

TWO-DIMENSIONAL Ti_3CNT_x CARBONITRIDE MXene: A REVIEW OF SYNTHESIS, STRUCTURE, CHARACTERIZATION AND PROSPECTIVE APPLICATIONS

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ARTICLE INFO

Received: 22 July 2026
Revised: 29 July 2026
Accepted: 04 September 2026

Keywords:

MXene; Ti_3CNT_x ; carbonitride; MAX phase; selective etching; nitrogen incorporation; photocatalysis; electrochemical energy storage; heavy metal adsorption; oxidation stability

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ABSTRACT

Two-dimensional transition metal carbonitride (Ti_3CNT_x) MXene has attracted growing scientific interest as a multifunctional nanomaterial, yet systematic reviews consolidating its synthesis, properties, and applications remain scarce compared to its carbide analogue $\text{Ti}_3\text{C}_2\text{T}_x$. This review provides a comprehensive account of Ti_3CNT_x , covering MAX ($\text{M}_{n+1}\text{AX}_n$) phase precursor synthesis, selective etching routes (hydrofluoric acid (HF)-based, (MILD), and fluorine-free methods), and exfoliation strategies yielding single-layer nanosheets. The structural consequences of partial carbon-to-nitrogen substitution are discussed, including termination-dependent changes in lattice parameters, interlayer spacing, and electron density near the Fermi level. Nitrogen incorporation modifies the electronic structure of Ti_3CNT_x by redistributing the density of states near the Fermi level and influencing its charge-transport and optical behavior. Reported studies generally indicate metallic or near-metallic electronic characteristics, while specific surface terminations, defects, and compositional configurations may lead to semiconducting-like features. The mechanical, optical, electrochemical, catalytic, and adsorption properties of Ti_3CNT_x are critically examined with particular attention to the dependence of reported performance on composition, surface chemistry, morphology, synthesis conditions, and testing protocols. Ti_3CNT_x has demonstrated promising lithium-ion storage performance, including an experimentally reported discharge capacity of approximately 300 mAh g^{-1} under specific cycling conditions. Its photocatalytic behavior is discussed primarily in the context of heterostructured and photocatalysis-assisted systems, where Ti_3CNT_x can contribute to interfacial charge transfer and charge separation. Direct quantitative comparisons with $\text{Ti}_3\text{C}_2\text{T}_x$ are considered only where experimental conditions are sufficiently comparable; otherwise, reported values are treated as material- and system-specific rather than evidence of universal superiority.

Electromagnetic interference shielding, heavy metal adsorption, gas sensing, and photothermal cancer therapy applications are also reviewed. Current limitations-including synthesis reproducibility, ambient oxidation, and production cost-are critically evaluated. Fluorine-free synthesis, machine learning-assisted compositional design, and Ti_3CNT_x -based heterostructures are identified as priority directions for future research.

Introduction

In 2011, Naguib et al. reported the first synthesis of a two-dimensional transition-metal carbide, $\text{Ti}_3\text{C}_2\text{T}_x$, establishing the MXene family as a new class of two-dimensional materials [1]. This novel class of materials, termed MXenes, is represented by the general formula $\text{M}_{(n+1)}\text{X}_n\text{T}_x$, where M denotes an early transition metal (Ti, V, Nb, Mo, among others), X represents carbon and/or nitrogen atoms, and T_x refers to surface functional groups (-OH, -O, -F, -Cl). The synthesis pathway, key physicochemical advantages, and emerging applications of Ti_3CNT_x MXene are schematically summarized in **Figure 1** [2].

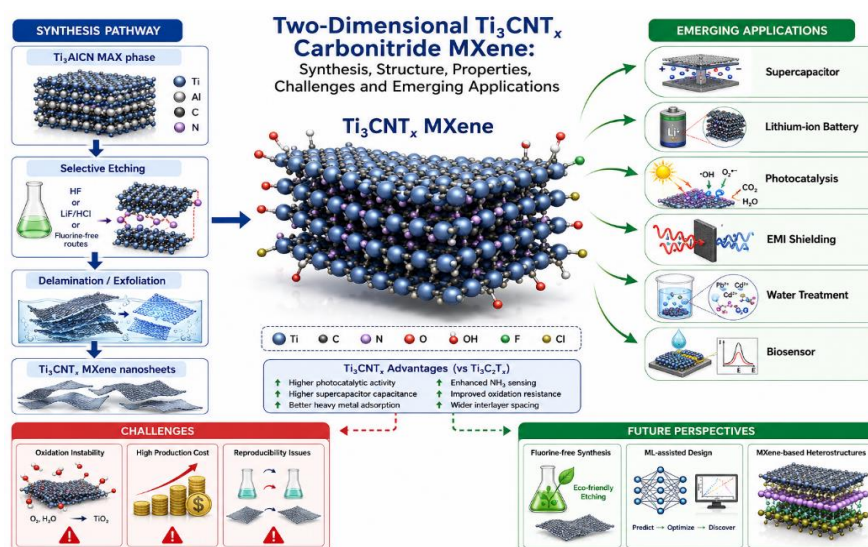


Figure 1. Schematic illustration of the synthesis pathway, advantages, and applications of 2D Ti_3CNT_x MXene (redrawn by the authors based on Ref. [1])

Over the past decade, the MXene family has expanded rapidly, now encompassing more than 30 experimentally confirmed and over 100 theoretically predicted compositions. Within this family, $\text{Ti}_3\text{C}_2\text{T}_x$ remains the most extensively studied and best-characterized member [3]. This prominence is largely attributed to its relatively accessible synthesis, high electrical conductivity, hydrophilic surface chemistry, and strong electrochemical performance [3]. Nevertheless, $\text{Ti}_3\text{C}_2\text{T}_x$ has several limitations. In particular, its relatively narrow electrochemical operating window, limited photocatalytic activity, and relatively rapid oxidation in oxygen-containing environments have prompted researchers to search for MXene materials with new compositions. This need has provided the basis for the extensive investigation of Ti_3CNT_x , a carbonitride MXene [4]. Unlike $\text{Ti}_3\text{C}_2\text{T}_x$, Ti_3CNT_x is a hybrid carbonitride MXene in which carbon (C) and nitrogen (N) atoms coexist within the X layer. As can be seen from its chemical formula, C and N atoms may be arranged alternately or randomly within the same layer, resulting in significant changes in the material's properties. [5] Nitrogen atoms possess one more valence electron than carbon atoms. This difference alters the density of electronic states (DOS) at the Fermi level of Ti_3CNT_x and modulates its metallic conductivity [6]. First-principles calculations based on density functional theory (DFT) have demonstrated that the electron density in Ti_3CNT_x is redistributed relative to that in $\text{Ti}_3\text{C}_2\text{T}_x$, thereby facilitating the formation of catalytically active sites [7][8]. While $\text{Ti}_3\text{C}_2\text{T}_x$ is generally characterized by metallic behavior, the incorporation of nitrogen into Ti_3CNT_x modifies the electronic structure through changes in orbital hybridization and the density of states near the Fermi level. In particular, the interaction between Ti 3d and N 2p orbitals can redistribute electronic states and alter charge-transport characteristics relative to $\text{Ti}_3\text{C}_2\text{T}_x$. Although idealized Ti_3CNT_x structures are generally predicted to retain metallic character, specific surface terminations, defects, and compositional configurations may modify the electronic structure and, in some cases, lead to semiconducting-like features. Therefore, the electronic properties of Ti_3CNT_x should be considered

composition- and surface-chemistry-dependent rather than being described by a universal intrinsic bandgap [4].

Nitrogen incorporation can also modify the surface electronic structure and adsorption behavior of Ti_3CNT_x , although the magnitude and direction of these effects depend on surface terminations, defects, and composition.

The review highlights fluorine-free synthesis, machine learning-assisted compositional design, and Ti_3CNT_x -based heterostructures as promising directions for future research. Figure 2 illustrates a representative LiF-HCl etching route for the synthesis of Ti_3CNT_x MXene from the Ti_3AlCN MAX phase, followed by surface functionalization.

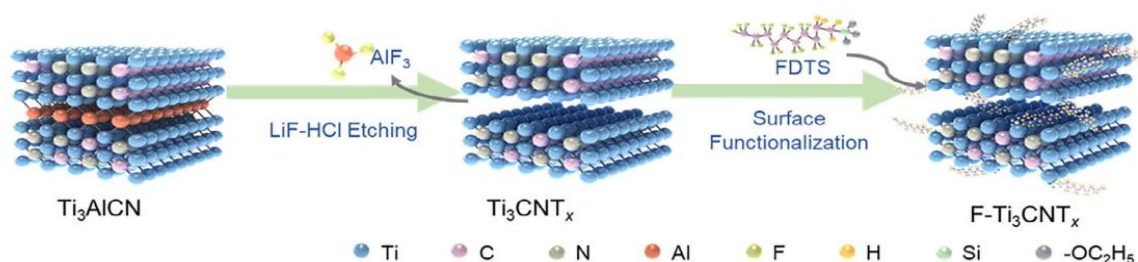


Figure 2. Schematic illustration of the synthesis of Ti_3CNT_x MXene from the Ti_3AlCN MAX phase through selective LiF-HCl etching and subsequent surface functionalization. Reproduced from Yang et al., *Adv. Mater. Interfaces*, 2025, 12, 2400969. Licensed under CC BY 4.0 [9].

Furthermore, the formation of stronger Ti-N bonds has been reported to improve the thermal and chemical stability of Ti_3CNT_x compared with $\text{Ti}_3\text{C}_2\text{T}_x$, which is beneficial for practical applications.

In recent years, scientific interest in Ti_3CNT_x has increased substantially, as reflected by the growing number of publications on its synthesis, properties, stability, and emerging applications. However, comprehensive review articles that systematically address the synthesis, stability, and photocatalytic properties of Ti_3CNT_x within a single framework remain limited [4].

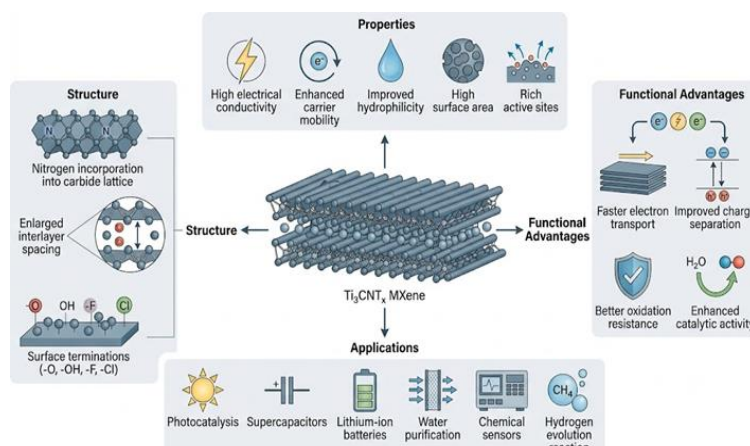


Figure 3. Schematic overview of the structure-property-application relationships in Ti_3CNT_x MXene, illustrating how nitrogen incorporation influences physicochemical properties and enables diverse technological applications (Created by the authors).

As illustrated in Figure 3, nitrogen incorporation can modify the structural and electronic characteristics of Ti_3CNT_x , which may influence its catalytic, electrochemical, and environmental performance.

Although recent reviews have comprehensively discussed carbonitride MXenes as a broader class of two-dimensional materials, a focused assessment of Ti_3CNT_x remains necessary because its structural, electronic, surface-chemical, and application-related characteristics can differ substantially from those of both conventional $\text{Ti}_3\text{C}_2\text{T}_x$ and other carbonitride MXenes. The present

review therefore focuses specifically on Ti_3CNT_x and provides an integrated analysis of its synthesis from Ti-Al-C-N MAX phases, selective etching and exfoliation strategies, structural and surface-chemical characteristics, and the effects of carbon-to-nitrogen substitution on its physicochemical properties. Particular emphasis is placed on establishing structure-property relationships and critically evaluating Ti_3CNT_x -specific experimental evidence alongside theoretical and comparative studies. In addition, the review examines the reported and emerging applications of Ti_3CNT_x in photocatalysis, energy storage, electromagnetic interference shielding, sensing, and related fields, while explicitly distinguishing experimentally demonstrated performance from values inferred from other MXene systems or theoretical calculations. This Ti_3CNT_x -centered perspective is intended to complement previous broad reviews of carbonitride MXenes and to identify material-specific challenges and research opportunities that remain insufficiently addressed.

The search covered publications available from 2011 through 2025. Studies were included when they reported experimental or theoretical investigations directly related to Ti_3CNT_x or titanium carbonitride MXenes, including synthesis, structure, surface chemistry, physicochemical properties, stability, or applications. Studies on $\text{Ti}_3\text{C}_2\text{T}_x$ and other MXene compositions were retained only when they provided relevant comparative or fundamental information. Publications lacking sufficient information on material composition, preparation, characterization, or application context, as well as studies outside the defined scope of this review, were excluded.

The search strategy employed combinations of keywords related to the material and its major research areas, including “ Ti_3CNT_x ”, “ Ti_3CN ”, “titanium carbonitride MXene”, “carbonitride MXene”, “MXene synthesis”, “MXene etching”, “photocatalysis”, “energy storage”, “electromagnetic interference shielding”, and “sensing”. Additional keyword combinations were considered to identify studies addressing nitrogen incorporation, surface functionalization, oxidation stability, and structure–property relationships.

Particular emphasis was placed on studies specifically reporting Ti_3CNT_x or closely related titanium carbonitride MXenes. Publications concerning $\text{Ti}_3\text{C}_2\text{T}_x$ and other MXene compositions were also considered when they provided relevant comparative information or fundamental insights into MXene synthesis, structure, surface chemistry, stability, or physicochemical properties. However, data obtained from non- Ti_3CNT_x MXenes were not considered as direct experimental evidence for Ti_3CNT_x -specific properties.

The identified literature was critically evaluated according to the material composition, synthesis or preparation method, experimental or theoretical approach, reported properties, and application context. Particular attention was given to distinguishing experimentally measured results from density functional theory (DFT) calculations and proposed mechanisms. Where quantitative values or mechanistic interpretations originated from $\text{Ti}_3\text{C}_2\text{T}_x$, other MXene compositions, or theoretical studies, their relevance to Ti_3CNT_x was considered separately rather than treating them as direct experimental evidence for Ti_3CNT_x .

Accordingly, this review provides an integrated assessment of Ti_3CNT_x carbonitride MXene, covering its synthesis, structural and surface-chemical characteristics, stability, physicochemical properties, and emerging applications. Particular attention is given to structure–property relationships and to comparisons with $\text{Ti}_3\text{C}_2\text{T}_x$ where sufficiently comparable evidence is available. Current challenges in synthesis, reproducibility, stability, and practical application are critically discussed, together with prospective research directions for Ti_3CNT_x -based materials [2].

2. Synthesis methods: From MAX phase to Ti_3CNT_x nanosheets.

2.1. Synthesis of MAX phases: Methods for obtaining Ti_3AlCN and other solid solution powders.

The first and most critical step in the Ti_3CNT_x MXene synthesis process is the synthesis of its precursor, the MAX phase. MAX phases are layered ternary compounds represented by the general formula $\text{M}_{(n+1)}\text{AX}_n$, where A is primarily a Group IIIA or IVA element (Al, Si, Ga, Ge,

etc.)[10]. For Ti_3CNT_x , the precursor MAX phase is Ti_3AlCN , which contains both carbon and nitrogen atoms [11].

Solid-State Reaction Method. A conventional approach described in the literature involves mixing Ti, Al, TiC, and TiN powders, or alternative carbon and nitrogen precursors, in stoichiometric ratios. The resulting mixture is subsequently sintered at temperatures ranging from 1350 °C to 1500 °C under an inert argon or nitrogen atmosphere for 2-4 h to produce Ti_3AlCN powder [6][10]. The microstructural quality and phase purity of the final product depend strongly on the purity, particle size distribution, and compositional homogeneity of the starting powders[11].

Spark Plasma Sintering (SPS) Method. This approach involves passing a pulsed electric current through a loaded sample, which induces a rapid localized temperature increase, allowing the synthesis to complete within 5-10 minutes. Compared to conventional methods, SPS is distinguished by a significantly reduced processing time, the formation of a fine-grained, homogeneous microstructure, and the capability to yield high-density products. However, the widespread adoption of this technique remains constrained by relatively high equipment and operational costs [12].

Gas-Phase Reaction Method (Chemical Vapor Deposition, CVD). In the CVD approach, gaseous Ti-containing precursors along with carbon and nitrogen sources (CH_4 , N_2 , or NH_3) react at elevated temperatures on a substrate surface. This method is well-suited for the deposition of Ti_3AlCN in thin film form; however, its applicability to large-scale production remains limited[13], [14].

The synthesized Ti_3AlCN powder is characterized by X-ray diffraction (XRD) analysis. Its characteristic reflections are reported at $2\theta = 9\text{-}10^\circ$ (002 plane) and $38\text{-}40^\circ$ (104 plane). Obtaining a high-quality MAX phase directly determines the efficiency of the subsequent etching step, as a poorly sintered or impurity-containing MAX phase inevitably leads to a low-yield or inferior-quality MXene product[15].

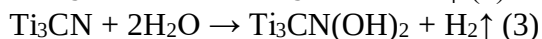
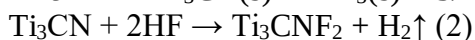
In summary, among the available MAX phase synthesis routes, solid-state reaction remains the most practical and widely adopted method for laboratory-scale Ti_3AlCN production owing to its simplicity and scalability. SPS offers superior microstructural control but is limited by equipment cost, while CVD is better suited for thin-film applications rather than bulk powder synthesis. Regardless of the chosen method, achieving high phase purity and compositional homogeneity in the Ti_3AlCN precursor is of paramount importance, as these factors directly govern the quality and yield of the resulting Ti_3CNT_x MXene. Future efforts should focus on optimizing solid-state synthesis parameters to minimize impurity phases, particularly at nitrogen-rich compositions, where formation of phase-pure materials can become more challenging.

2.2. Acidic etching: selective extraction of the A layer

The selective etching of MAX phases is based on the preferential removal of the A-layer, while the transition-metal carbide/nitride layers are preferentially retained to form the characteristic layered MXene structure. During etching, the removal of the A-element is accompanied by surface functionalization, resulting in the formation of surface terminations (T_x), such as -O, -OH, and -F, depending on the etching chemistry and subsequent treatment conditions.

2.2.1. Etching with hydrofluoric acid (HF)

HF-based etching is historically the first and remains the most widely used method for Ti_3CNT_x synthesis[6], [16]. Simplified representations of the fluoride- and hydroxyl-terminated surface formation during HF-based etching can be expressed as follows:



HF-based etching is an established route for selectively removing the Al layers from Ti_3AlCN MAX phases to obtain Ti_3CNT_x . Reported outcomes depend strongly on etchant strength,

temperature, reaction time, precursor composition, and subsequent washing and delamination. Excessively aggressive conditions can increase defect formation, whereas insufficient etching can leave residual MAX-phase material [17],[16]. Because these parameters are highly system-specific, direct comparison of reported etching conditions should be made only when precursor composition and processing protocols are comparable.

The primary drawback of HF-based etching is the extreme toxicity and corrosivity of the acid, necessitating specialized protective equipment and adapted laboratory facilities.

2.2.2. Mixture of mineral acids and fluoride salts (MILD method)

The Minimally Intensive Layer Delamination (MILD) approach uses a mixture of LiF and HCl to generate fluoride species in situ during the etching process, providing an alternative to direct HF-based etching [18]

As illustrated in Figure 4, the MILD synthesis of single-layered Ti_3CNT_x MXene involves two sequential steps: microwave-assisted HCl/LiF etching of the Ti_3AlCN MAX phase (4 h), followed by TMAOH delamination (24 h) to yield a stable aqueous single-layer dispersion.

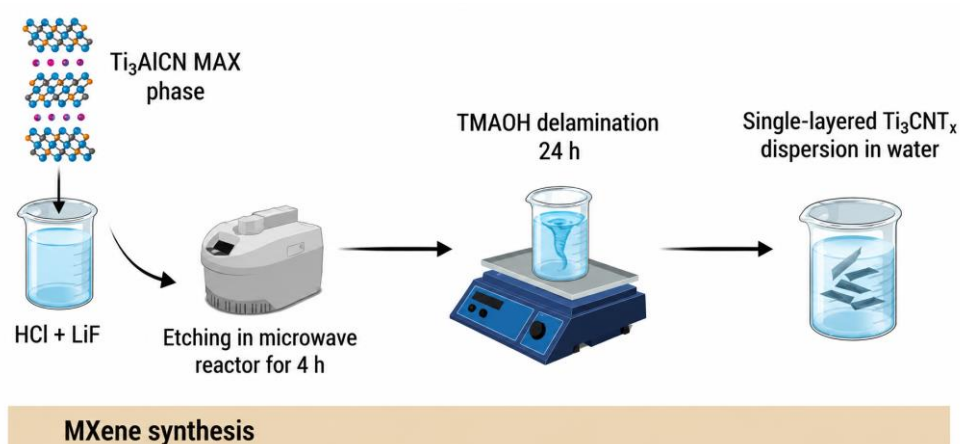
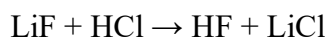


Figure 4. Schematic illustration of the synthesis of single-layered Ti_3CNT_x MXene: selective etching of Ti_3AlCN MAX phase using HCl/LiF in a microwave reactor (4 h), followed by TMAOH delamination (24 h) to obtain a stable single-layered Ti_3CNT_x aqueous dispersion. Reproduced from Purbayanto et al., ACS Appl. Mater. Interfaces, 2023, 15, 44075-44086. Licensed under CC BY 4.0 [17].



The MILD approach uses a fluoride salt/mineral-acid system to generate the active etching environment in situ and can facilitate simultaneous intercalation and subsequent delamination[17][19]. Reported Ti_3CNT_x products obtained by this route show that morphology, surface termination, flake dimensions, and colloidal stability depend on the exact precursor and processing conditions[16]. Therefore, the literature supports MILD as an important alternative to direct HF-based processing, while Ti_3CNT_x -specific optimization remains necessary[20].

Overall, while HF etching remains the most established method for Ti_3CNT_x synthesis, the MILD approach represents a significant advancement in terms of safety and product quality. The emergence of fluorine-free routes, including molten salt and electrochemical etching, holds particular promise for environmentally sustainable large-scale production, though their optimization for Ti_3CNT_x -specific conditions requires further investigation.

2.3. Exfoliation (Delamination)

The product obtained by acidic etching is multilayer MXene (ml-MXene). An additional exfoliation (delamination) step is required to obtain single- or few-layer nanosheets (fl-MXene).

Several intercalation agents have been explored for Ti_3CNT_x delamination. DMSO (dimethyl sulfoxide), owing to its large molecular size, penetrates between MXene layers and

expands the interlayer spacing when ml-MXene is immersed for 18-24 hours, followed by ultrasonication; successful intercalation is confirmed by a downward shift of the d_{002} peak in XRD analysis [17]. TMAOH (tetramethylammonium hydroxide) has been reported as an effective intercalation agent for Ti_3CNT_x , where its relatively large TMA^+ cation can facilitate interlayer expansion and subsequent layer separation under suitable sonication conditions [21]. A more recent alternative, choline chloride (ChCl), offers the advantage of high water solubility and biologically safe, and Ti_3CNT_x nanosheets prepared by this route have been reported to exhibit superior colloidal stability. Depending on the intercalant and processing conditions, a final ultrasonication step may be used to facilitate further delamination. Probe sonicators generally provide higher energy input than bath sonicators; however, excessive sonication can fragment the nanosheets and reduce their lateral dimensions, making optimization of sonication amplitude and duration important [17].

Collectively, the choice of delamination method significantly influences the lateral size, layer number, and colloidal stability of the resulting Ti_3CNT_x nanosheets. TMAOH intercalation has been reported as an effective approach for producing stable Ti_3CNT_x single-layer dispersions under suitable processing conditions. The use of alternative intercalants, including choline chloride, also provides opportunities to modify the delamination process and surface characteristics of the resulting nanosheets.

2.4. Green and Fluorine-Free Synthesis Methods

Environmental and safety concerns associated with HF and fluoride salts have prompted researchers to develop alternative, "green" synthesis routes for Ti_3CNT_x [20].

Alkaline etching using concentrated NaOH solutions has been investigated as a fluorine-free approach for selectively removing the Al layer from Ti_3AlCN . However, the etching efficiency for Ti_3CNT_x has been reported to be lower than that achieved for $Ti_3C_2T_x$, limiting its current applicability [22], [23].

Electrochemical (electrolytic) etching employs the MAX phase as an anode in an aqueous electrolyte, enabling Al removal under controlled electrochemical conditions without the use of fluoride-containing etchants [9]. In hydrothermal approaches, etching is performed under elevated temperature and pressure, and some reported processes can combine etching with partial delamination [17]. Molten-salt (Lewis acid) etching utilizes salts such as $ZnCl_2$ or $NaCl/KCl$ eutectics at elevated temperatures to remove the A-layer without fluoride-containing reagents. Such treatments can introduce chlorine-containing surface terminations and provide an alternative route for tuning the surface chemistry of Ti_3CNT_x [24].

Collectively, fluorine-free synthesis methods remain at an early stage of development for Ti_3CNT_x . Further optimization of etching conditions, phase purity, surface chemistry, and delamination is required to achieve reproducible material quality comparable to that obtained by established fluoride-based routes. Nevertheless, these approaches offer important opportunities to reduce the use of hazardous fluoride-containing reagents and to introduce alternative surface terminations, making them promising directions for more sustainable Ti_3CNT_x processing.

3. Crystal Structure and Surface Chemistry

3.1. Crystal lattice parameters and atomic arrangement

Ti_3CNT_x adopts a hexagonal crystal structure belonging to the $P6_3/mmc$ space group, sharing the general layered architecture of $Ti_3C_2T_x$ but exhibiting several structurally significant differences arising from the coexistence of carbon and nitrogen atoms in the X layers [5].

The SEM micrographs of $Ti_3AlC_{1.5}N_{0.5}$ and Ti_3AlCN in Figure 5 show the characteristic layered morphology of the carbonitride MAX phases. Both compositions exhibit a lamellar structure, while differences in grain morphology and lamellar appearance can be observed with increasing nitrogen content. These morphological variations are consistent with the compositional dependence of the crystal structure and lattice parameters reported for $Ti_3AlC_{2-\gamma}N_\gamma$. However, the SEM images alone do not establish a direct relationship between nitrogen content, interlayer cohesion, and subsequent etching efficiency.

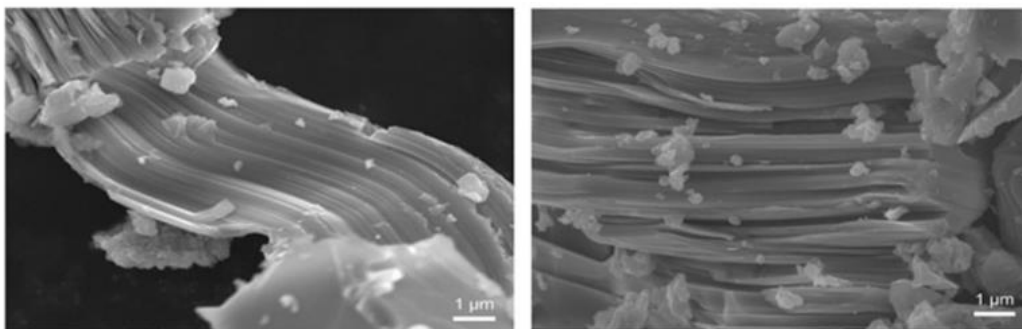


Figure 5. SEM micrographs for $\text{Ti}_3\text{AlC}_{1.5}\text{N}_{0.5}$ and Ti_3AlCN phases, respectively. Reproduced from Zhang et al., Two-dimensional carbonitride MXenes: From synthesis to properties and applications, 2024, 6, e609. Licensed under CC BY 4.0 [2]

Higher-resolution structural characterization of Ti_3AlCN is provided by transmission electron microscopy. The TEM image reveals the nanoscale lamellar architecture of the Ti_3AlCN precursor at a scale of 50 nm, showing the tightly stacked, parallel layer arrangement characteristic of 312-type MAX phases. The individual lamellae are well-defined and continuous, with no obvious evidence of significant delamination or severe structural disorder. These observations are consistent with the layered morphology of the sintered precursor and provide a structural basis for subsequent selective etching [15].

High-resolution TEM reveals well-defined lattice fringes in the Ti_3AlCN precursor, further confirming its crystalline structure. The observed lattice characteristics are consistent with the compositional modification associated with C/N substitution in $\text{Ti}_3\text{AlC}_{2-\gamma}\text{N}_\gamma$. Increasing nitrogen content has been experimentally associated with changes in both the in-plane and out-of-plane lattice parameters, reflecting composition-dependent changes in interatomic distances and lattice distortion. Therefore, the structural evolution of $\text{Ti}_3\text{AlC}_{2-\gamma}\text{N}_\gamma$ should be interpreted in terms of composition-dependent lattice modification rather than attributed solely to differences in the nominal atomic radii of C and N.

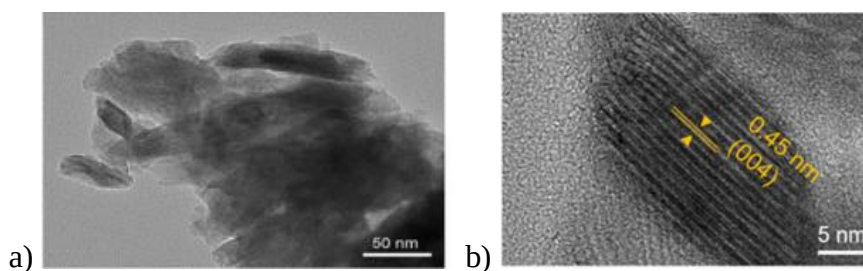


Figure 6. TEM (a) and HRTEM (b) images of Ti_3AlCN . Reproduced from Zhang et al., J. Adv. Ceram., 2024, 13(9), 1473-1481. Licensed under CC BY 4.0 [2].

The morphological transformation resulting from selective etching of the Ti_3AlCN precursor is clearly demonstrated in the SEM images of the resulting Ti_3CNT_x MXene (Figure 7, panels a and b). The acid-etched Ti_3CNT_x displays the characteristic accordion-like multilayer morphology with well-defined stacked lamellae separated by interlayer gaps. The individual MXene layers appear relatively smooth and continuous, with interlayer spacing associated with the removal of Al and the presence of surface terminations and intercalated species [2].

In contrast, the molten-salt-etched Ti_3CNT_x exhibits a different lamellar morphology, which can be associated with the distinct processing conditions used during etching. The molten-salt route also produces different surface chemistry, with Cl-containing terminations reported for Ti_3CNCl_2 -based MXene materials[25].

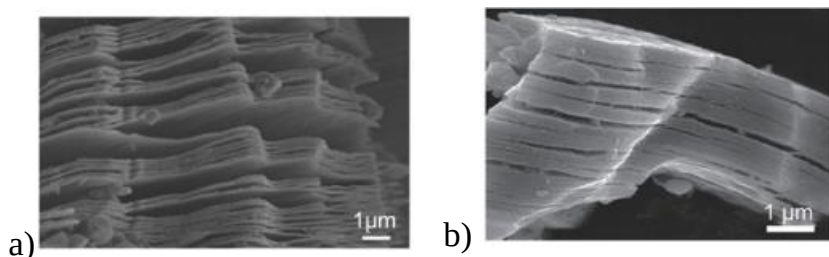


Figure 7. a) SEM image of Ti_3CNT_x obtained by etching Ti_3AlCN with 30% HF solution for 21 h. Reproduced from Zhang et al., Carbon Energy, 2024, 6, e609. Licensed under CC BY 4.0 [1]. b) SEM image of Ti_3CNT_x obtained by etching Ti_3AlCN with CuCl_2 molten salt. Reproduced from Zhang et al., Carbon Energy, 2024, 6, e609. Licensed under CC BY 4.0 [2]

X-ray diffraction (XRD) analysis indicates that Ti_3CNT_x exhibits composition- and termination-dependent lattice parameters. Reported in-plane lattice parameters are generally close to those of $\text{Ti}_3\text{C}_2\text{T}_x$, while variations in the C/N ratio can modify the lattice dimensions. Experimental and theoretical studies indicate that increasing N content can induce lattice contraction through changes in interatomic distances and lattice distortion associated with C/N substitution. The out-of-plane lattice parameter and interlayer spacing, in contrast, are strongly affected by surface terminations and intercalated species. Therefore, reported lattice parameters should be interpreted with respect to composition, surface chemistry, and measurement conditions rather than treated as universal constants[26].

DFT calculations for specific surface-terminated Ti_3CNT_x models indicate lattice parameters in the approximate range of 3.00-3.07 Å, while experimentally measured values depend on composition, surface termination, and synthesis conditions. Therefore, lattice parameters reported for Ti_3CNT_x should be interpreted in relation to the specific structural model and experimental conditions rather than as universal values for all Ti_3CNT_x materials[26]

Each Ti_3CNT_x monolayer consists of a seven-atomic-layer sandwich arranged, from top to bottom, as $\text{T}_x\text{-Ti-(C/N)-Ti-(C/N)-Ti-T}_x$, with the overall thickness determined by the atomic arrangement and surface termination. The central Ti layers, located between the X layers, contribute to the structural integrity of the MXene sheet [27].

The arrangement of C and N atoms within the two X layers of Ti_3CNT_x remains an open and actively debated question. Three structural models have been proposed: an ordered model, in which C and N occupy separate X layers (C-Ti-N-Ti-C or N-Ti-C-Ti-N stacking), thermodynamically favored according to DFT calculations; a disordered model, in which C and N are distributed across both X layers; and a cluster model, in which C- and N-rich nanoscale domains coexist within the same layer. Although first-principles calculations favor specific ordered arrangements on energetic grounds, experimental determination of the precise C/N distribution remains challenging [6], [1].

In the XRD pattern of Ti_3CNT_x , several features can be used for phase identification and structural assessment, including the low-angle (002) reflection associated with the interlayer structure, higher-order reflections such as (006) and (008) that provide information on stacking periodicity, and the attenuation or disappearance of MAX-phase reflections following Al removal. The exact position of these reflections can vary with C/N composition, surface termination, intercalated species, hydration state, and processing conditions. Consequently, differences between Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ XRD patterns should be interpreted in the context of these structural and chemical variables rather than attributed exclusively to nitrogen incorporation [9].

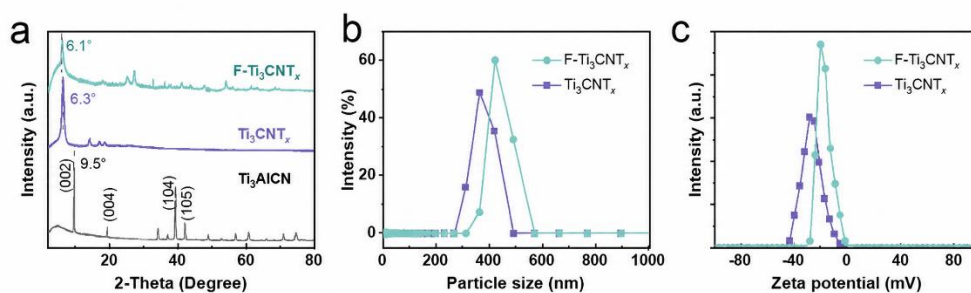


Figure 8. a) XRD patterns of Ti_3AlCN , Ti_3CNT_x , and $\text{F-Ti}_3\text{CNT}_x$ powders. b) Particle size distribution of Ti_3CNT_x and $\text{F-Ti}_3\text{CNT}_x$ in water dispersion. c) Zeta potential values of Ti_3CNT_x and $\text{F-Ti}_3\text{CNT}_x$ in water dispersion. Reproduced from Yang et al., *Adv. Mater. Interfaces*, 2025, 12, 2400969. Licensed under CC BY 4.0[9].

Taken together, the available crystallographic evidence indicates that the lattice parameters and interlayer spacing of Ti_3CNT_x are sensitive to composition, surface termination, intercalation chemistry, and synthesis conditions. Importantly, changes in the in-plane lattice parameter should be distinguished from variations in the out-of-plane lattice parameter and interlayer spacing, as these structural dimensions can respond differently to C/N substitution, surface functionalization, and intercalated species. The unresolved question of C/N ordering within the X layer remains an important structural issue in carbonitride MXene research and requires further experimental investigation using compositionally well-defined samples.

3.2. Surface Functional Groups (T_x): Effect of -O, -OH, -F, and -Cl Terminations on Material Stability

The surface of Ti_3CNT_x is typically terminated by surface functional groups, collectively denoted as T_x , whose identity and relative abundance depend on the synthesis route and post-processing conditions. These terminations can substantially influence the electronic structure, hydrophilicity, electrochemical behavior, and stability of the material [28].

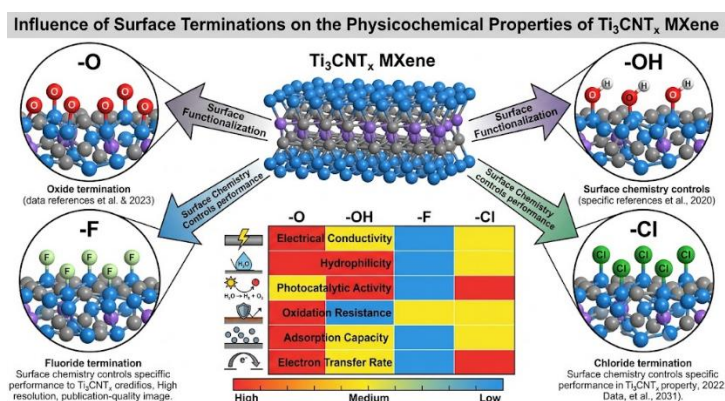


Figure 9. Qualitative heat-map representation of the reported influence of surface terminations (-O, -OH, -F, and -Cl) on selected physicochemical properties of Ti_3CNT_x MXene, including electrical conductivity, hydrophilicity, photocatalytic behavior, oxidation resistance, adsorption, and electron-transfer characteristics. The relative levels shown are qualitative representations based on trends reported in the reviewed literature and are not intended as normalized quantitative values. Created by the authors based on the reviewed literature.

As shown in Figure 9, surface chemistry plays an important role in determining the properties and performance of Ti_3CNT_x MXene. Oxygen-containing terminations can modify electronic structure and charge-transfer characteristics, while hydroxyl groups generally contribute to hydrophilicity and colloidal interactions. Fluorine-containing terminations can also alter surface electronic properties and interfacial charge-transfer behavior. Therefore, the effect of a given

termination should be interpreted in relation to its abundance, the overall surface composition, and the specific application.

Fluoride terminations (-F) are commonly associated with HF- and fluoride-salt-based etching routes and can substantially modify the surface electronic and interfacial properties of Ti_3CNT_x . Their presence may affect surface reactivity, ion accessibility, charge-transfer behavior, and electrochemical response. Consequently, controlling the abundance of -F terminations is an important consideration in tailoring Ti_3CNT_x for electrochemical and photocatalytic applications[29], [30].

Hydroxyl terminations (-OH) can arise during aqueous etching and washing steps and generally contribute to the hydrophilic character of Ti_3CNT_x , facilitating interactions with aqueous electrolytes and reactant solutions. In photocatalytic systems, surface hydroxyl groups may participate in interfacial reactions and can influence the generation of reactive oxygen species, depending on the surface electronic structure and reaction conditions. However, the relationship between -OH abundance and oxidation stability is not universal and depends on the overall surface chemistry and environmental conditions[28].

Oxide terminations (-O) form either by thermal dehydration of -OH groups at elevated temperatures or through direct reaction with oxygen. The resulting Ti-O bonds are covalent and thermally stable, and DFT calculations indicate that -O-rich Ti_3CNT_x exhibits a distinct work function relative to -F- or -OH-terminated variants, offering a handle for tuning electron transfer properties in catalytic and electronic applications [31].

Chloride terminations (-Cl) represent a relatively recent addition to the surface chemistry of MXenes and can be introduced through chloride-containing etching or molten-salt routes. Ti_3CNCl_2 -based MXene materials have been investigated for catalytic applications, where surface termination and interfacial electronic structure can influence hydrogen adsorption and charge-transfer behavior. However, the effects of -Cl termination on Ti_3CNT_x remain less extensively established than those of -O, -OH, and -F, and further systematic studies are needed to clarify the underlying mechanisms [32].

Surface termination composition is routinely assessed using a combination of complementary characterization techniques. X-ray photoelectron spectroscopy (XPS) resolves the chemical states of Ti, C, N, F, and O through their respective core-level spectra and can provide information on the relative abundance and chemical environment of surface species[17]. Fourier-transform infrared spectroscopy (FTIR) can identify characteristic vibrational features associated with Ti-O, Ti-OH, and Ti-F environments. Solid-state ^{13}C and ^{15}N NMR spectroscopy can provide information on the local chemical environments of X-layer atoms, while thermogravimetric analysis (TGA) can be used to assess overall thermal stability and changes in mass associated with surface species during heating [27].

As shown in Figure 10, XPS analysis of Ti_3CNT_x and $\text{F-Ti}_3\text{CNT}_x$ films reveals distinct differences in surface termination chemistry across the Ti 2p, C 1s, O 1s, N 1s, and F 1s core-level spectra.

The available evidence indicates that surface termination strongly influences Ti_3CNT_x properties, but no single termination can be considered universally optimal. The effects of -O, -OH, -F, and -Cl depend on composition, morphology, processing history, and the target application. Accordingly, termination engineering should be treated as an application-specific strategy rather than a general route to improved performance.

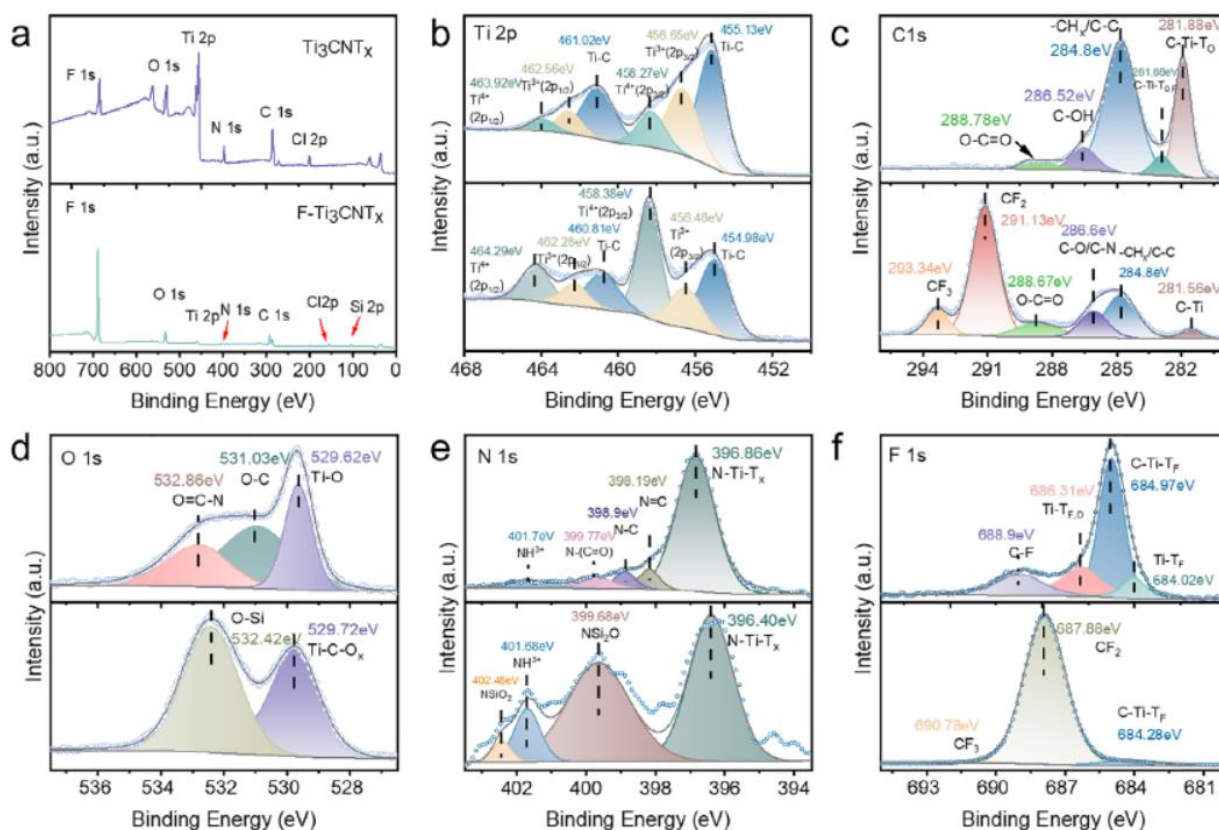


Figure 10. a) The XPS spectra survey of drop-cast Ti_3CNT_x and $\text{F-Ti}_3\text{CNT}_x$ films. The high-resolution XPS spectra of b) Ti 2p, c) C 1s, d) O 1s, e) N 1s, and f) F 1s of Ti_3CNT_x film (top) and $\text{F-Ti}_3\text{CNT}_x$ film (bottom). Reproduced from Yang et al., *Adv. Mater. Interfaces*, 2025, 12, 2400969. Licensed under CC BY 4.0 [7].

3.3. Oxidation Mechanism of Ti_3CNT_x and Strategies for Enhancing Chemical Stability

One of the significant practical challenges limiting the broader application of Ti_3CNT_x is its susceptibility to oxidative degradation under environmental conditions, particularly during prolonged exposure to oxygen and moisture. The oxidation stability of Ti_3CNT_x is therefore an important consideration for its storage, processing, and practical use[33].

Ti_3CNT_x oxidation is a multifactorial process influenced by water and oxygen exposure, surface termination, defects, morphology, and environmental conditions [38]. Oxidation can involve progressive changes in the Ti-containing framework and the formation of TiO_2 -rich products, while structural degradation becomes more pronounced with prolonged environmental exposure. The available evidence does not justify assigning a single oxidation mechanism or rate to all Ti_3CNT_x samples. Reported stabilization strategies include protective coatings, controlled storage, and surface functionalization; their effectiveness is likewise dependent on material form and processing conditions [38,40,41]. Figure 11 provides a source-specific example of surface functionalization that substantially changes wettability and maintains the reported contact-angle response under the tested conditions [7].

As demonstrated in Figure 11, surface functionalization of Ti_3CNT_x with FDTs results in a pronounced wettability transition from hydrophilic ($\text{CA} = 83.31^\circ$) to superhydrophobic ($\text{CA} = 153.12^\circ$), with the functionalized $\text{F-Ti}_3\text{CNT}_x$ film maintaining stable contact angles across a wide pH range (pH 1-11) and in various salt solutions over 30 days.

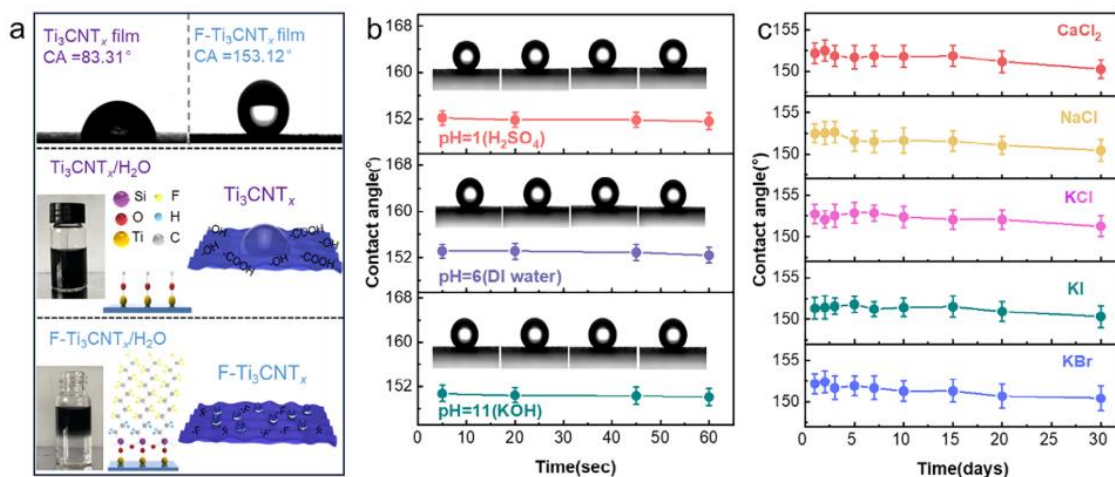


Figure 11. Surface chemistry characterization of Ti_3CNT_x and $\text{F-Ti}_3\text{CNT}_x$ films: (a) digital photographs and contact angle (CA) analysis of $\text{Ti}_3\text{CNT}_x/\text{H}_2\text{O}$ and $\text{F-Ti}_3\text{CNT}_x/\text{H}_2\text{O}$ - functionalization transforms the surface from hydrophilic to superhydrophobic (CA: $83.31^\circ \rightarrow 153.12^\circ$); (b) contact angle stability of $\text{F-Ti}_3\text{CNT}_x$ film at various pH conditions (pH 1, 6, 11); (c) variation in CA over 30 days in different salt solutions (CaCl_2 , NaCl , KCl , KI , KBr) simulating artificial sweat composition. Reproduced from Yang et al., *Adv. Mater. Interfaces*, 2025, 12, 2400969. Licensed under CC BY 4.0 [9].

Interlayer engineering, protective coatings, and surface-termination control have been investigated as possible approaches to reducing environmental degradation of MXenes. For Ti_3CNT_x specifically, direct evidence remains limited and the effectiveness of each strategy depends on the material architecture and processing history. These approaches should therefore be evaluated using Ti_3CNT_x -specific stability measurements rather than inferred directly from $\text{Ti}_3\text{C}_2\text{T}_x$ or other MXenes.

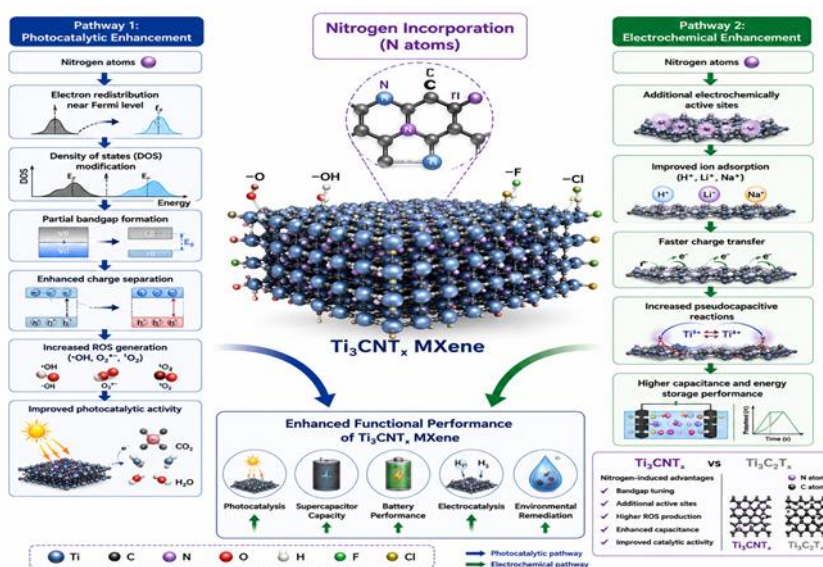


Figure 12. Nitrogen-induced structure-property-application relationship in Ti_3CNT_x MXene. Created by the authors

As schematically illustrated in Figure 12, nitrogen incorporation can modify the structure-property-application relationships of Ti_3CNT_x through changes in electronic structure, surface chemistry, and interfacial reactivity. The magnitude and direction of these effects depend on C/N composition, surface termination, defects, morphology, and the application-specific environment;

therefore, the figure is intended as a conceptual framework rather than evidence of universal superiority over $\text{Ti}_3\text{C}_2\text{T}_x$.

The above discussion underscores that oxidation stability of Ti_3CNT_x is a multifactorial challenge requiring coordinated consideration of synthesis conditions, storage environment, and surface engineering. Protective coatings, including atomic layer deposition (ALD), and controlled storage under inert atmospheres have been investigated as approaches for mitigating environmental degradation, while termination engineering and heterostructure design provide additional strategies for modifying surface reactivity and stability. However, the effectiveness and long-term durability of these approaches require further systematic evaluation using Ti_3CNT_x -specific stability measurements under standardized environmental conditions.

4. Unique Physicochemical Properties

4.1. Electrical Conductivity: High Density of States at the Fermi Level and Metallic Behavior

The electrical conductivity of Ti_3CNT_x is an important physicochemical property that strongly influences its potential performance in energy storage, electrocatalysis, electromagnetic interference shielding, and other charge-transport-related applications.

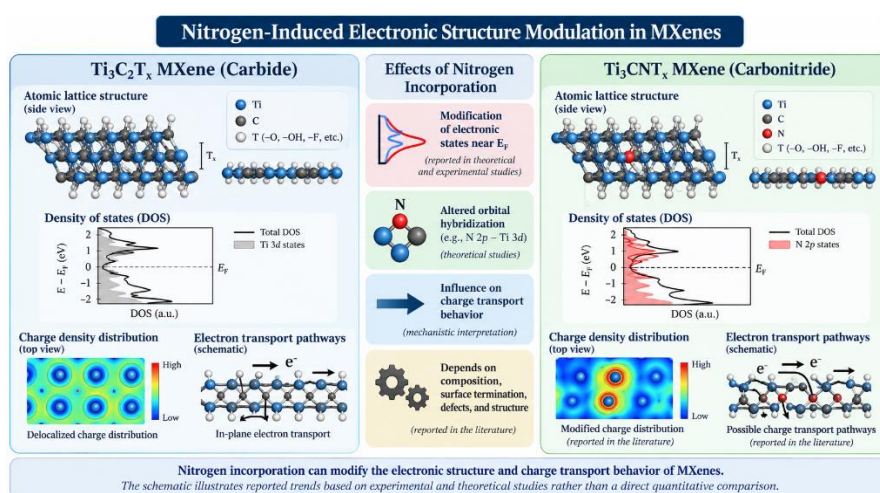


Figure 13. Schematic illustration of nitrogen-induced electronic-structure modulation in Ti_3CNT_x MXene compared with $\text{Ti}_3\text{C}_2\text{T}_x$.

The figure summarizes reported changes in electronic density of states, charge-density distribution, and possible charge-transfer pathways based on experimental and theoretical studies. The schematic is intended to illustrate reported trends rather than represent a direct quantitative comparison.

As illustrated schematically in Figure 13, nitrogen incorporation can modify the electronic structure of Ti_3CNT_x relative to $\text{Ti}_3\text{C}_2\text{T}_x$. Reported studies indicate changes in the density of states and charge-density distribution associated with the presence of N within the X layer. These electronic modifications may influence charge transport and interfacial electron-transfer behavior, although the magnitude and direction of the effect depend on composition, defects, surface terminations, and structural configuration.

Theoretical studies of Ti_3CNT_x generally indicate metallic or near-metallic electronic structures, with substantial electronic states around the Fermi level[8]. Incorporation of N into the X layer modifies the calculated density of states and electronic structure relative to carbide MXenes. In particular, interactions involving N 2p and Ti 3d states can contribute to changes in the distribution of electronic states near the Fermi level. [34]. However, the calculated electronic properties depend on the assumed C/N configuration, surface termination, and defect structure.

Accordingly, theoretical predictions should be interpreted in relation to the specific structural model considered.

These electronic-structure modifications provide a possible basis for differences in the electrical and catalytic behavior reported for Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$. Nevertheless, experimentally observed properties are also strongly influenced by defects, morphology, surface termination, film thickness, and processing history.

Reported electrical conductivity values for Ti_3CNT_x vary considerably depending on the synthesis route, flake thickness, intercalation state, surface termination, and film morphology. Therefore, rather than assigning a single conductivity range to all Ti_3CNT_x samples, it is more appropriate to consider the electrical response in relation to the specific preparation and measurement conditions. Experimental studies have demonstrated that processing and intercalation can substantially modify the measured conductivity of Ti_3CNT_x , while individual flakes can exhibit metallic-like intrinsic transport behavior [8].

Temperature-dependent transport measurements indicate that the electrical response of Ti_3CNT_x depends strongly on its processing and intercalation state. While intrinsic Ti_3CNT_x can exhibit metallic behavior, as-prepared multilayer films may show semiconductor-like temperature dependence because of intercalated species and interflake transport. Removal of intercalated species can therefore lead to a transition toward more metallic-like transport behavior, demonstrating that the measured macroscopic response does not necessarily represent the intrinsic electronic character of an individual Ti_3CNT_x flake[8]

Surface termination provides an additional experimentally relevant parameter for controlling the electrical properties of Ti_3CNT_x . Reported differences among -O-, -OH-, and -F-containing surfaces indicate that surface chemistry can alter the electronic states near the Fermi level and consequently influence charge transport[35]. The specific conductivity values reported for different termination compositions should, however, be interpreted within the corresponding synthesis, morphology, and measurement conditions rather than treated as universal values[8].

The electronic structure may also be modified by surface termination and defect states. Some theoretical and experimental studies have suggested that specific surface-terminated or defect-containing Ti_3CNT_x configurations can exhibit semiconducting-like electronic features. Such behavior should not be regarded as an intrinsic property of all Ti_3CNT_x samples, because the electronic structure depends strongly on composition, surface chemistry, and defect concentration[35].

Taken together, the available evidence indicates that the electronic and electrical properties of Ti_3CNT_x are governed by the combined effects of C/N composition, surface termination, defects, and morphology. Experimental studies demonstrate substantial variation in conductivity among Ti_3CNT_x samples, while theoretical calculations provide insight into how C/N substitution and surface chemistry modify the electronic states near the Fermi level. The reported coexistence of metallic or near-metallic behavior with semiconducting-like features in selected samples suggests that Ti_3CNT_x possesses potentially tunable electronic characteristics. However, establishing a reproducible relationship between synthesis conditions, surface chemistry, electronic structure, and functional performance requires further systematic experimental and theoretical investigation. Future studies should therefore focus on establishing reproducible relationships between C/N composition, surface termination, defect concentration, and electronic transport properties using complementary experimental characterization and theoretical calculations.

4.2. Optical Properties: Light Absorption, Free-Carrier and Plasmonic Effects

Ti_3CNT_x has been reported to show broad optical absorption extending across portions of the UV-visible-NIR region, although the spectral response depends on composition, termination, thickness, morphology, and measurement conditions[36]. Its optical behavior has been associated with interband electronic transitions and, in metallic samples, free-carrier or plasmonic

contributions. These features make Ti_3CNT_x of interest for photothermal and optoelectronic applications, while photocatalytic relevance depends on the coupled semiconductor and interface.

The plasmonic and free-carrier optical response of Ti_3CNT_x may provide several photocatalytically relevant effects, depending on the material structure and excitation conditions. Local electromagnetic-field enhancement can increase the intensity of light near the MXene surface, while plasmon or free-carrier decay may generate energetic charge carriers that can participate in interfacial processes. In addition, absorption of near-infrared radiation can produce photothermal heating, which may influence thermally assisted catalytic reactions. The relative contribution of these effects depends on composition, surface termination, morphology, carrier density, and the coupled reaction system. Optical conductivity calculations have also been used to relate the frequency-dependent optical response of Ti_3CNT_x to its electronic transport behavior [37]. Single- and few-layer Ti_3CNT_x nanosheets can exhibit substantial attenuation of visible light, whereas multilayer films generally show much lower optical transmission. Consequently, film thickness and layer number are important parameters for controlling the optical response of Ti_3CNT_x in optoelectronic applications [27] - a transparency comparable to that of monolayer graphene ($\sim 2.3\%$). Multilayer films are essentially opaque across the visible range, and for optical device applications requiring controlled transmittance, single- or few-layer Ti_3CNT_x is therefore preferred. Additionally, weak photoluminescence (PL) has been observed in Ti_3CNT_x [38], tentatively attributed to localized bandgap states arising at nanosheet edges and defect sites rather than bulk electronic transitions. While the origin of this PL signal remains incompletely understood, it opens a potential avenue for biological imaging applications.

Collectively, the optical properties of Ti_3CNT_x indicate its potential as a broadband light-absorbing and optoelectronic material.

Beyond light absorption, Ti_3CNT_x has also been demonstrated as an electron-transport layer in perovskite solar cells, where a Ti_3CNT_x -based device achieved a power conversion efficiency of 20.16% and showed improved operational stability [39].

Its optical response is strongly influenced by nanosheet thickness, surface termination, defect structure, composition, and intercalation state. These factors can modify light absorption, plasmonic behavior, photothermal conversion, and charge-carrier dynamics. Although some studies have reported favorable optical or near-infrared responses for Ti_3CNT_x relative to $\text{Ti}_3\text{C}_2\text{T}_x$, the available evidence does not support a universal superiority of one material over the other. Differences in synthesis conditions, morphology, surface chemistry, film thickness, and measurement methodology can substantially affect the observed optical response. Therefore, direct comparison between Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ should be restricted to studies conducted under comparable experimental conditions. Integration of Ti_3CNT_x with suitable semiconductor or two-dimensional materials may further enable application-specific control of light absorption, interfacial charge transfer, and photothermal effects.

4.3. Mechanical Properties: Flexibility and Strength of Thin Films and Aerogels

The mechanical properties of Ti_3CNT_x are strongly influenced by its composition, defect structure, surface chemistry, layer thickness, and processing history. Studies have demonstrated that Ti_3CNT_x nanosheets can combine high mechanical stiffness with the flexibility characteristic of two-dimensional materials, making them promising for flexible electronics, protective coatings, and lightweight composite structures. The mechanical response is also affected by nanosheet architecture and interactions between individual layers. In particular, reducing layer thickness and controlling defects can influence the balance between stiffness, flexibility, and mechanical stability. However, direct quantitative comparison between Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ remains challenging because reported mechanical properties depend strongly on sample preparation, nanosheet dimensions, defect concentration, surface termination, and measurement methodology. Therefore, the mechanical advantages of Ti_3CNT_x should be considered application-specific rather than as evidence of universal superiority over $\text{Ti}_3\text{C}_2\text{T}_x$.

Reported mechanical properties of Ti_3CNT_x vary substantially with composition, defect density, nanosheet dimensions, surface termination, and measurement methodology. Quantitative comparison with $\text{Ti}_3\text{C}_2\text{T}_x$ should therefore be limited to studies using comparable specimen geometry, thickness, environmental conditions, loading mode, and measurement protocols. The available literature supports the mechanical potential of Ti_3CNT_x nanosheets, but does not justify assigning a universal mechanical advantage to either MXene.

Ti_3CNT_x nanosheets can exhibit considerable mechanical flexibility, which is particularly relevant for flexible and wearable devices. Their ultrathin two-dimensional architecture allows them to accommodate bending and deformation, while the mechanical response can be influenced by defects, surface chemistry, and interactions between individual layers. Flexible Ti_3CNT_x -based films have therefore attracted interest for applications in flexible electronics, supercapacitors, and sensors. Raman spectroscopy provides complementary structural information, allowing changes in vibrational modes and defect-related features to be investigated. [40]. Relative to $\text{Ti}_3\text{C}_2\text{T}_x$, all Raman peaks in Ti_3CNT_x exhibit slight frequency shifts consistent with the mass and force-constant changes introduced by N incorporation. The full width at half maximum (FWHM) of Raman lines serves as a practical indicator of defect density in synthesized samples [41][42]. Three-dimensional aerogel architectures derived from Ti_3CNT_x nanosheets provide an additional strategy for combining low density, mechanical resilience, and interconnected porous structures. The open porous network can facilitate mechanical recovery while providing a large accessible surface area and interconnected pathways, making Ti_3CNT_x -based aerogel structures potentially useful for electromagnetic shielding, thermal management, and electrochemical applications. However, the mechanical and functional performance of these porous architectures depends strongly on the fabrication method, density, pore structure, nanosheet arrangement, and interfacial interactions. Therefore, further systematic studies are required to establish reliable relationships between aerogel structure and mechanical or functional performance.

Overall, recent experimental evidence demonstrates that multilayer Ti_3CNT_x coatings exhibit distinct mechanical and tribological behavior, including load-dependent friction, wear resistance, and tribofilm formation[43]. Nevertheless, Ti_3CNT_x -specific mechanical datasets remain considerably less developed than those available for $\text{Ti}_3\text{C}_2\text{T}_x$. Reliable comparison between the two materials requires matched specimen geometry, thickness, surface termination, environmental conditions, loading mode, and measurement methodology. Future studies should therefore combine nanoindentation, tensile or bending measurements, tribological testing, and structural characterization to establish reproducible relationships between C/N composition, surface chemistry, defects, morphology, and mechanical performance.

5. Emerging Applications

5.1. Electrochemical Energy Storage

5.1.1. Supercapacitors

Supercapacitors occupy an intermediate position between conventional capacitors and batteries in the electrochemical energy-storage landscape, combining high power density, rapid charge–discharge capability, and long cycle life. Ti_3CNT_x has attracted interest as a potential electrode material because its layered structure, mixed C/N composition, and surface chemistry provide opportunities for tuning interfacial charge-storage behavior.

Charge storage in Ti_3CNT_x -based electrodes may involve both electric double-layer capacitance (EDLC) and pseudocapacitive contributions. EDLC originates primarily from electrostatic accumulation of electrolyte ions at the electrode–electrolyte interface, whereas pseudocapacitive behavior can arise from reversible surface redox processes and ion interactions involving transition-metal surface sites. The relative contribution of these mechanisms depends on surface termination, electrolyte composition, electrode architecture, interlayer spacing, and operating conditions. Because much of the mechanistic understanding of MXene charge storage has been established using $\text{Ti}_3\text{C}_2\text{T}_x$ and related systems, these mechanisms should be considered as a general framework rather than as exclusively Ti_3CNT_x -specific behavior. [44].

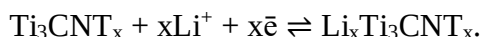
For Ti_3CNT_x , reported electrochemical charge-storage performance depends strongly on electrode architecture, surface chemistry, C/N composition, interlayer spacing, electrolyte composition, and testing protocol[45]. Nitrogen incorporation may provide an additional route for modifying the electronic structure and surface interactions of titanium carbonitride MXenes, potentially affecting ion adsorption and charge-storage processes[33]. However, the available literature does not provide sufficient evidence to establish a universal capacitance advantage of Ti_3CNT_x over $\text{Ti}_3\text{C}_2\text{T}_x$.

Electrochemical impedance spectroscopy (EIS) can provide information on ion transport, interfacial resistance, and charge-transfer characteristics in MXene-based electrodes. For Ti_3CNT_x , however, the available experimental evidence remains comparatively limited, and extracted transport parameters should be interpreted in relation to electrode morphology, surface termination, electrolyte composition, and measurement methodology. Interlayer engineering and hybridization with complementary electroactive materials represent potential strategies for improving electrolyte accessibility and charge-storage performance, although their effectiveness should be demonstrated using Ti_3CNT_x -specific experimental systems.

Long-term stability under humidity, oxidation, and repeated electrochemical cycling remains an important consideration for Ti_3CNT_x -based supercapacitor electrodes. Further Ti_3CNT_x -specific studies are required to establish reproducible relationships between composition, surface chemistry, electrode architecture, charge-storage mechanism, and long-term cycling stability.

5.1.2. Anode materials for Lithium-Ion and Post-Lithium batteries

Lithium-ion batteries remain widely used for portable electronics, electric vehicles, and stationary energy-storage systems. Ti_3CNT_x has been investigated as an anode material for lithium-ion storage, with its electrochemical behavior depending on C/N composition, surface termination, electrode architecture, and cycling conditions. Lithium storage in Ti_3CNT_x -based electrodes can involve ion intercalation together with surface and interfacial charge-storage processes[19]. A simplified representation of lithium incorporation can be expressed as:



A representative study demonstrated that a highly defective Ti_3CNT_x fiber-membrane electrode can serve as an anode substrate for lithium-metal batteries, achieving a Coulombic efficiency of approximately 99.1% and stable cycling over 1000 cycles. The enhanced performance was attributed to the high surface area, strong lithiophilicity, and Ti-vacancy defects of the Ti_3CNT_x structure[46]

Experimental studies of titanium carbonitride MXenes have demonstrated that their layered architecture can accommodate reversible alkali-ion storage, while electrochemical performance remains sensitive to nanosheet morphology, interlayer accessibility, surface chemistry, and electrode processing. In particular, Ti_3CNT_x -based electrodes have been investigated for lithium-ion storage, with reported performance depending on the preparation route and electrode configuration [47]. Initial irreversible capacity losses may arise from interfacial reactions and solid-electrolyte-interphase formation, as observed in MXene-based electrode systems.

Sodium-ion storage has also been investigated for titanium carbonitride MXenes. Their layered structure and tunable interlayer environment can provide pathways for Na^+ accommodation, while the electrochemical response depends on composition, surface termination, electrode architecture, and electrolyte chemistry. Ti_3CNT_x and related titanium carbonitride MXenes have therefore been considered as potential sodium-storage materials. However, quantitative comparison between different studies should be restricted to experiments performed using comparable electrode compositions and electrochemical protocols.

Potassium-ion storage represents another potential application for titanium carbonitride MXenes. The larger ionic radius of K^+ introduces additional transport and structural constraints, while the layered architecture of carbonitride MXenes may provide opportunities for ion accommodation. Nevertheless, Ti_3CNT_x -specific evidence for potassium-ion storage remains

limited, and further experimental studies are required before reliable performance comparisons can be established. [48].

Multivalent-ion systems, including zinc-ion storage, also represent a potential direction for MXene-based electrodes. However, the available evidence for Ti_3CNT_x in such systems remains comparatively limited. Accordingly, zinc-ion and other multivalent-ion applications should currently be considered emerging research directions rather than established performance areas for Ti_3CNT_x .

Across these battery chemistries, Ti_3CNT_x shows potential for ion-storage applications because its layered structure, tunable interlayer environment, and mixed C/N composition provide opportunities for controlling ion transport and interfacial charge storage. Nevertheless, the reported electrochemical behavior varies substantially with composition, surface termination, interlayer engineering, electrode architecture, electrolyte chemistry, and testing protocol. Direct evidence supporting a universal battery-performance advantage of Ti_3CNT_x over $\text{Ti}_3\text{C}_2\text{T}_x$ is currently insufficient. Future studies should therefore focus on establishing composition-structure-performance relationships, improving initial Coulombic efficiency and long-term cycling stability, and developing reproducible electrode architectures for alkali- and multivalent-ion storage.

5.2. Electromagnetic Interference (EMI) Shielding

The rapid proliferation of electronic devices has made electromagnetic interference (EMI) an increasingly critical engineering challenge, driving demand for high-performance shielding materials that are simultaneously lightweight, flexible, and processable. Ti_3CNT_x has attracted increasing interest as a potential material for EMI shielding and microwave absorption applications.

EMI attenuation in Ti_3CNT_x -based materials can involve a combination of reflection, absorption, and multiple internal reflection. Electrical conductivity can contribute to reflection, whereas dielectric losses, interfacial polarization, and multiple internal reflections can contribute to absorption within multilayer or porous architectures. Importantly, the relative contribution of these mechanisms depends on conductivity, thickness, morphology, surface chemistry, frequency, and composite architecture. Direct comparison with $\text{Ti}_3\text{C}_2\text{T}_x$ therefore requires matched specimen geometry and measurement conditions[27].

Direct Ti_3CNT_x studies demonstrate that microwave and EMI-related performance can be substantial, including absorption-dominated behavior under appropriate processing conditions. For example, Ti_3CNT_x nanosheets have shown strong microwave absorption in the X and Ku bands, while thermal processing and layered architecture can markedly influence the electromagnetic response[16],[33]. These findings indicate the application potential of Ti_3CNT_x without implying a universal performance advantage over $\text{Ti}_3\text{C}_2\text{T}_x$.

Overall, Ti_3CNT_x should be considered a promising alternative platform for EMI shielding and microwave absorption, particularly where absorption-dominated attenuation, low-dimensional architecture, or lightweight structures are desirable. However, the magnitude of its advantage or disadvantage relative to $\text{Ti}_3\text{C}_2\text{T}_x$ remains application- and condition-dependent. Future studies should report thickness, density, frequency range, conductivity, reflection/absorption/transmission contributions, and testing geometry consistently to enable reliable cross-study comparison.

5.3. Catalysis and Environmental Remediation

5.3.1. Hydrogen Evolution Reaction (HER) and Oxygen Reduction Reaction (ORR)

Green hydrogen production has emerged as one of the most strategically important directions in modern energy research, and Ti_3CNT_x has attracted growing attention as an electrocatalyst for water-splitting reactions[49].

The HER activity of Ti_3CNT_x is influenced by its conductive Ti-C-N framework, surface termination, defect structure, composition, morphology, electrolyte, pH, catalyst loading, substrate, and electrochemical normalization method. Nitrogen incorporation can modify the electronic environment of surface Ti sites and thereby affect hydrogen adsorption and charge-transfer processes. However, the available literature does not justify assigning a single universal HER

overpotential, Tafel slope, exchange current density, or hydrogen adsorption free-energy range to Ti_3CNT_x [50]. Direct comparisons with $\text{Ti}_3\text{C}_2\text{T}_x$ or Pt/C should therefore be restricted to studies using comparable catalyst architectures and electrochemical protocols. Theoretical calculations are valuable for interpreting how N incorporation may alter adsorption energetics, but calculated descriptors should be clearly distinguished from experimentally measured catalytic performance.

ORR has also been considered as a potential application of carbonitride MXene-based electrocatalysts. Nitrogen incorporation provides an additional route for modifying the electronic structure and the interaction of surface sites with oxygen-containing intermediates. However, Ti_3CNT_x -specific experimental evidence for ORR remains limited compared with the available HER literature. Therefore, nitrogen incorporation alone should not be interpreted as evidence of intrinsically superior ORR activity, and further Ti_3CNT_x -specific studies under standardized conditions are required to establish reliable structure-activity relationships.

5.3.2. Heavy Metal and Organic Dye Removal

Industrial wastewater containing heavy metal ions and synthetic dyes poses significant environmental challenges. Ti_3CNT_x -containing materials have been explored for adsorption and photocatalysis-assisted pollutant removal, but the available Ti_3CNT_x -specific evidence remains comparatively limited. Adsorption behavior is expected to depend on surface termination, defect structure, pH, ionic strength, and the identity and concentration of the target contaminant; therefore, mechanistic and quantitative claims should be restricted to the specific material and experimental conditions reported in each study[51].

The catalytic performance of Ti_3CNT_x MXene is strongly associated with its electronic structure, abundant active sites, and efficient charge-transfer capability. Nitrogen incorporation promotes charge separation and accelerates electron migration, which are beneficial for photocatalytic degradation and environmental remediation processes. Figure 14 presents the proposed photocatalytic mechanism of Ti_3CNT_x MXene under light irradiation.

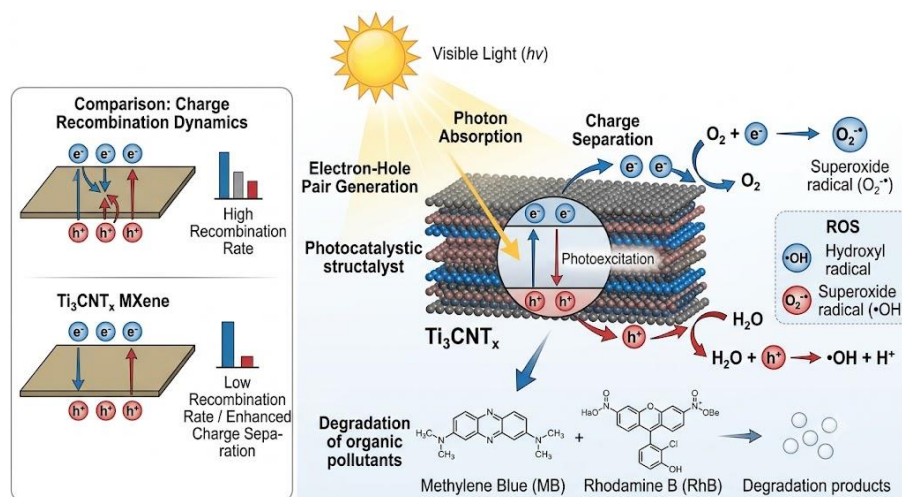


Figure 14. Proposed photocatalytic mechanism of Ti_3CNT_x MXene for catalytic and environmental remediation applications. Under light irradiation, photogenerated electrons and holes participate in the formation of reactive oxygen species (ROS), including $\text{O}_2^{\bullet-}$ and $\bullet\text{OH}$ radicals, which facilitate the degradation of organic pollutants. Nitrogen incorporation enhances charge separation and suppresses electron-hole recombination, thereby improving photocatalytic efficiency (Created by the authors based on the reviewed literature).

Reported adsorption performance for Ti_3CNT_x -containing materials is strongly dependent on surface chemistry, defect structure, adsorbate concentration, pH, ionic strength, and experimental protocol. Because the available evidence is heterogeneous and some adsorption data are reported for other MXene compositions, quantitative adsorption capacities should be interpreted as study-specific rather than as universal values for Ti_3CNT_x [52].

Photocatalytic degradation of organic pollutants has been investigated for Ti_3CNT_x - containing systems, including methylene blue, rhodamine B, tetracycline, and bisphenol A. In many reported studies, Ti_3CNT_x functions as an electron-transfer or cocatalytic component within hybrid photocatalysts rather than as an isolated light-absorbing semiconductor. Reported degradation performance varies substantially with catalyst composition, heterostructure architecture, surface termination, pollutant concentration, catalyst loading, light source, and irradiation time[53].

Table 1

Condition-aware comparison of Ti_3CNT_x - and $\text{Ti}_3\text{C}_2\text{T}_x$ -based systems in photocatalytic pollutant degradation.

Pollutant / reaction	Ti_3CNT_x -based systems	$\text{Ti}_3\text{C}_2\text{T}_x$ -based systems	Comparative interpretation
Methylene blue (MB)	Photocatalytic degradation has been reported, particularly in hybrid/heterostructured systems	Photocatalytic degradation and catalytic-assisting roles have been widely reported	Direct comparison requires matched catalyst composition, loading, light source, concentration, and irradiation time
Rhodamine B (RhB)	Degradation reported in Ti_3CNT_x - containing photocatalytic systems	Degradation reported in $\text{Ti}_3\text{C}_2\text{T}_x$ -containing systems	Reported efficiencies are system-specific and should not be interpreted as evidence of universal superiority
Tetracycline	Promising photocatalytic degradation reported in Ti_3CNT_x - based systems	$\text{Ti}_3\text{C}_2\text{T}_x$ -based photocatalytic systems have also been investigated	Heterostructure composition and experimental conditions strongly influence performance
Bisphenol A (BPA)	Emerging application in photocatalytic/environmental-remediation systems	$\text{Ti}_3\text{C}_2\text{T}_x$ -based systems have been investigated more extensively	Comparative performance remains condition-dependent
Overall photocatalytic role	Can act as an interfacial electron-transfer/cocatalytic component in hybrid photocatalysts	Commonly used as a conductive electron-transfer/cocatalytic component	The role of MXene depends strongly on interface structure, surface termination, and the coupled semiconductor

As summarized in Table 1, Ti_3CNT_x - and $\text{Ti}_3\text{C}_2\text{T}_x$ -based systems have both demonstrated potential for photocatalytic and photocatalysis-assisted pollutant removal. However, reported degradation efficiencies depend strongly on catalyst composition, surface termination, heterostructure architecture, pollutant concentration, catalyst loading, light source, and irradiation time. Therefore, available literature does not support a universal conclusion that Ti_3CNT_x consistently outperforms $\text{Ti}_3\text{C}_2\text{T}_x$ in photocatalytic applications[54].

The available evidence suggests that Ti_3CNT_x may provide useful interfacial and electronic characteristics in selected heterostructured photocatalysts, whereas $\text{Ti}_3\text{C}_2\text{T}_x$ benefits from a substantially larger experimental literature base. Consequently, photocatalytic performance should be evaluated on a system-specific basis using matched experimental conditions rather than by comparing isolated removal percentages reported across different studies[20].

Overall, the available evidence indicates that Ti_3CNT_x has meaningful potential for environmental remediation, particularly through adsorption, reductive adsorption, and catalytic advanced oxidation processes. However, the evidence base is heterogeneous, and Ti_3CNT_x -specific photocatalytic studies remain less extensive than studies of $\text{Ti}_3\text{C}_2\text{T}_x$. Consequently, pollutant-removal performance should be evaluated on a system-specific basis, taking into account surface termination, defect structure, preparation route, contaminant concentration, pH, adsorbent or catalyst loading, light source where applicable, oxidant concentration, and reaction time. Direct

comparisons between Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ should be restricted to experiments performed under matched conditions.

5.4. Sensors and Biomedical Applications

Ti_3CNT_x is being explored for gas, mechanical, electrochemical, and environmental sensing because of its electrical conductivity, accessible surface, and tunable surface chemistry. The available Ti_3CNT_x -specific sensing literature remains more limited than that for $\text{Ti}_3\text{C}_2\text{T}_x$, and reported detection limits and response metrics depend strongly on analyte concentration, humidity, film thickness, electrode architecture, device geometry, and signal definition. Nitrogen incorporation may modify adsorption and charge-transfer behavior, but claims of systematically enhanced sensing relative to $\text{Ti}_3\text{C}_2\text{T}_x$ require matched experimental or computational evidence. Therefore, sensing performance should be reported on a device- and analyte-specific basis rather than as universal detection ranges.

In electrochemical biosensing, Ti_3CNT_x may serve as a conductive electrode or interfacial material because of its accessible surface and tunable surface chemistry. Such platforms can be combined with molecular recognition elements, enzymes, or other functional layers to translate analyte interactions into measurable electrochemical signals. However, Ti_3CNT_x -specific biosensing studies remain comparatively limited, and quantitative detection metrics should be interpreted in relation to the electrode architecture, recognition chemistry, analyte concentration range, and measurement protocol.

In the biomedical domain, Ti_3CNT_x has attracted exploratory interest because of its optical absorption, photothermal behavior, and surface chemistry. Potential applications include photothermal or multimodal therapeutic platforms and bioelectronic interfaces. At present, however, these applications remain at an early research stage, and claims regarding photothermal conversion efficiency, cell-killing performance, or clinical relevance should be restricted to specific experimental systems and exposure conditions rather than generalized to Ti_3CNT_x as a whole[55].

Taken together, the sensor and biomedical literature indicates that Ti_3CNT_x has potential as a multifunctional platform, but the evidence base is heterogeneous and substantially smaller than that for more extensively studied MXenes. Translating laboratory demonstrations into reliable devices or biomedical applications will require reproducible material synthesis, well-defined surface chemistry, standardized performance metrics, and systematic evaluation of long-term stability and safety.

6. Comparative Analysis: Ti_3CNT_x versus $\text{Ti}_3\text{C}_2\text{T}_x$

6.1. Side-by-Side Property Comparison

Although Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ belong to the same MXene family, the incorporation of nitrogen into the carbonitride lattice results in notable differences in their physicochemical and functional properties. Comparative evaluation of key performance indicators is essential for understanding their suitability for specific applications[6]. Figure 15 summarizes the relative performance of Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ across multiple categories reported in the literature.

Comparative Visualization Methodology. Because the reported values for Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ are obtained under different experimental conditions, direct normalization against the highest literature-reported value may introduce study-dependent bias[17]. Therefore, the comparison presented in Figure 15 is intended to illustrate reported qualitative trends rather than provide an absolute ranking of material performance. The relative categories were assigned based on the direction and consistency of trends reported in the literature, while recognizing that differences in synthesis, surface termination, morphology, testing conditions, and measurement protocols can substantially affect the reported values[8].

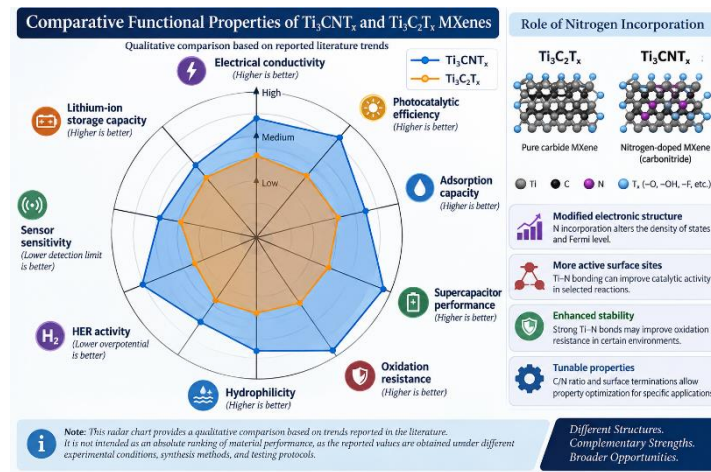


Figure 15. Qualitative comparison of Ti_3CNT_x and $Ti_3C_2T_x$ across selected functional properties based on trends reported in the literature. The figure is intended to illustrate comparative trends rather than provide an absolute ranking of material performance.

As shown in Figure 15, Ti_3CNT_x and $Ti_3C_2T_x$ exhibit distinct performance profiles across the selected functional categories. Ti_3CNT_x shows favorable trends in several areas, particularly those associated with surface chemistry, catalytic activity, and electrochemical behavior, whereas $Ti_3C_2T_x$ retains advantages in properties such as electrical conductivity and EMI shielding. These differences should be interpreted in the context of material composition, surface termination, morphology, synthesis conditions, and application-specific testing protocols rather than as evidence of universal superiority of one MXene over the other[56].

Table 2 provides a comparative summary of selected physicochemical, electrochemical, and functional properties of Ti_3CNT_x and $Ti_3C_2T_x$, together with the corresponding literature references.

Table 2

Balanced, condition-aware comparison of Ti_3CNT_x and $Ti_3C_2T_x$ MXenes

Parameter	$Ti_3AlCN \rightarrow Ti_3CNT_x$	$Ti_3AlC_2 \rightarrow Ti_3C_2T_x$	Comparative interpretation
Etching approach	HF-based, MILD, molten-salt and other routes reported	HF-based, MILD, electrochemical and other routes widely reported	Route selection strongly affects surface chemistry and defect structure
Process severity	Condition-dependent; Ti-N-containing MAX phases may require tailored processing	Condition-dependent	Direct comparison requires matched precursor and protocol
Delamination	Sensitive to intercalation, termination and layer cohesion	Sensitive to intercalation, termination and layer cohesion	Architecture and surface chemistry determine exfoliation outcome
Product yield / quality	Strongly synthesis-dependent	Strongly synthesis-dependent	No universal yield advantage should be assigned
Scale-up maturity	Less mature	More established	Ti_3CNT_x requires further process optimization

Overall, the comparison in Table 2 indicates that Ti_3CNT_x and $Ti_3C_2T_x$ possess complementary property profiles rather than a universally superior performance hierarchy. Nitrogen incorporation can modify the electronic structure, surface chemistry, defect characteristics, and interfacial behavior of carbonitride MXenes, which may be advantageous for selected applications. At the same time, $Ti_3C_2T_x$ may retain advantages in other properties, including electrical conductivity and established synthesis and processing routes. Therefore, the

relative suitability of these MXenes should be evaluated according to the specific application and experimental conditions.

6.2. Synthesis and Processing Comparison

The synthesis of Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ involves related processing concepts but differs in precursor chemistry and compositional control. For Ti_3CNT_x , controlling the C/N ratio and obtaining phase-pure Ti_3AlCN are particularly important. These differences can affect etching behavior, surface termination, defect formation, and the reproducibility of the final MXene. Because reported processing windows vary between studies, direct numerical comparison of synthesis conditions should be avoided unless the precursor composition and protocols are closely matched.

The etching behavior of Ti_3AlCN is sensitive to precursor composition and processing conditions. Reported studies use different etching chemistries and processing windows, so the literature does not support a single universal set of conditions or a universal yield advantage for Ti_3CNT_x over $\text{Ti}_3\text{C}_2\text{T}_x$.

Table 3

Comparison of HF etching parameters for Ti_3AlCN and Ti_3AlC_2 MAX phases

<i>Parameter</i>	<i>Ti_3AlCN (for Ti_3CNT_x)</i>	<i>Ti_3AlC_2 (for $\text{Ti}_3\text{C}_2\text{T}_x$)</i>
Reported HF concentration	10-30 %	5-30 %
Reported temperature	25-40 °C	22-35 °C
Reported duration	24-72 h	18-48 h
MILD method efficiency	Moderate	High
Product yield	55-70 %	65-80 %

Differences in etching behavior between Ti_3AlCN and Ti_3AlC_2 can arise from changes in precursor composition and bonding environment. The magnitude of these differences is study-dependent and should be evaluated using matched precursor and etching protocols.

Delamination behavior depends on interlayer chemistry, intercalation, surface termination, and processing history. Ti_3CNT_x -specific studies indicate that suitable intercalation strategies can facilitate layer separation, but direct comparison with $\text{Ti}_3\text{C}_2\text{T}_x$ should be made only under matched conditions [7,18].

6.3. Detailed Photocatalytic Performance Comparison

Given that photocatalytic applications constitute the central focus of this review, the mechanistic and quantitative aspects of photocatalytic performance reported for Ti_3CNT_x -based systems warrant dedicated discussion[52].

At the mechanistic level, $\text{Ti}_3\text{C}_2\text{T}_x$ generally exhibits metallic or highly conductive electronic characteristics and therefore is commonly employed as a conductive component or cocatalyst rather than as a standalone semiconductor photocatalyst. In hybrid systems with semiconductors such as TiO_2 , g- C_3N_4 , or BiVO_4 , $\text{Ti}_3\text{C}_2\text{T}_x$ can facilitate interfacial electron transport and suppress charge recombination. Ti_3CNT_x likewise generally retains metallic-like electronic characteristics, while nitrogen incorporation modifies the density of states and electronic structure near the Fermi level. Specific surface terminations, defects, and compositional configurations may introduce semiconducting-like features in particular theoretical models or experimentally investigated samples; however, these observations should not be interpreted as evidence for a universal intrinsic bandgap of Ti_3CNT_x . Accordingly, in photocatalytic systems Ti_3CNT_x is more appropriately considered a conductive and interfacial charge-transfer component that can facilitate electron transport and charge separation when coupled with suitable semiconductor materials[52].

Nitrogen incorporation may additionally influence surface electronic structure, adsorption behavior, defect formation, and interfacial charge-transfer processes, all of which can affect photocatalytic or photocatalysis-assisted reactions. However, the specific contribution of nitrogen to reactive oxygen species (ROS) generation depends on the material composition, surface termination, defect concentration, and reaction environment. Therefore, ROS formation should be

discussed on the basis of the particular Ti_3CNT_x -based system and experimental evidence rather than attributed universally to nitrogen sites alone. For example, Ti_3CN -containing TiO_2 heterostructures have been reported to exhibit enhanced ROS formation during dye degradation, with superoxide, singlet oxygen, and hydroxyl radicals implicated in the reaction mechanism. In such systems, however, the observed ROS generation reflects the combined behavior of the semiconductor-MXene heterostructure rather than an intrinsic property of Ti_3CNT_x alone[57].

Similarly, although Ti_3CNT_x has been demonstrated to participate in singlet-oxygen-mediated oxidation processes, particularly in defect-engineered and peroxymonosulfate-activated systems, these results should not be directly generalized to conventional visible-light photocatalysis[58].

Because the reported photocatalytic and photocatalysis-assisted pollutant-removal performances of Ti_3CNT_x -based materials vary substantially with catalyst composition, dosage, pollutant concentration, solution pH, irradiation wavelength and intensity, reaction volume, and irradiation time, direct numerical comparison between different studies should be interpreted with caution unless the experimental conditions are closely matched. Table 5 therefore summarizes representative reported results together with the available experimental conditions to provide a more transparent basis for comparison.

Table 5 summarizes representative reported photocatalytic results together with the available experimental conditions to provide a more transparent basis for comparison.

Pollutant / reaction	Photocatalyst	Removal / conversion (%)	Catalyst dosage	Pollutant concentration	pH	Light source	Time	Ref.
MB	$\text{Ti}_3\text{CN}/\text{TiO}_2$ - Ti_3CN heterostructure	97	0.5 mg	25 mg/L	NR	UV, 365 nm, 44.8 W	30 min	[57]
RhB	Ti_3CNT_x -based thin film	Discoloration observed; not directly quantified as suspension photocatalytic degradation	Thin film	70 mg/L	NR	UV 365 nm / white light	up to 120 min	[18]

The 97% methylene-blue removal reported for the $\text{TiO}_2/\text{Ti}_3\text{CN}$ heterostructure should not be interpreted as the intrinsic photocatalytic efficiency of pristine Ti_3CNT_x . In the reported experiment, the Ti_3CN -containing heterostructure exhibited substantially higher ROS formation than pristine Ti_3CN , TiO_2 , and photolysis controls, indicating that the enhanced degradation arose from the combined semiconductor-MXene system[57].

The RhB result is also not directly comparable with suspension photocatalysis because the reported Ti_3CNT_x material was used as a thin film rather than as a dispersed photocatalyst. Therefore, the result is retained as evidence of Ti_3CNT_x -based photoactive surface behavior but is not assigned as a universal degradation efficiency for Ti_3CNT_x [17].

Rather than assigning a universal performance advantage to Ti_3CNT_x over $\text{Ti}_3\text{C}_2\text{T}_x$, the available literature suggests that nitrogen-containing MXenes can provide favorable electronic, surface-chemical, and interfacial charge-transfer characteristics in selected photocatalytic or photocatalysis-assisted systems. In several studies, Ti_3CNT_x has been incorporated into heterostructures or composite photocatalysts, where its conductive nature and surface functional groups can facilitate charge separation and interfacial electron transport. Consequently, the reported degradation efficiencies should be considered material- and system-specific rather than as intrinsic values applicable to all Ti_3CNT_x samples.

The revised comparison therefore distinguishes experimentally demonstrated performance from broader mechanistic interpretation and reports the principal reaction conditions whenever

these are available in the original studies. Where a parameter was not specified in the source, it is indicated as “NR” (not reported) rather than estimated.

6.4. Application-Specific Recommendations

Based on the comparative analysis presented in Sections 6.1-6.3, Ti_3CNT_x and $\text{Ti}_3\text{C}_2\text{T}_x$ exhibit application-dependent advantages rather than a universal performance hierarchy. Ti_3CNT_x shows particular promise in photocatalysis and environmental remediation when its nitrogen-modified electronic structure, surface chemistry, and interfacial charge-transfer characteristics are beneficial under the specific conditions employed. $\text{Ti}_3\text{C}_2\text{T}_x$ may retain advantages in applications where high electrical conductivity, established processing routes, or cost considerations are dominant. For electrochemical energy storage, sensing, electrocatalysis, and photothermal applications, the reported performance differences depend strongly on composition, surface termination, morphology, synthesis procedure, and testing conditions. Therefore, material selection should be based on the requirements of the specific application rather than on a general assumption that Ti_3CNT_x is superior to $\text{Ti}_3\text{C}_2\text{T}_x$.

$\text{Ti}_3\text{C}_2\text{T}_x$ may retain advantages in applications where high electrical conductivity and established processing characteristics are particularly important, including electromagnetic interference shielding and high-conductivity electrode applications. However, these advantages should not be interpreted as universal, since the performance of both $\text{Ti}_3\text{C}_2\text{T}_x$ and Ti_3CNT_x depends on surface termination, flake morphology, defect density, film or electrode architecture, and measurement conditions. $\text{Ti}_3\text{C}_2\text{T}_x$ may also remain attractive for large-scale and cost-sensitive applications because of its comparatively mature synthesis and processing history, whereas Ti_3CNT_x offers opportunities for property tuning through nitrogen incorporation. Thus, the selection between $\text{Ti}_3\text{C}_2\text{T}_x$ and Ti_3CNT_x should be guided by the specific functional requirements and processing constraints of the intended application.

In many practical deployment scenarios, neither material needs to be selected exclusively. $\text{Ti}_3\text{C}_2\text{T}_x/\text{Ti}_3\text{CNT}_x$ bilayer electrode architectures and van der Waals heterostructures may provide complementary functional characteristics by integrating the high electrical conductivity of $\text{Ti}_3\text{C}_2\text{T}_x$ with the composition- and surface-chemistry-dependent electrochemical and photocatalytic characteristics of Ti_3CNT_x . Such hybrid architectures may facilitate simultaneous optimization of charge transport, interfacial charge transfer, and light-assisted processes, particularly in photoelectrochemical systems where multiple functional requirements must be satisfied. However, the actual benefits of these architectures remain dependent on interfacial structure, component ratio, surface termination, morphology, and operating conditions.

7. Challenges and Future Perspectives

7.1. Synthesis homogeneity and quality control of Ti_3CNT_x

One of the most significant challenges in Ti_3CNT_x research is the difficulty of obtaining high-quality, homogeneous, and reproducible product. This challenge arises from several interconnected factors[59].

The stoichiometry of Ti_3AlCN MAX phase synthesis is highly sensitive to processing conditions. Small deviations in sintering temperature, duration, or atmosphere composition can substantially alter product phase composition: a temperature of 1380 °C instead of the target 1400 °C, for example, has been reported to yield secondary Ti_3AlC_2 and TiN phases that compromise subsequent MXene quality. Furthermore, the C:N ratio in the X layer can deviate significantly from the nominal 1:1 stoichiometry, ranging from 0.7:1.3 to 1.3:0.7 in practice. These compositional variations introduce batch-to-batch inconsistency and make interlaboratory reproducibility difficult to achieve[60], [61].

Lateral nanosheet dimensions and layer number distributions obtained by exfoliation follow broad statistical distributions - typically 0.5-15 μm in lateral size - rather than the narrow, standardized size profiles required for industrial applications. Density gradient centrifugation and

membrane filtration have been employed to narrow these distributions, but neither approach has yet achieved sufficient scalability or efficiency for large-scale manufacturing [62].

Etching and exfoliation inevitably introduce structural defects - vacancies, dislocations, edge defects, and chemical impurities - at nanosheet surfaces and edges. While certain defect types can enhance photocatalytic activity by providing additional active sites, they generally degrade electrical conductivity and mechanical strength. A quantitative methodology for assessing defect density and its property consequences in Ti_3CNT_x remains incompletely developed; advanced characterization techniques such as positron annihilation spectroscopy (PAS) and atom probe tomography (APT) have only recently begun to be applied to this material system [63].

Surface termination composition (-O/-OH/-F/-Cl ratio) is a critical determinant of MXene properties yet remains difficult to control with precision. Batch-to-batch variation in surface chemistry - particularly problematic for electrochemical and catalytic applications - represents a reproducibility bottleneck. Post-synthetic functionalization strategies including high-temperature annealing and chemical substitution reactions are being explored to address this limitation, but reliable protocols for targeted termination engineering have not yet been established [64].

7.2. Environmental Oxidation and Stabilization Strategies

The susceptibility of Ti_3CNT_x to oxidative degradation in ambient conditions remains one of the most actively investigated challenges in the field, directly limiting the material's practical deployment lifetime.

Oxidation kinetics of Ti_3CNT_x depend on environmental exposure, including humidity, oxygen and water availability, temperature, surface termination, defect density, and storage configuration. Direct studies demonstrate that environmental stability can vary substantially with material form and surface modification. Accordingly, specific degradation rates or storage lifetimes should not be generalized across different Ti_3CNT_x samples without considering the experimental conditions [17].

Several stabilization strategies have been investigated, including controlled storage, polymer or oxide encapsulation, graphene-based barriers, and surface-termination engineering. Direct Ti_3CNT_x studies indicate that protective surface modification can substantially improve environmental stability, but the magnitude of improvement depends on film architecture and coating chemistry [38]. Figure 11 provides a representative, source-specific example of wettability stabilization after surface functionalization [7].

Paradoxically, controlled partial oxidation of Ti_3CNT_x can be exploited rather than suppressed: surface TiO_2 formation generates $\text{Ti}_3\text{CNT}_x/\text{TiO}_2$ heterojunctions that enhance photocatalytic activity through favorable band alignment. However, protocols for achieving reproducible and spatially controlled partial oxidation remain underdeveloped, and this "productive oxidation" strategy currently represents an emerging rather than established approach [65].

7.3. Large-Scale Production Cost and Technological Scale-Up Challenges

The large-scale production of Ti_3CNT_x remains an important challenge for its practical implementation. Unlike the extensively studied $\text{Ti}_3\text{C}_2\text{T}_x$ system, Ti_3CNT_x synthesis is still largely demonstrated at laboratory scale, and the availability of suitable Ti_3AlCN MAX-phase precursors, control of carbon-nitrogen composition, and reproducible selective etching remain important considerations. Recent Ti_3CNT_x studies have continued to focus on improving synthesis efficiency and reducing processing time, highlighting the need for further process development toward scalable production [16],[19]

Scale-up is further complicated by the multistep nature of Ti_3CNT_x preparation, which includes MAX-phase synthesis, selective removal of the Al layer, washing and purification, and, when required, delamination or post-processing. Maintaining uniform reaction conditions during scale-up is particularly important because variations in temperature, reagent concentration, mixing, and etching kinetics can influence Al removal, surface termination, defect density, and the resulting structural and electronic properties.

Etching and purification also represent important engineering and environmental considerations. Conventional fluoride-containing routes require appropriate corrosion-resistant equipment, process control, and treatment of acidic and fluoride-containing waste streams. Consequently, fluorine-free or reduced-fluoride approaches, including molten-salt and electrochemical strategies, are of particular interest for future scale-up. However, these approaches still require Ti_3CNT_x -specific optimization to establish reproducible phase purity, surface chemistry, yield, and material performance[19].

Processing conditions can also substantially influence the defect structure and resulting properties of Ti_3CNT_x . Chen et al. demonstrated that controlled acid treatment can introduce Ti-vacancy defects and modify the electrochemical behavior of Ti_3CNT_x , highlighting the sensitivity of the material to processing-induced structural changes[66].

Another important challenge is the reproducibility of Ti_3CNT_x properties at larger production scales. Variations in the C/N ratio, residual Al content, surface termination, flake thickness, defect concentration, and degree of delamination may affect the electrical, optical, electrochemical, and catalytic behavior of the resulting material. Therefore, future scale-up studies should evaluate not only production yield but also batch-to-batch consistency and structure-property relationships.[67].

At present, a reliable Ti_3CNT_x -specific industrial production cost cannot be established from the available literature. Reported laboratory procedures provide useful information about material consumption, processing steps, and energy-intensive operations, but these data are insufficient to define a validated cost per gram at industrial scale. Accordingly, quantitative production-cost estimates are not assigned here. Future techno-economic analyses should consider precursor cost, energy consumption during MAX-phase synthesis, etching and purification requirements, water and waste treatment, process yield, equipment depreciation, and quality-control requirements.

Overall, the most credible routes toward scalable Ti_3CNT_x production involve improving precursor synthesis, developing more efficient and environmentally compatible etching strategies, reducing washing and purification requirements, and establishing continuous or semi-continuous processing methods. Importantly, these approaches should be evaluated using standardized metrics that include yield, purity, surface chemistry, defect concentration, flake dimensions, energy consumption, waste generation, and batch-to-batch reproducibility.

7.4. Future Research Directions

Despite significant progress in the synthesis and application of Ti_3CNT_x MXene, several scientific and technological challenges still limit its large-scale implementation. Future research should focus on developing environmentally friendly synthesis routes, improving structural stability, optimizing surface chemistry, and designing multifunctional heterostructures. A roadmap highlighting the major development pathways and future application opportunities of Ti_3CNT_x MXene is presented in Figure 16.

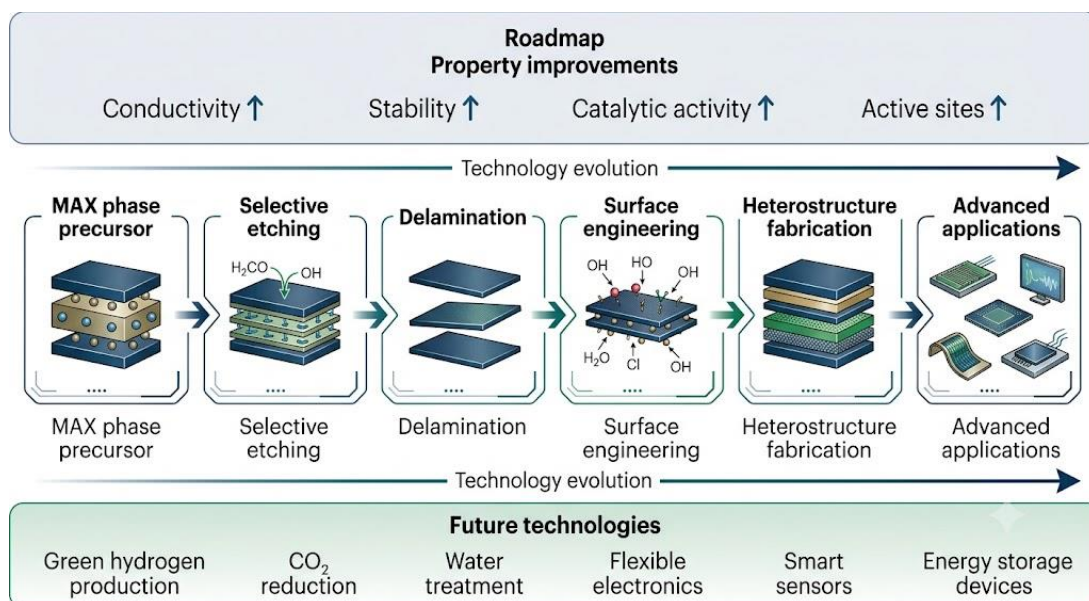


Figure 16. Future development roadmap of Ti_3CNT_x MXene, illustrating the relationships between synthesis strategies, property optimization, and emerging technological applications. Advances in etching methods, delamination techniques, surface engineering, and heterostructure fabrication are expected to enhance conductivity, stability, and catalytic performance, enabling next-generation applications in hydrogen production, CO_2 reduction, environmental remediation, sensing, and energy storage (Created by the authors based on the reviewed literature).

As illustrated in Figure 16, future progress in Ti_3CNT_x research will depend on the integration of advanced synthesis techniques with rational surface engineering approaches. The development of fluorine-free etching methods, oxidation-resistant structures, and multifunctional composites is expected to accelerate the transition of Ti_3CNT_x MXene from laboratory-scale studies to practical industrial applications.

Machine learning (ML) and artificial intelligence methods represent promising future tools for accelerating Ti_3CNT_x research. In principle, ML-assisted interatomic potentials, high-throughput calculations, and data-driven models could help explore relationships among C/N composition, surface termination, defects, and material properties. Such approaches should be treated as prospective research strategies, because their reliability will depend on the quality, size, and chemical consistency of the underlying Ti_3CNT_x datasets.

The construction of heterostructures combining Ti_3CNT_x with complementary two-dimensional or semiconductor materials is another promising research direction. For example, $\text{Ti}_3\text{CNT}_x/\text{g-C}_3\text{N}_4$, $\text{Ti}_3\text{CNT}_x/\text{MoS}_2$, and $\text{Ti}_3\text{CNT}_x/\text{BiVO}_4$ architectures could be investigated to determine whether interfacial charge transfer, band alignment, and catalytic-site coupling can improve photocatalytic or electrocatalytic performance. These systems should presently be regarded as proposed research directions rather than established examples of universal performance enhancement.

Biomedical applications of Ti_3CNT_x also warrant systematic investigation, particularly in areas involving photothermal behavior, biosensing, and bioelectronic interfaces. Future work should first establish cytocompatibility, surface stability, degradation behavior, and reproducibility before claims regarding therapeutic or implantable applications can be assessed. Multimodal platforms combining Ti_3CNT_x with other functional materials may be explored, but their performance must be evaluated on a system-specific basis.

In environmental and industrial applications, future studies could examine Ti_3CNT_x for CO_2 reduction, nitrogen-related electrocatalysis, water treatment, and solar-driven photothermal processes. The potential contribution of N-containing sites to adsorption and activation is a useful hypothesis for computational and experimental investigation, but it should not be presented as an established superiority over carbide MXenes without direct evidence. Standardized

electrochemical, photocatalytic, and stability measurements will be essential for determining whether Ti_3CNT_x offers practical advantages in these emerging applications.

Looking across these directions, a coherent picture emerges: the most impactful future advances in Ti_3CNT_x science will likely arise from the convergence of computational design, heterostructure engineering, and application-specific surface chemistry control. The combination of tunable electronic properties, N-containing surface chemistry, and structural versatility makes Ti_3CNT_x an interesting platform for further investigation alongside other MXene materials. Establishing application-specific advantages will require well-controlled experimental comparisons and validated structure-property relationships.

Conclusions

This review has systematically examined the synthesis, crystal structure, physicochemical properties, emerging applications, and future research directions of two-dimensional Ti_3CNT_x carbonitride MXene. The principal conclusions are summarized below.

Regarding synthesis and structure: The quality of Ti_3CNT_x is strongly influenced by the homogeneity and phase purity of its Ti_3AlCN MAX-phase precursor. Solid-state synthesis remains an important route for preparing MAX-phase precursors, while SPS and CVD-based approaches provide additional opportunities for controlling phase formation and microstructure. In the etching step, MILD and fluorine-free approaches have emerged as alternatives to conventional HF-based routes, with potential benefits in process safety and control. TMAOH and choline chloride have also been explored as intercalation and delamination agents for Ti_3CNT_x . Crystallographic studies generally support a hexagonal structure, while the precise atomic ordering of C and N within the X layers remains an active area of investigation. Surface termination chemistry, including -O, -OH, -F, and -Cl species, is strongly dependent on the synthesis and post-treatment conditions and can substantially influence the resulting material properties.

Regarding physicochemical properties: Ti_3CNT_x generally exhibits metallic or near-metallic electronic characteristics, while nitrogen incorporation modifies the density of states and charge distribution relative to $\text{Ti}_3\text{C}_2\text{T}_x$. However, the resulting electronic behavior depends on composition, surface termination, defects, and structural configuration, and semiconducting-like features may occur under specific conditions. The physicochemical properties of Ti_3CNT_x - including electrical, optical, mechanical, electrochemical, and surface characteristics - are therefore strongly dependent on synthesis history and material structure. These dependencies highlight the importance of controlling composition, termination chemistry, morphology, and defect structure when designing Ti_3CNT_x for specific applications.

Regarding applications: Ti_3CNT_x demonstrates promising photocatalytic, electrochemical, sensing, adsorption, and photothermal characteristics, but the magnitude and direction of performance differences relative to $\text{Ti}_3\text{C}_2\text{T}_x$ are strongly dependent on material composition, surface termination, morphology, synthesis conditions, and testing protocols. The available literature therefore does not support a universal conclusion that Ti_3CNT_x consistently outperforms $\text{Ti}_3\text{C}_2\text{T}_x$ across all applications. Instead, the two MXenes should be considered complementary materials whose performance advantages are application-specific.

Regarding challenges and outlook: Three major challenges remain important for the broader development of Ti_3CNT_x : synthesis reproducibility and compositional control, environmental oxidation and surface stability, and the economic and technical requirements associated with scale-up. Future efforts should therefore focus on fluorine-free or reduced-fluoride synthesis, improved stabilization strategies such as protective coatings and encapsulation, and scalable processing approaches. Computational methods, including machine-learning-assisted materials design, may further support the exploration of composition-structure-property relationships. Ti_3CNT_x -based heterostructures, including $\text{Ti}_3\text{CNT}_x/\text{g-C}_3\text{N}_4$, $\text{Ti}_3\text{CNT}_x/\text{MoS}_2$, and $\text{Ti}_3\text{CNT}_x/\text{BiVO}_4$ systems, represent promising research directions for photocatalytic and photoelectrochemical applications, although their performance should be validated under well-defined and comparable experimental

conditions. Biomedical and other emerging applications should likewise be regarded as prospective research areas requiring further experimental validation.

Overall, Ti_3CNT_x represents a promising member of the two-dimensional MXene family with a diverse range of tunable physicochemical properties and emerging applications. Its practical potential will depend on continued improvements in synthesis reproducibility, compositional and surface-termination control, oxidation stability, scalable processing, and device integration. Future studies combining well-controlled experiments with theoretical analysis will be particularly important for establishing reliable structure-property relationships and determining the application-specific advantages of Ti_3CNT_x relative to other MXenes.

Acknowledgments

This study was supported by institutional budgetary funding from the Center for Advanced Technologies under the Academy of Sciences of the Republic of Uzbekistan.

Declaration of generative AI and AI-assisted technologies

During the preparation of this manuscript, the authors used ChatGPT (OpenAI, GPT-5.6 Sol) to assist with text translation and the creation of selected schematic figures. All AI-assisted text and graphical content was critically reviewed, checked for scientific accuracy, and revised as necessary by the authors. Particular attention was paid to scientific terminology, chemical notation, figure labels, and consistency with the cited literature. The authors take full responsibility for the accuracy, integrity, and final content of the manuscript and its figures.

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