

Removal of Pharmaceutical Pollutants from Aquatic Mediums Using MXene Nanocomposites: Mechanisms, Advances, and Challenges

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ABSTRACT

Pharmaceutical pollutants are now seen as one of the growing environmental problems worldwide. They remain in water for long periods, accumulate in ecosystems, and can contribute to antimicrobial resistance. Most traditional wastewater treatment systems cannot remove these substances efficiently because of their strong chemical stability and complex molecular structures. In recent studies, two-dimensional materials called MXenes, made of transition metal carbides and nitrides, have shown strong potential for removing pharmaceutical compounds. Their layered design, wide surface area, and reactive sites make them effective through several mechanisms such as electrostatic attraction, hydrogen bonding, π - π stacking, photocatalytic degradation, and electrochemical oxidation. When MXenes are combined with other materials like polymers, metal oxides (for example, TiO₂ and ZnO), or carbon-based substances, their performance and stability improve even more. In addition, they can be reused through regeneration methods like solvent washing or electrochemical reactivation without losing much efficiency. Overall, MXenes provide a promising and sustainable solution for the treatment of pharmaceutical wastewater.

INTRODUCTION

In recent years, pharmaceutical (PhACs) pollutants have garnered increasing global attention due to their widespread presence in aquatic environments and their persistent occurrence in water sources, which pose significant threats to both ecosystems and public health (Gouveia *et al.*, 2024; Sabra *et al.*, 2024). These pollutants comprise a diverse array of compounds, including antibiotics, antidepressants, and analgesics, which enter aquatic systems via domestic wastewater, industrial effluents, and medical waste (Aus der Beek *et al.*, 2015).

Although, PhACs may be present at low concentrations in water bodies, the cumulative effects of these compounds can lead to profound ecological disruptions, including behavioral alterations and interference with endocrine functions in aquatic organisms (Wilkinson *et al.*, 2022). Furthermore, the persistence of PhACs in aquatic environments heightens the risk of antimicrobial resistance, representing a major public health concern (Serwecińska, 2020). A

key concern is the poor biodegradability of many of these compounds, leading to their accumulation and the amplification of their toxicity over time (**Kantang *et al.*, 2009**).

For example, antibiotics such as metronidazoles are highly persistent, resisting conventional wastewater treatments, accumulating in aquatic environments, disrupting microbial communities, and promoting antibiotic resistance (**Singh *et al.*, 2024**). Similarly, paracetamol (acetaminophen), a widely used analgesic and antipyretic, enters the environment through hospital wastewater, improper disposal, and untreated wastewater (**Mostafa *et al.*, 2024**). These examples illustrate that, even at low concentrations, PhACs can persist in aquatic systems and pose substantial environmental risks due to their chemical stability and potential toxicity. Many other PhACs exhibit similar characteristics, contributing to extensive ecological and public health concerns (**Kantang *et al.*, 2025**).

Pharmaceutical active compounds (PhACs) are increasingly detected in aquatic ecosystems, where they exert adverse effects on fish physiology and survival. Individually, PhACs disrupt endocrine regulation, impair reproduction, and alter behavior, while chronic exposure leads to bioaccumulation and weakened immune responses. Studies have shown that waterborne pharmaceuticals can cause developmental, neurological, and reproductive disorders in fish, threatening population stability (**Dediu *et al.*, 2022**). When combined with other pollutants such as heavy metals, pesticides, or microplastics, the impacts are magnified through synergistic interactions, resulting in oxidative stress, tissue damage, and impaired metabolic pathways (**Younis & Almutairi, 2025**). These combined stressors not only compromise fish health and biodiversity but also pose serious risks to human health through consumption of contaminated fish, including potential toxicity and the spread of antimicrobial resistance (**Estrada-Almeida *et al.*, 2024**). Thus, the presence of PhACs—alone or in mixtures—represents a critical challenge for aquatic ecosystem integrity and food.

Conventional wastewater treatment systems, including biological treatment and sedimentation, are generally inadequate for the complete removal of micropollutants due to their complex chemical properties and high stability (**Kanaujiya *et al.*, 2019**). Moreover, the absence of uniform and enforceable regulations governing the discharge of pharmaceuticals underscores the urgent need for advanced wastewater treatment technologies (**Ibrahim *et al.*, 2023**). Research indicates that over 50% of pharmaceuticals can escape conventional treatment, highlighting the necessity for innovative and effective remediation strategies (**Pal, 2018**).

Consequently, exploring environmentally sustainable treatment approaches, such as the application of nanomaterials and multifunctional materials, is imperative (**Patel *et al.*, 2019**; **Alharbi *et al.*, 2025**; **Younis *et al.*, 2025**). Advanced materials, notably MXene, a two-dimensional transition metal carbide or nitride, have demonstrated exceptional efficiency in removing PhACs pollutants from water (**González-Poggini *et al.*, 2021**). Its layered structure, abundant surface functional groups, high surface area, and strong adsorption capacity enable effective contaminant removal through adsorption and oxidation mechanisms (**Kabir *et al.*,**

2024). This evidence underscores the promising role of advanced materials in mitigating PhACs pollution in aquatic systems.

2. MXenes and their properties

2.1. Structural characteristics and composition

MXenes represent an emerging class of quasi-two-dimensional materials obtained through the selective etching of the “A” layers from ternary carbides or nitrides known as MAX phases, which have the general formula $M_{n+1}AX_n$.

In this formula, M denotes a transition metal (e.g., Ti, V, Nb), a corresponds to an element from groups 13 or 14—most commonly aluminum (Al)—and X represents carbon and/or nitrogen, with n typically ranging from 1 to 3 and X represents carbon and/or nitrogen. The integer n (typically n = 1, 2, or 3) denotes the number of transition metal (M) layers in the precursor MAX phase, which directly influences the resulting MXene's structure and properties. For example, in Ti_3AlC_2 (where n=3), the etching of the Al layer yields a three-layer Ti_3C_2 MXene (e.g., $Ti_3C_2T_x$). (Rai *et al.*, 2025).

The selective etching process transforms the MAX phase into the MXene structure, represented by the formula $M_{n+1}X_nT_x$, where T_x indicates surface termination groups such as –O, –OH, and –F. These surface terminations substantially modify the material's surface chemistry, electronic properties, and overall functionality (Kubitza *et al.*, 2023).

Consequently, MXenes exhibit unique structural and chemical characteristics that distinguish them from conventional two-dimensional materials and underpin their diverse applications in environmental remediation, energy storage, and catalysis.

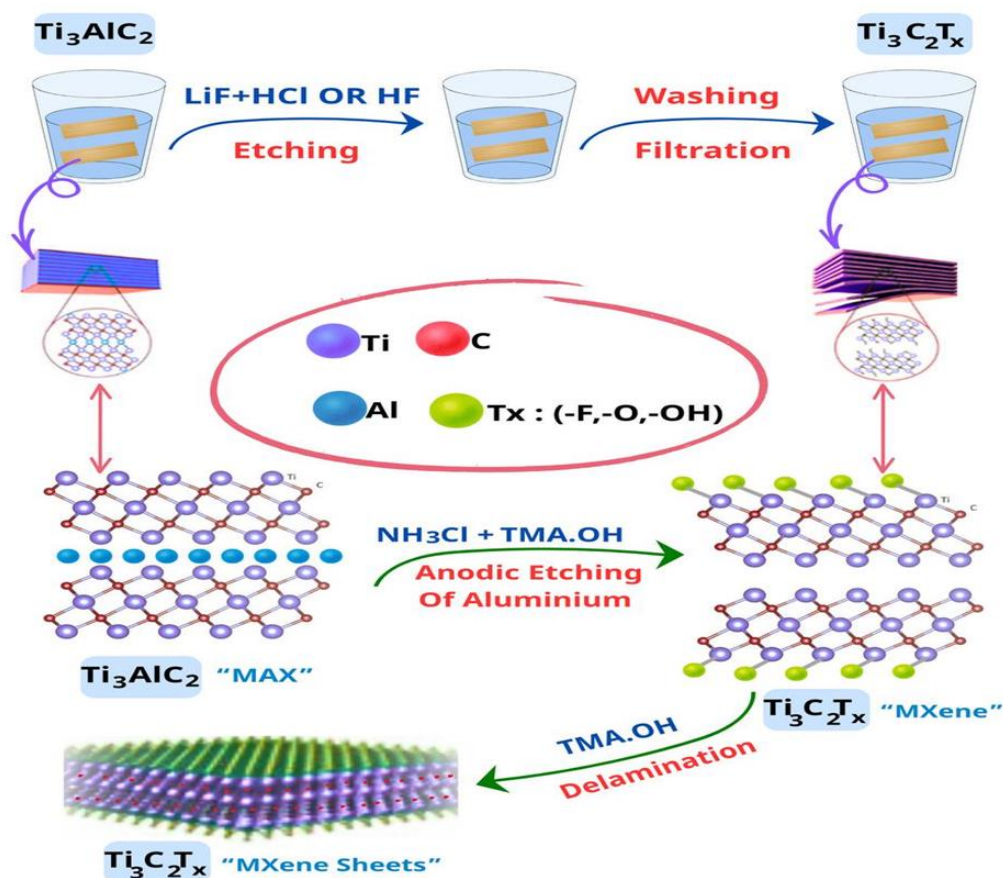


Fig. 1. Illustration of the etching process from MAX phase to MXene nanosheets. The original MAX structure (M–A–X) undergoes selective chemical etching by (HF OR HCL/LiF) to remove the A layer (e.g., Al), resulting in a layered accordion-like MXene ($\text{M}_{n+1}\text{X}_n\text{T}_x$) structure with surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$), which significantly alter surface chemistry and properties

This structural architecture endows MXenes with several defining characteristics :

Ordered two-dimensional structure: MXenes possess strong M– bonds and relatively weaker M–A bonds, which facilitate the selective etching process from the MAX phase precursor (Kubitza et al., 2023).

Accordion-like layered morphology: Their metallic layers form a high specific surface area, and the layered configuration provides tunable interlayer spacing, enhancing properties such as ion storage capacity, hydrophilicity, adsorption, and catalytic activity (Sun et al., 2024; Cai et al., 2025).

Compositional versatility: MXenes can incorporate single or multiple transition metals within the M layers, allowing precise control over electronic and chemical properties. For instance, they can exist as single-metal variants, such as $\text{Ti}_3\text{C}_2\text{T}_x$, or as multi-metal solid solutions, such as $(\text{Mo}, \text{Ti})_3\text{C}_2\text{T}_x$, enabling fine-tuning of electrical conductivity, mechanical strength, and chemical reactivity to suit specific application requirements (Michalowski & Mathis, 2022).

Furthermore, the combination of diverse transition metals and surface terminations contributes to the broad spectrum of MXene properties, making them highly suitable for applications in energy storage, electromagnetic interference shielding, and other advanced technological domains (**Zou et al., 2022; Li et al., 2023**).

2.1.1 Surface terminations and interaction with pollutants:

In $\text{Ti}_3\text{C}_2\text{T}_x$ and related MXenes, the type and proportion of surface terminations ($\text{T}_x = -\text{O}, -\text{OH}, -\text{F}$, etc.) critically influence hydrophilicity, surface charge, the availability of active sites, and specific adsorption mechanisms (**Jiang, 2025**). Terminations rich in $-\text{OH}$ and $-\text{O}$ generally enhance water wettability and provide hydrogen-bond donors and acceptors, which strengthen interactions with polar pharmaceuticals and oxygenated contaminants through hydrogen bonding, electrostatic attraction, and inner-sphere complexation. Additionally, these terminations facilitate ion transport through hydrated interlayers (**Rems et al., 2024**).

In contrast, $-\text{F}$ terminations are typically less hydrophilic and may passivate active sites, often reducing adsorption capacity and interfacial reactivity toward aqueous micropollutants (**Jiang, 2025**). Comparative studies indicate that MXenes synthesized via fluoride-free or low-F etching routes, resulting in higher $-\text{O}/-\text{OH}$ fractions, exhibit superior adsorption and separation performance for antibiotics and dyes compared to HF-etched, F-terminated counterparts (**Tawalbeh et al., 2023**).

Both density-functional theory calculations and experimental reports further demonstrate stronger binding energies and more extensive hydrogen-bond networks on $-\text{OH}$ -terminated surfaces than on $-\text{F}$ -terminated surfaces. This observation aligns with the higher uptake and faster adsorption kinetics observed for polar solutes in water (**Sanga et al., 2024**). Collectively, tailoring MXene surface terminations toward $-\text{O}/-\text{OH}$ dominance—through etchant selection, post-treatments, or mild oxidation—represents an effective strategy to enhance pharmaceutical removal, whereas high $-\text{F}$ coverage is generally unfavorable for aqueous adsorption applications (**Rems et al., 2024; Jiang, 2025**).

2.1.2. Common etching techniques and impact on MXene properties:

The synthesis of MXenes commonly involves etching techniques such as direct hydrofluoric acid (HF) treatment or the use of HCl/LiF mixtures. HF etching effectively removes the A-layer (e.g., Al in Ti_3AlC_2); however, it often generates excessive $-\text{F}$ terminations and introduces structural defects, which can compromise surface reactivity and reduce mechanical stability (**Kiran et al., 2025**).

In contrast, etching with HCl/LiF produces HF in a controlled manner, typically resulting in MXenes with a higher proportion of $-\text{O}/-\text{OH}$ terminations, fewer structural defects, and improved layer integrity (**Wyatt et al., 2024**). Comparative studies demonstrate that while HF-etched MXenes may suffer from defect-induced instability, LiF/HCl -derived MXenes retain better crystallinity, larger interlayer spacing, and enhanced adsorption and electrochemical performance (**Mendoza-Sánchez et al., 2023; Jia et al., 2025**).

Therefore, the selection of the etching route directly influences the surface termination chemistry, defect density, and overall structural integrity of MXenes, ultimately affecting their suitability for various applications.

2.2 Synthesis methods

MXenes are generally synthesized by selectively removing the A layer from MAX phases, followed by intercalation and delamination to produce few-layered or single-layered flakes. The chosen synthesis route critically determines the surface terminations ($T_x = -O, -OH, -F, -Cl$, etc.), defect density, interlayer spacing, and flake size, which in turn influence adsorption properties as well as electrochemical and structural stability (Zhang *et al.*, 2022; Wang *et al.*, 2024).

2.2.1 Etching routes :

2.2.1.1 Direct HF etching:

Concentrated HF efficiently removes Al (or other A elements) from MAX phases (e.g., $Ti_3AlC_2 \rightarrow Ti_3C_2T_x$), generating accordion-like multilayer MXenes with $-F, -OH$, and $-O$ terminations. While this method is both rapid and scalable, the strong HF can introduce point defects (such as Ti vacancies), structural disorder, and reduced interlayer spacing, potentially compromising electrical conductivity and mechanical integrity if parameters such as acid concentration, reaction time, temperature, and particle size are not carefully controlled (Zhang *et al.*, 2022).

2.2.1.2 In Situ Hydrofluoric acid (LiF/HCl):

The combination of LiF and HCl produces HF *in situ* and simultaneously intercalates Li^+ during etching, resulting in a “clay-like” MXene that is easier to delaminate. This milder approach preserves the layered structure, reduces defect density, and yields a higher $-O/-OH$ ratio with larger interlayer spacing compared to direct HF etching. Additionally, it enhances flake size retention and colloidal stability, which are essential for applications in membranes and adsorbents (Shen *et al.*, 2021; Wang *et al.*, 2024).

2.2.1.3 Electrochemical etching (Low-fluoride):

Electrochemical anodic removal of A layers provides precise control over defect densities and surface terminations without the need for bulk HF handling. This greener approach is also suitable for scalable MXene production (Chan *et al.*, 2024).

2.2.1.4 Lewis acid / molten salt etching (Halide terminations):

Etching in molten Lewis-acidic salts (e.g., $ZnCl_2, CuCl_2$) or halogen-rich environments produces MXenes with halide terminations (e.g., $Ti_3C_2Cl_2$) while minimizing water exposure. This method expands the diversity of surface terminations, increases interlayer spacing, and enhances thermal and chemical stability. Furthermore, $-Cl$ terminations can later be exchanged for $-O/-OH$ via hydrolysis if required (Li *et al.*, 2019).

2.2.2 Process variations:

Several processing parameters, including the solid-to-liquid ratio, MAX particle size, caustic concentration, temperature, reaction time, agitation, and atmospheric conditions, significantly influence MXene yield, defect density, surface terminations, and flake size. Additionally, thorough washing to near-neutral pH is crucial to remove residual salts and acids, ensuring the stabilization of colloidal suspensions (**Benchakar *et al.*, 2020**).

Table 1. Summarized each etching method advantages and limitations according to the intended MXene application

Etching Method	Resulting MXene Properties	Advantages	Limitations
HF etching	High surface functionalization (–OH, –F), thin layers, good conductivity.	Simple, widely used, produces high-quality MXenes.	Highly toxic, hazardous handling, environmental concerns.
LiF/HCl etching	Controlled layer delamination, abundant –OH terminations, good hydrophilicity.	Safer than concentrated HF, tunable etching, easier scalability.	Longer reaction time, lower yield than HF.
Electrochemical etching	Precise control over surface chemistry, less –F termination, adjustable layer thickness.	Green method, less toxic, tunable properties.	Requires electrochemical setup, slower process, limited to some MXenes.
Molten salt etching	Produces fluoride-free MXenes, good conductivity, thermally stable.	Can produce novel terminations, scalable, high thermal stability.	High temperature required, energy intensive, equipment corrosion.

A comparison of the etching methods summarized above reveals that each approach has distinct advantages and limitations that directly influence MXene properties and potential applications. Direct HF etching remains the most widely used due to its efficiency and scalability, producing accordion-like multilayer MXenes with abundant –F/–OH/–O terminations. However, the process is highly hazardous, and the induced structural defects or narrower interlayer spacing can compromise conductivity and mechanical stability if reaction conditions are not carefully optimized.

The LiF/HCl *in situ* method offers a milder alternative, improving delamination, preserving layered structures, and increasing –O/–OH terminations. This enhances colloidal stability and makes MXenes more suitable for membrane or adsorbent applications. Nonetheless, reaction

times are longer, and yields are typically lower than direct HF, which may limit industrial scalability.

Electrochemical etching provides a greener and safer route, with tunable defect density and surface chemistry. While promising for environmentally friendly production, this method requires specialized equipment and is slower, limiting its applicability to some MXene types. Molten salt/Lewis acid etching expands surface chemistry possibilities and allows halide terminations, offering thermal and chemical stability advantages. However, high temperatures and energy-intensive conditions may pose practical challenges and increase equipment corrosion risks.

It is also important to note that most studies were conducted under controlled laboratory conditions (e.g., pure water) rather than real wastewater systems, and sample sizes were often limited. Conflicting results in the literature, particularly regarding the influence of surface terminations on adsorption or electrochemical performance, indicate the need for systematic studies comparing different etching routes under realistic operational conditions. This critical perspective highlights that while the choice of etching method can optimize MXene properties for specific applications, careful consideration of safety, scalability, and environmental relevance is essential for translating laboratory findings into practical use.

2.3 Intercalation and delamination

Delamination is a crucial step in converting multilayer MXenes into few- or single-layer flakes by increasing interlayer spacing and weakening interflake interactions. Common intercalants include dimethyl sulfoxide (DMSO), urea, tetrabutylammonium hydroxide (TBAOH), and small cations such as Li^+ , Na^+ , or K^+ , which are typically introduced during or after the etching process (Hu *et al.*, 2023; Wang *et al.*, 2024).

Mild sonication or shear mixing is commonly employed to separate MXene layers; however, excessive sonication can fragment the flakes and increase defect density, making the optimization of processing conditions essential (Hu *et al.*, 2023; Wang *et al.*, 2024). The quality of delaminated MXenes can be assessed by stable colloidal suspensions, shifts in the (002) XRD peak, flake thickness around 1–2 nm as measured by AFM, and high conductivity in formed films. Over-processing may lead to oxidation and compromised performance (Shen *et al.*, 2021).

MXenes, particularly $\text{Ti}_3\text{C}_2\text{T}_x$, are susceptible to oxidation in aqueous and atmospheric environments. To prolong shelf life and preserve flake size and electrical conductivity—critical factors for reproducible environmental applications—storage under low temperatures, oxygen-poor conditions, controlled pH, and the addition of antioxidants is recommended (Chan *et al.*, 2024; Kruger *et al.*, 2024).

2.4 Surface functionalization and modification techniques

Surface modification techniques are crucial for enhancing MXene performance across a variety of applications, including energy storage, sensing, and biomedical fields. The main approaches include :

2.4.1 Intercalation and delamination:

These processes involve the insertion of molecules between MXene layers, weakening interlayer bonds and facilitating the separation into individual sheets (**Jothibas et al., 2025**). For example, tannic acid has been employed as a bio-exfoliating agent for $\text{Ti}_3\text{C}_2\text{T}_x$ MXene, effectively achieving layer separation without compromising environmental properties (**Ali et al., 2025; Mussa et al., 2025**).

2.4.2 Polymer-based surface functionalization:

Polymers provide an efficient means of modifying MXene surfaces. For instance, RGD peptide-functionalized MXene nanoconjugates have been developed to improve tumor-targeting efficiency and enhance photothermal therapeutic performance (**Kim et al., 2025**).

2.4.3 Chemical deposition of surface functional groups:

Chemical deposition techniques are employed to introduce functional groups onto MXene surfaces, thereby improving their chemical and physical properties (**Mullani et al., 2025**). For example, $\text{Ti}_3\text{C}_2\text{T}_x$ has been modified using aryl diazonium compounds, which enhances interactions in solution and broadens potential application areas (**Han et al., 2025; Huang 2025**).

3. Mechanisms of pharmaceutical removal using mxenes

3.1 Adsorption mechanisms

3.1.1 Electrostatic interactions:

Electrostatic interactions play a predominant role in the adsorption of pharmaceuticals onto MXene surfaces, particularly for charged drug molecules in aqueous environments. MXenes, such as $\text{Ti}_3\text{C}_2\text{T}_x$, possess abundant surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$) that impart a negative surface charge under neutral or slightly basic conditions, with zeta potentials typically ranging from -20 to -40 mV (**Kim et al., 2021**). This negative charge strongly attracts positively charged pharmaceutical species, including various antibiotics and cationic drugs such as tetracycline, ciprofloxacin, and amoxicillin, through Coulombic attraction (**Abdul Ghani et al., 2023**).

The magnitude and direction of electrostatic interactions are influenced by solution pH, which affects both MXene surface charge (via protonation /deprotonation of surface terminations) and the ionization state of the pharmaceutical molecules (**Jeon, 2021**). At low pH, protonation of MXene surface groups reduces negative charge, weakening electrostatic attraction. Conversely, under near-neutral or alkaline conditions, the surface becomes highly negatively charged, enhancing adsorption of cationic drugs. Solution ionic strength also plays a critical role, as high salt concentrations can screen electrostatic forces and reduce adsorption capacity (**Ahmaruzzaman, 2022**).

Electrostatic interactions often act synergistically with hydrogen bonding and π - π interactions, resulting in high adsorption efficiencies for pharmaceuticals containing multiple functional groups (Zeng *et al.*, 2024). Comparative studies indicate that MXenes with higher -O/-OH surface terminations and fewer structural defects exhibit stronger electrostatic affinity toward positively charged drug species, due to enhanced surface charge density and hydrophilicity (Othman *et al.*, 2022).

3.1.2 π - π Interactions:

π - π interactions significantly contribute to the adsorption of antibiotics on MXene surfaces because of the aromatic structures present in both the adsorbent and adsorbate. These interactions are primarily mediated by the delocalized π -electron clouds of the antibiotic aromatic rings and the conjugated structures in MXenes (Zeng *et al.*, 2024). Surface terminations such as -O, -OH, and -F modulate the electronic properties and surface energy of MXenes, thereby influencing the extent of π - π interactions (Janjhi *et al.*, 2023). Furthermore, these interactions are highly pH-dependent, as protonation states of functional groups on both MXene and antibiotic molecules alter electron density and, consequently, interaction strength (Sanga *et al.*, 2023).

3.1.3 Hydrogen bonding:

Hydrogen bonding constitutes another dominant mechanism for the adsorption of antibiotics onto MXene-based materials (Zeng *et al.*, 2024). Functional groups such as -O and -OH on MXene surfaces act as hydrogen bond donors or acceptors, facilitating strong interactions with heteroatoms (e.g., N, O) present in antibiotic molecules. The density and spatial distribution of these surface functional groups significantly influence both the number and stability of hydrogen bonds formed (Janjhi *et al.*, 2023). Moreover, pH strongly affects hydrogen bonding by altering the ionization states of both the MXene surface and the antibiotic molecules, leading to variations in bond strength and adsorption efficiency (Sanga *et al.*, 2023).

3.2 Photocatalytic degradation

Photocatalytic degradation represents an efficient approach for removing antibiotics from water using MXenes. Upon exposure to light, MXenes absorb photons and generate electron-hole pairs. These charge carriers subsequently react with water and oxygen to produce reactive oxygen species (ROS), such as hydroxyl radicals ($\bullet$ OH) and superoxide anions ($\bullet$ O₂⁻), which attack antibiotic molecules and break them down into smaller, less harmful compounds. The efficiency of this process is strongly influenced by the separation of electron-hole pairs, the presence and type of surface functional groups, and the light absorption properties of MXenes (Xu *et al.*, 2023; Irfan & Khan, 2024).

3.3 Electrochemical Oxidation and Reduction

Electrochemical oxidation and reduction have emerged as effective methods for the removal of pharmaceutical contaminants from aqueous environments, with MXenes serving as

promising electrode materials due to their unique physicochemical properties. When a voltage is applied to MXene electrodes, electron-hole pairs are generated, promoting the formation of ROS, such as hydroxyl radicals ($\bullet\text{OH}$) at the anode surface. These highly reactive species degrade complex pharmaceutical molecules into smaller, less harmful compounds (Abdul Ghani *et al.*, 2022). The efficiency of electrochemical processes depends on parameters including applied voltage, electrode surface area, and the presence of supporting electrolytes (Tawalbeh *et al.*, 2023).

MXenes, particularly $\text{Ti}_3\text{C}_2\text{T}_x$, exhibit high electrical conductivity and large surface area, rendering them suitable for electrochemical applications (Bilibana 2023). Moreover, their surface chemistry, encompassing functional groups such as $-\text{OH}$, $-\text{O}$, and $-\text{F}$, can be tailored to enhance both reactivity and stability during electrochemical reactions (Hussain *et al.*, 2024). Studies have demonstrated that MXene-based electrodes can effectively remove PhACs via electrochemical oxidation and reduction, underscoring their potential in wastewater treatment technologies (Abbasi *et al.*, 2025).

This method is noted for its effectiveness in removing pharmaceutical contaminants (PhACs) generically. While it doesn't single out a specific class like the other sections, the context of the entire manuscript section strongly implies its application across various types, with a common focus on antibiotics.

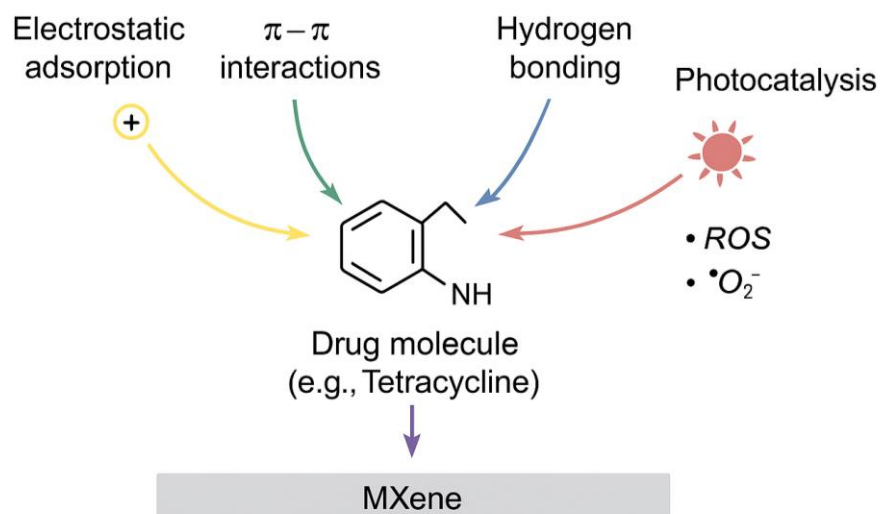


Fig. 2. Schematic representation of pharmaceutical pollutant removal Mechanisms by MXenes

Additionally, integrating MXenes with other materials, such as carbon-based composites or conductive polymers, has been explored to further enhance electrochemical performance. These hybrid systems improve charge transfer rates and increase stability, making them more effective for long-term applications in pharmaceutical removal from water (Pouramini *et al.*, 2023). In summary, MXenes present a viable solution for the

electrochemical remediation of pharmaceutical contaminants, owing to their high conductivity, customizable surface chemistry, and potential for hybridization with other materials, which continues to drive research and development in environmental remediation (Iravani & Varma, 2022).

Table 2. Summary of the major mechanisms by which MXenes remove pharmaceutical contaminants, along with representative drug examples and key operational factors influencing performance

Removal Mechanism	Description	Examples of Target Drugs	Key Influencing Factors
Electrostatic Interaction	Coulombic attraction between negatively charged MXene surfaces and positively charged pharmaceutical species.	Tetracycline, Ciprofloxacin, Amoxicillin.	Solution pH (neutral–basic enhances adsorption), ionic strength (high salt weakens interaction), surface –O/–OH terminations.
π–π Interaction	π – π stacking between aromatic rings of pharmaceutical molecules and the conjugated MXene surface.	Sulfonamides, Fluoroquinolones.	pH-dependent protonation state, type of surface terminations (–O/–OH enhance interaction).
Hydrogen Bonding	Formation of hydrogen bonds between –O/–OH groups on MXene surfaces and heteroatoms (N, O) in drug molecules.	Antibiotics containing –NH ₂ or –OH groups.	pH (affects donor/acceptor availability), density of surface functional groups.
Photocatalytic Degradation	Light-excited MXenes generate electron–hole pairs, producing ROS ($\bullet$ OH, $\bullet$ O ₂ [–]) that degrade pharmaceuticals.	Tetracycline, Sulfonamides.	Light intensity and wavelength, charge separation efficiency, surface chemistry.
Electrochemical Oxidation/Reduction	Applied voltage at MXene electrodes generates ROS, enabling oxidation or reduction of pharmaceuticals.	Metformin, Ciprofloxacin.	Applied potential, electrode surface area, electrolyte type.

Table (2) highlights the diverse mechanisms through which MXenes remove pharmaceutical contaminants, revealing both the strengths and limitations of each pathway. Electrostatic interactions, while highly effective for cationic pharmaceuticals under neutral to alkaline

conditions, are sensitive to solution chemistry, particularly ionic strength, which can reduce adsorption efficiency in real wastewater with high salinity. π – π interactions and hydrogen bonding provide additional selectivity for aromatic and polar drug molecules, yet their performance is pH-dependent and may decline in highly acidic or basic environments. Photocatalytic degradation offers a promising route for complete mineralization of pharmaceuticals but often suffers from electron–hole recombination and requires optimized light sources, limiting large-scale application. Similarly, electrochemical oxidation provides precise control over contaminant degradation but may be energy-intensive and susceptible to electrode fouling over multiple cycles. Overall, while the combination of these mechanisms enables MXenes to achieve superior removal efficiency compared to conventional adsorbents, future studies should focus on integrating multiple mechanisms synergistically (e.g., adsorption–photocatalysis systems) and validating their performance under real wastewater conditions to ensure practical scalability and long-term stability.

4. MXene-based nanocomposites

MXene-based nanocomposites represent a versatile class of materials that combine MXenes with polymers, metal oxides, and carbon-based compounds, thereby significantly enhancing their structural stability, conductivity, and multifunctional performance. These hybrid systems are particularly valuable for environmental remediation, energy storage, and biomedical applications due to their tunable physicochemical properties.

4.1 Hybrid materials with polymers

The incorporation of polymers such as poly(vinyl alcohol) (PVA), polyaniline (PANI), and polyethylene oxide (PEO) enhances the flexibility, mechanical strength, and environmental stability of MXene-based systems. Polymer integration also improves dispersibility and prevents MXene layer restacking, resulting in superior electrochemical performance and increased adsorption capacity for the pollutant removal (Ali *et al.*, 2025).

4.2 Hybrid materials with metal oxides

Coupling MXenes with metal oxides, such as TiO₂, forms heterojunctions that facilitate charge separation and improve light-harvesting efficiency. TiO₂@MXene composites have demonstrated outstanding photocatalytic activity, achieving over 97% removal of tetracycline under visible light irradiation (Qiang *et al.*, 2022; Liu *et al.*, 2024). Furthermore, advanced hybrid systems such as sonophotocatalytic MXene/TiO₂–WS₂ composites have been shown to accelerate degradation kinetics through the synergistic effects of photoexcitation and ultrasonic activation (Ranjith *et al.*, 2023).

4.3 Hybrid materials with carbon-based compounds

The hybridization of MXenes with carbon-based materials, including graphene oxide and carbon nanotubes, further enhances electrical conductivity and mechanical stability. These

carbon-based hybrids offer a large surface area and strong interactions with organic contaminants, making them particularly effective for water purification and adsorption-driven processes (Amani *et al.*, 2025).

4.4 Synergistic effects for enhanced removal performance

MXene-based nanocomposites frequently exhibit synergistic effects, in which the combination of MXenes with other components yields performance that surpasses the sum of the individual materials.

Enhanced photocatalytic degradation: MXene–ZnO composites display superior photocatalytic activity compared to their individual counterparts. MXenes expand ZnO's light absorption range and surface area, leading to higher hydroxyl radical generation and achieving up to ~96% tetracycline removal under UV irradiation (Karakaş *et al.*, 2025).

Efficient photocatalyst design (CF/MXene): Ternary nanocomposites formed by integrating MXenes with copper and iron oxide nanostructures (CF/MXene) demonstrate rapid adsorption and photocatalytic degradation of dyes such as Rhodamine B, achieving ~94% removal within 120 minutes under visible light. This improvement is attributed to enhanced charge separation and reactive species generation (Katubi *et al.*, 2024).

MXene as a co-catalyst in hybrid photocatalysts: MXenes, when incorporated into hybrid systems such as MOFs, polymers, or graphene, act as conductive co-catalysts, enabling faster charge transfer and improving photocatalytic degradation of PhACs through efficient interfacial electron transport (Iravani & Varma, 2022).

Although the above examples clearly demonstrate the exceptional performance of MXene-based nanocomposites in pollutant removal, it is essential to critically assess their practical limitations and challenges to gain a comprehensive understanding of their applicability in real-world scenarios.

Overall, MXene-based nanocomposites exhibit remarkable potential for pharmaceutical removal owing to their synergistic properties, which combine the high conductivity and large surface area of MXenes with the enhanced stability and multifunctionality of polymers, metal oxides, and carbon materials. The prevention of MXene restacking by polymers, formation of heterojunctions with metal oxides, and conductive networks with carbon-based compounds collectively lead to superior adsorption, photocatalytic, and electrochemical performance compared to pristine MXenes.

Nevertheless, several challenges remain before these systems can be applied at scale. Achieving uniform dispersion and strong interfacial bonding between MXenes and secondary components is still difficult, which may hinder reproducibility and active site accessibility. In addition, many studies report results under idealized laboratory conditions, potentially overestimating performance relative to real wastewater systems containing competing ions, natural organic matter, and fluctuating pH. The long-term structural stability, regeneration

efficiency, and potential secondary contamination from nanocomposite leaching also require more systematic investigation.

Future work should focus on scalable, environmentally benign synthesis methods, precise tuning of interfacial chemistry, and testing under realistic conditions. Life-cycle and techno-economic assessments will be essential to evaluate the practicality of MXene-based nanocomposites for sustainable pharmaceutical wastewater treatment.

5. Impacts of pharmaceutical pollutants on ecosystem :

5.1 Effects of PhACs on fish

Many studies have shown that pharmaceutical active compounds (PhACs) can harm fish even when they are present in very small amounts. Some drugs can disturb hormone levels and change fish behavior or growth patterns (**Grădinariu, 2025**). Continuous exposure to these substances often leads to oxidative stress because antioxidant enzymes such as superoxide dismutase (SOD) and catalase (CAT) become less effective. An imbalance like this can harm fish by damaging their tissues, reducing their ability to reproduce, and in severe cases, leading to death (**Aib et al., 2025**). Some substances—particularly antidepressants and synthetic hormones—have also been connected to changes in behavior and reproduction, such as the feminization of male fish (**Punginelli et al., 2024**). Altogether, these studies highlight how leftover pharmaceuticals in water pose a serious risk to fish health and the balance of aquatic ecosystems.

5.2 Combined effects of PhACs with other pollutants

The danger becomes greater when PhACs mix with other pollutants such as heavy metals, pesticides, or microplastics (**Aladl et al., 2025; El-Sayed et al., 2025**). Research has found that this combination increases toxicity through what is called the “cocktail effect” (**Aib et al., 2025**). Microplastics can adsorb to pharmaceuticals and carry them inside fish bodies, which leads to higher accumulation and stronger toxic effects (**Arienzo & Donadio, 2023**). These mixtures can weaken the immune system, cause inflammation, and affect growth and reproduction. What makes this issue more serious is that these pollutants can move through the food chain, reaching humans who consume contaminated fish (**Punginelli et al., 2024**). Understanding these combined effects is crucial for developing safer and more sustainable wastewater treatment solutions.

6. Regeneration and reusability

6.1 Material stability and resistance to fouling

The long-term performance of MXene-based materials is critically dependent on their structural stability and resistance to fouling (**Lee et al., 2023**). MXenes are prone to oxidation and surface degradation under environmental conditions, which can gradually diminish their functional properties (**Taberi et al., 2025**). To address these challenges, several stabilization strategies have been proposed, including surface passivation, polymer encapsulation, and

hybridization with other nanomaterials. These modifications enhance chemical robustness, reduce fouling, and extend the operational lifespan of MXenes, which is particularly critical for applications involving repeated exposure to harsh environments, such as catalysis, energy storage, and water purification (Baig *et al.*, 2024; Meskher *et al.*, 2025).

6.2 Regeneration methods and lifecycle performance

Efficient regeneration is essential to maintain the functional performance of MXene-based materials across multiple operational cycles. A range of physical and chemical approaches—such as solvent washing, thermal treatment, and electrochemical regeneration—have been investigated to restore active sites and remove fouling contaminants (Jabeen *et al.*, 2025).

Recent studies highlight the quantitative impact of these methods: SI-Ti₃C₂T_x MXene achieved nearly complete regeneration within five minutes using an electrochemical approach, maintaining a ~99.7% removal rate even after multiple adsorption–regeneration cycles (Abdul Ghani *et al.*, 2021). Furthermore, surface engineering strategies, such as decorating Ti₃C₂T_x with Au nanoparticles and –F terminations, have significantly extended lifecycle performance, allowing up to 600 stable cycles compared to only 100 cycles for pristine MXene (Yoon *et al.*, 2025). These findings demonstrate that optimized regeneration protocols and rational material design can minimize structural degradation and sustain high performance, thereby improving the cost-effectiveness and environmental viability of MXene-based systems.

6.3 Long-term application potential

MXene-based materials show strong promise for long-term applications owing to their excellent structural stability, electrical conductivity, and tunable surface chemistry (Protyai *et al.*, 2024). In practical devices, Ti₃C₂T_x electrodes used in PDLC smart windows maintained stable switching behavior for 365 days without noticeable degradation (Kumar *et al.*, 2023). In energy storage, MXene–reduced graphene oxide aerogel electrodes retained over 95% of their initial capacitance after 75,000 charge–discharge cycles at 5A. g^{−1} (Wang *et al.*, 2019). Similarly, in water treatment, Ti₃C₂T_x/CNF-14 composites demonstrated 84.71% capacity retention after 50 cycles, with adsorption capacity fully recoverable after regeneration (Lei *et al.*, 2023).

Collectively, these results emphasize that integrating surface functionalization, nanocomposite design, and optimized regeneration strategies is key to enabling MXene-based systems to maintain consistent performance over prolonged operation, ultimately supporting their scalability and real-world implementation (Baig *et al.*, 2024; Akhter & Maktedar, 2025).

Table 3. MXene-based materials demonstrate remarkable pharmaceuticals removal efficiency and durability across different regeneration methods and operational cycles

Drug / Pollutant	Most Effective Regeneration Method	Notes / Performance
Ciprofloxacin	Electrochemical	Complete regeneration in 5 min; removal rate ~99.7% after multiple cycles (Abdul Ghani et al., 2021).
Tetracycline	Solvent washing	Efficient removal; slight capacity loss after 5 cycles; requires longer contact time (Chen et al., 2023).
Ciprofloxacin + Au@F-Ti ₃ C ₂ T _x	Electrochemical + Surface Engineering	Extended cycling lifespan to 600 cycles vs 100 cycles for pristine MXene (Yoon et al., 2025).
Rhodamine B	Photocatalytic	MXene synthesized via ultrasonication exhibited high efficiency in the degradation of Rhodamine B and Methylene Blue, demonstrating its potential for wastewater purification (Kumar et al., 2024).
Ti ₃ C ₂ T _x MXene (in PDLC smart window device)	Electrochemical / Device Operation	Maintained structural integrity and electrochemical performance for up to 365 days of continuous operation (Lee et al., 2023).

Table (3) provides a comprehensive comparison of several studies investigating the performance and regeneration behavior of Ti₃C₂T_x MXene-based materials for the removal of pharmaceutical and dye pollutants, as well as their applications in electrochemical devices. The comparative analysis reveals a clear variation in regeneration efficiency and cycling stability depending on the type of pollutant, treatment mechanism, and structural modification of the material.

According to **Abdul Ghani et al. (2021)**, electrochemical regeneration stands out as one of the most efficient approaches. The intercalated Ti₃C₂T_x MXene achieved complete regeneration within only five minutes while maintaining a removal rate of approximately 99.7% after multiple adsorption–regeneration cycles. This indicates excellent electron transfer ability and rapid reusability with minimal loss of efficiency. However, the study was limited to a single pollutant and controlled laboratory conditions, which restricts the generalization of these findings to more complex multi-contaminant systems.

In contrast, the work of **Chen et al. (2023)** on tetracycline demonstrated that solvent washing could effectively regenerate the active sites of MXene. Nonetheless, a slight reduction in adsorption capacity was observed after five consecutive cycles, and a longer contact time was

required to achieve full removal. These findings suggest that conventional solvent-based regeneration may be insufficient for long-term applications, as it can lead to partial degradation of the active surface sites. Hence, electrochemical regeneration presents a more controllable and sustainable alternative.

The study by **Yoon *et al.* (2025)** further emphasizes the role of surface engineering as a promising strategy to enhance MXene's structural and electrochemical stability. The modification of the surface using Au@F $\text{Ti}_3\text{C}_2\text{T}_x$ significantly extended the cycling lifespan from around 100 to 600 cycles. Although these results were obtained in the context of lithium-metal batteries, they provide compelling evidence that surface modification can improve the structural robustness and electronic stability of MXene—features that can be advantageously applied to electrochemical regeneration systems for water treatment.

Furthermore, **Kumar *et al.* (2024)** highlighted the potential of photocatalytic degradation as an environmentally friendly pathway for wastewater purification. The MXene synthesized via ultrasonication showed remarkable photocatalytic activity toward the degradation of Rhodamine B and Methylene Blue, achieving near-complete removal within a short period and maintaining good stability over successive cycles. This approach is attractive due to its solvent-free and energy-efficient nature, yet it remains limited under turbid water conditions or in the presence of competing ions that can hinder light absorption.

Meanwhile, **Lee *et al.* (2023)** investigated the long-term structural and operational stability of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene in electrochemical and smart device applications such as PDLC smart windows. Their results confirmed that the material maintained its structural integrity and electrochemical performance for up to one year (365 days) of continuous operation, demonstrating excellent environmental and electrochemical stability. Such durability makes MXene a promising material for long-term applications, whether in smart devices or continuous-flow electrochemical treatment systems.

Overall, the analysis reveals that electrochemical regeneration remains the most efficient and rapid approach among all regeneration methods, while solvent washing and thermal techniques show relatively lower stability and efficiency over repeated use. Recent research clearly indicates that improving MXene's performance and durability is closely tied to surface functionalization and structural optimization, which enhance both its electronic properties and resilience under operational stress. However, most of these studies are still confined to laboratory-scale conditions. Therefore, future work should focus on large-scale and real-water systems involving multi-pollutant environments to validate the long-term stability, regeneration capability, and structural integrity of MXene-based materials in realistic applications.

7. Comparative analysis

7.1 Comparison between MXenes and conventional adsorbents/catalysts

MXenes consistently demonstrate superior adsorption and catalytic efficiency compared to conventional materials, primarily due to their large surface area, hydrophilic surfaces, and abundance of surface functional groups ($-\text{OH}$, $-\text{O}$, $-\text{F}$), which enhance interactions with

pollutants and reactants. For example, MXenes have achieved adsorption capacities of up to 214 mg/g for U^{6+} ions, markedly outperforming many traditional adsorbents (**Dehghani et al., 2025; Mussa et al., 2025**).

In terms of selectivity, MXenes offer the advantage of tunable surface chemistry, enabling preferential adsorption or targeted catalytic activity for specific molecules. This provides a clear improvement over conventional adsorbents, which often rely on non-specific physical interactions (**He et al., 2025; Mussa et al., 2025**).

From an economic perspective, while conventional adsorbents are generally cheaper per unit, MXenes can achieve higher efficiency with smaller material quantities, potentially reducing overall material requirements for comparable pollutant removal (**Elouardi et al., 2024**).

Regarding scalability, advances in synthesis techniques, including electrochemical etching and molten salt methods, have enabled the production of MXenes at a scale suitable for industrial applications (**Elouardi et al., 2024**). Nonetheless, the need for precise control over surface functionalization and layer structure remains a minor limitation, as slight variations in synthesis can affect adsorption capacity or catalytic performance.

Overall, MXenes represent a significant improvement over conventional adsorbents and catalysts in efficiency, selectivity, and material utilization, with only minor concerns regarding reproducibility and structural sensitivity under specific conditions.

8. Challenges

8.1 Obstacles in large-scale MXene synthesis

The practical implementation of MXenes at an industrial scale faces significant challenges. Conventional hydrofluoric acid (HF) etching, while effective for removing the A-layer, poses severe safety risks, generates corrosive waste streams, and requires strict regulatory compliance, complicating large-scale production (**He et al., 2024**). Alternative approaches, such as *in-situ* HF (LiF/HCl), electrochemical etching, or molten-salt methods, reduce these hazards but still encounter difficulties in controlling flake size, surface terminations ($-O/-OH/-F/-Cl$), and maintaining consistent yields.

MXenes, including $Ti_3C_2T_x$, are highly susceptible to oxidation during synthesis, storage, and processing. This susceptibility can degrade electrical conductivity, collapse interlayer structures, and alter surface chemistry, which directly affects adsorption and electrochemical performance (**Iqbal et al., 2021; Cai & Kim, 2025**). Furthermore, batch-to-batch variability in surface terminations can influence hydrophilicity, interlayer spacing, and overall functionality, complicating reproducibility (**Kumar et al., 2023; Lee et al., 2023**).

Scale-up introduces additional challenges, such as increased defect formation, layer restacking, and reduced delamination efficiency. Achieving uniform flake size and morphology is critical for reproducible performance in membranes, electrodes, and other applications. Moreover, extensive washing to remove residual acids or salts is necessary to stabilize colloidal suspensions, but this process can be resource-intensive, affecting operational efficiency (**Shuck et al., 2021; Carey & Barsoum, 2022**).

8.2 Environmental safety concerns :

Despite their remarkable properties, MXenes present environmental safety challenges. Potential toxicity to aquatic and terrestrial ecosystems is a major concern, as nanosheets may induce oxidative stress or cytotoxic effects in certain microbial and plant models (Xiang *et al.*, 2025). In addition, MXenes can undergo partial oxidation under ambient conditions, forming byproducts that may alter their chemical behavior and interactions with ecosystems (Sahith *et al.*, 2025).

The lack of standardized guidelines for safe handling, disposal, and environmental monitoring further complicates their practical use and commercialization (Hansen *et al.*, 2024).

8.3 Integration into existing wastewater treatment infrastructure

Integrating MXenes into conventional wastewater treatment systems involves technical and operational challenges. Their nanoscale size and high reactivity can interfere with microbial communities in biological treatment units, potentially inhibiting biological processes (Abdul Rasheed *et al.*, 2024; Ye *et al.*, 2025).

Material recovery and long-term reuse are also critical considerations, as MXenes may experience surface changes that reduce adsorption capacity over multiple cycles (Abdul Ghani *et al.*, 2021). Scalability and process optimization remain obstacles for real-world applications. Performance in complex wastewater matrices can differ from laboratory conditions due to competing ions, organic matter, and pH variations (Tawalbeh *et al.*, 2023; Amani *et al.*, 2025). Embedding MXenes into composite membranes, polymer matrices, or supporting materials may improve handling, prevent nanoparticle leaching, and facilitate integration into existing infrastructure (Du *et al.*, 2024).

Table 5. Summary of the main challenges, strengths, and limitations of MXenes

Challenge / Category	Strengths	Limitations
Large-Scale MXene Synthesis	Multiple approaches available (HF, LiF/HCl, electrochemical, molten-salt) provide flexible production options	Safety hazards, batch-to-batch variability, difficulty controlling flake size and layers, extensive washing required
Stability and Oxidation Resistance	Surface modifications and protective additives improve oxidation resistance	High susceptibility to oxidation, affecting conductivity and surface chemistry
Integration into Wastewater Treatment Systems	MXenes can be incorporated into membranes or supporting materials	Potential interference with microbial communities, performance reduction over multiple cycles, practical deployment complexity

Removal of Pharmaceutical Pollutants from Aquatic Mediums Using MXene Nanocomposites

Environmental Safety	Exceptional pollutant removal and remediation potential	Possible ecological toxicity, nanoparticle accumulation in water and soil, lack of standardized regulatory guidelines
Regeneration and Reusability	Methods like solvent washing or electrochemical regeneration maintain performance	Some methods may cause surface degradation over repeated use, long-term performance needs further study

9. Future perspectives

MXene-based nanomaterials have demonstrated impressive capabilities for the removal of pharmaceutical pollutants, yet their journey from laboratory discovery to real-world application is still at an early stage. To accelerate this transition, the research community must shift from generic statements about “further study” toward clearly defined roadmaps that address fundamental scientific gaps and practical implementation barriers.

One of the most pressing directions lies in achieving atomic-level precision in tailoring MXene surfaces and interlayer structures. Controlling surface terminations and interlayer spacing with deterministic accuracy would allow the design of active sites that selectively capture or degrade pharmaceuticals with high efficiency. Coupled with this, the development of in-situ and operando characterization techniques capable of monitoring molecular interactions and degradation pathways directly on MXene surface will provide critical insights into their reaction mechanisms under realistic water treatment conditions.

Another promising avenue involves moving beyond the traditional use of MXene powders in suspension. While effective in laboratory-scale tests, powders pose challenges for handling, separation, and reuse. Future innovation will likely focus on engineering macroscopic MXene-based architectures such as three-dimensional printed monoliths, mechanically robust mixed-matrix membranes, and electrospun nanofibrous mats. These formats can facilitate integration into flow-through reactors, improve stability, and enable continuous operation under complex wastewater conditions. In parallel, embedding MXene-based sensors within treatment systems offers the opportunity to enable real-time monitoring of pharmaceutical concentrations, paving the way for smart, adaptive treatment technologies.

A further critical perspective concerns the sustainability of MXene production and deployment. Current etching and delamination routes are not inherently scalable or environmentally benign. Thus, the development of fluoride-free, waterbased, and energy-efficient synthesis strategies will be indispensable for industrial viability. At the same time, there is an urgent need to consider the full life cycle of MXene materials. Future work must examine not only performance metrics but also environmental fate, recyclability, and long-term cost effectiveness. Life-cycle assessments and techno-economic evaluations will be essential to validate claims of sustainability and ensure that MXene-based technologies can compete with or complement conventional treatment methods.

In summary, the future of MXene research in pharmaceutical pollutant removal will depend on three interconnected priorities: Precise structural and surface control at the atomic level; disruptive device-scale innovations for practical integration; and truly sustainable production and evaluation frameworks. Addressing these priorities will transform MXenes from an exciting laboratory material into a cornerstone of next-generation water purification technologies.

CONCLUSION

Pharmaceutical pollutants remain a pressing environmental and public health concern due to their persistence, bioaccumulation potential, and ability to induce antimicrobial resistance. This review highlights MXenes and their nanocomposites as a versatile platform for the removal of these contaminants, leveraging their unique two-dimensional architecture, high surface area, tunable surface terminations, and excellent electrical conductivity. The synergistic combination of adsorption, electrostatic interactions, hydrogen bonding, photocatalytic degradation, and electrochemical oxidation enables MXenes to achieve superior removal efficiencies compared to conventional adsorbents and catalysts.

MXene-based nanocomposites incorporating polymers, metal oxides, and carbon-based materials exhibit enhanced stability, improved charge separation, and increased adsorption capacity, offering significant advantages for practical wastewater treatment. Moreover, regeneration strategies such as electrochemical reactivation and solvent washing demonstrate the feasibility of repeated use, supporting cost-effectiveness and long-term operation.

In summary, MXenes and their composites present a promising toolkit for the sustainable removal of PhACs, bridging the gap between laboratory-scale innovation and real-world water treatment needs.

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