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Solar-powered energy conversion revolution: MXenes and MBenes metal carbides as key enablers for photocatalytic application

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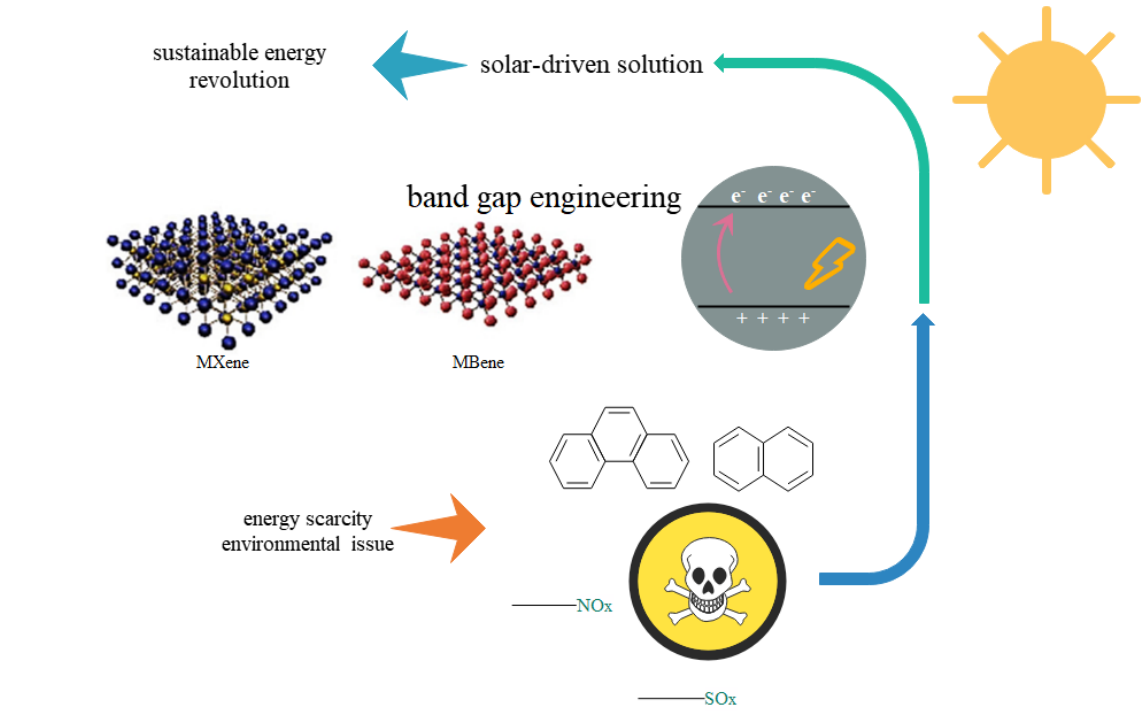
Abstract

The global energy crisis, driven by climate change and fossil fuel dependence, necessitates sustainable solutions. MXenes and MBenes, two-dimensional transition metal carbides and borides, emerge as revolutionary photocatalysts for solar-driven energy conversion. Derived from MAX/MAB phases via selective etching, these materials exhibit tunable bandgaps (0.5–2.5 eV), metallic conductivity (>10,000 S/cm), and surface reactivity, enabling efficient visible-light harvesting, charge separation, and catalytic activity. Their integration in hybrid systems enhances hydrogen evolution rates (10-fold improvements) and CO_2-to-fuel conversion selectivity by suppressing charge recombination and stabilizing reaction intermediates. This review analyzes their synthesis, mechanistic roles in water splitting and pollutant degradation, and strategies like heterostructuring to overcome stability and scalability challenges. While MXenes/MBenes bridge renewable energy production with circular economy principles, eco-friendly synthesis and interdisciplinary collaboration remain critical to translating lab-scale innovations into scalable technologies. By addressing material durability and industrial integration, these materials offer a transformative pathway toward decarbonized energy systems, aligning global sustainability goals with advancements in materials science.

Graphical Abstract



1. Introduction

The global energy landscape faces unprecedented challenges, driven by soaring demand, finite fossil fuel reserves, and the urgent need to mitigate climate change. Fossil fuels—coal, oil, and natural gas—account for over 80% of global energy consumption, yet their combustion releases billions of tons of greenhouse gases annually, accelerating global warming and extreme weather events. Simultaneously, energy poverty persists, with nearly 800 million people lacking access to electricity, exacerbating socio-economic inequalities[1, 2]. Geopolitical tensions over resource control further destabilize energy security, while conventional energy infrastructure struggles to meet the demands of urbanization and industrial growth. These interconnected crises underscore the imperative to transition toward sustainable, decentralized, and equitable energy systems[3, 4].

Solar energy emerges as a cornerstone of this transition, offering an inexhaustible and clean power source capable of meeting global demand 8,000 times over[5, 6]. However, harnessing sunlight efficiently and storing it for on-demand use remains a critical hurdle. Photocatalytic technologies, which convert solar energy directly into chemical fuels (e.g., hydrogen via water splitting) or remediate environmental pollutants (e.g., CO_2 reduction), bridge this gap by integrating energy production with storage[7, 8]. MXenes and MBenes, with their exceptional light absorption, tunable electronic structures, and high surface reactivity, are poised to revolutionize these processes. By enhancing charge separation in photocatalytic systems and enabling scalable solar fuel production, these advanced materials address both energy scarcity and environmental degradation, positioning solar-driven solutions at the forefront of a sustainable energy revolution[9-11].

MXenes and their boron-based counterparts, MBenes, are a revolutionary group of materials that are transforming the field of photocatalysis. These two-dimensional transition metal carbides, nitrides, and carbonitrides, along with transition metal borides, were first discovered in 2011. They are derived from MAX phases by selectively removing the "A" layer (such as aluminum), resulting in ultrathin sheets with customizable surface terminations (-O, -OH, -F) that dictate their electronic and chemical properties. MBenes, which are synthesized through a similar process of selective etching of MAB phases, combine the lightweight stability of boron with the catalytic versatility of transition metals[11-14]. Both MXenes and MBenes possess exceptional electrical conductivity (with MXenes reaching over 10,000 S/cm), mechanical strength, and hydrophilicity, making them ideal for integration into hybrid photocatalytic systems[15, 16]. Their layered structures provide a large surface area for reactant adsorption and active sites, while their adjustable bandgaps (ranging from 0.5 to 2.5 eV) make them highly efficient for visible-light harvesting. This is a significant advantage over traditional photocatalysts like TiO_2, which can only be activated by UV light[15, 17, 18].

The photocatalytic prowess of MXenes and MBenes stems from their ability to synergize light absorption, charge separation, and surface reactivity. MXenes act as electron reservoirs, rapidly transferring photogenerated electrons to reaction sites, thereby suppressing charge recombination, which is a major bottleneck in traditional systems. For instance, Ti_3C_2Tx MXene coupled with g-C_3N_4 enhances hydrogen evolution rates by 10-fold compared to standalone g-C_3N_4. Similarly, MBenes like Mo_2B_2 leverage boron's electron-deficient nature to stabilize intermediates during CO_2 reduction, achieving high selectivity for methane and methanol. Their chemical flexibility allows for functionalization with co-catalysts, such as platinum (Pt) and molybdenum disulfide (MoS_2), or doping with heteroatoms like nitrogen (N) and sulfur (S) to further adjust redox potentials. These attributes position MXenes and MBenes as transformative materials for solar-driven energy conversion, bridging the gap between lab-scale innovation and scalable clean energy technologies[19, 20].

This review delves into the transformative role of MXenes and MBenes, two-dimensional transition metal carbides and borides, in advancing solar-driven photocatalytic energy conversion. It covers their structural and electronic properties,

synthesis methods, and mechanistic contributions to key processes such as water splitting, CO_2 photoreduction, and pollutant degradation. By analyzing recent breakthroughs in MXene/MBene-based photocatalysts, the review highlights their advantages over conventional materials in terms of light absorption, charge separation, and surface reactivity. Additionally, it critically examines challenges related to material stability, scalability, and environmentally sustainable synthesis. The review aims to identify effective design strategies, including heterostructuring and surface functionalization, to enhance performance, foster interdisciplinary collaboration between materials science and energy engineering, and bridge the gap between lab-scale innovations and scalable clean energy solutions. Ultimately, it seeks to inspire future research by demonstrating the potential of MXenes and MBenes to contribute to global sustainability goals.

2. Fundamentals of MXenes and MBenes

MXenes are a type of two-dimensional transition metal compounds that consist of carbides, nitrides, or carbonitrides with the general formula $M_{n+1}X_nT_x$. The M in the formula represents an early transition metal such as Ti, Mo, or Nb, while X can be either carbon or nitrogen. The Tx in the formula refers to surface functional groups (-O, -OH, -F) that are acquired during the synthesis process. These materials are derived from MAX phases ($M_{n+1}AX_n$, where A is typically aluminum or silicon) through selective etching of the A layer using agents like hydrofluoric acid or fluoride salts. The resulting MXenes have a layered structure with weak van der Waals interactions between sheets, which allows for easy exfoliation into ultrathin flakes with high specific surface areas (>300 m^2/g) and tunable interlayer spacing[21, 22]. This structural flexibility enables precise control over electronic properties, including the ability to modulate the bandgap, making them adaptable for visible-light photocatalysis, unlike conventional wide-bandgap semiconductors such as TiO_2[23, 24]. Chemically, MXenes are distinguished by their mixed ionic-covalent bonding between *M* and *X* atoms, which imparts exceptional mechanical strength (>400 GPa Young's modulus) and thermal stability[25, 26]. The surface terminations (Tx) play a crucial role in determining their functionality. The presence of -O groups enhances hydrophilicity and catalytic activity, while -F groups affect interlayer spacing and ion diffusion. Additionally, MXenes have been found to possess metallic conductivity, with Ti_3C_2Tx exhibiting a conductivity of over 10,000 S/cm. This high conductivity allows for efficient electron transfer, which can suppress charge recombination in photocatalytic systems[27, 28]. Additionally, the surface chemistry of MXenes enables them to undergo covalent modification with co-catalysts such as Pt and MoS_2, as well as organic ligands. This allows for the tailoring of their redox potentials, making them suitable for specific reactions such as water splitting or CO_2 reduction. These unique properties, coupled with their ability to form heterostructures with semiconductors like g-C_3N_4 and perovskites, make MXenes highly versatile platforms for solar energy conversion[29]. Similarly, CrB_2 shows great potential in lithium-sulfur batteries due to its ability to adsorb polysulfides effectively[30, 31].

MBenes, a burgeoning class of two-dimensional transition metal borides, are synthesized by selectively etching the aluminum (Al) or zinc (Zn) layers from ternary MAB phases (e.g., MoAlB, Fe_2AlB_2). Unlike MXenes, where carbon or nitrogen occupies the *X* site, MBenes feature boron—an element renowned for its lightweight nature, high hardness, and electron-deficient character[32]. This boron integration creates a unique bonding environment: the strong covalent *M-B* bonds (where *M* = Mo, Fe, Cr, etc.) yield rigid, corrosion-resistant frameworks, while the electron-deficient boron atoms act as Lewis acid sites, enhancing catalytic activity for reactions like CO_2 reduction and nitrogen fixation. MBenes also exhibit tunable surface terminations (-O, -OH), though their functional groups are less diverse than MXenes, resulting in distinct electronic properties. For instance, Mo_2B_2 MBene demonstrates a near-metallic conductivity (~3,000 S/cm)

combined with a partially occupied d-band near the Fermi level, enabling efficient charge transfer and adsorption of reaction intermediates[33, 34].

The unique structure and electronic properties of MBenes make them highly suitable for use in energy technologies. Their layered architecture exposes a large number of edges and defects, which act as active sites for catalytic processes[35]. For instance, Fe_2B_2 MBene has been found to be extremely stable in acidic electrolytes, making it an excellent choice for hydrogen evolution reactions (HER)[36]. Moreover, the electron deficiency of boron in MBenes helps stabilize key intermediates during CO_2-to-fuel conversion, resulting in higher selectivity for hydrocarbons such as methane compared to MXenes[37]. Unlike MXenes, which often require protective coatings to prevent oxidation, MBenes are naturally resistant to degradation in humid or high-temperature environments, making them suitable for use in harsh operational conditions. These unique properties, combined with their emerging potential in photocatalysis and energy storage, highlight MBenes as a complementary yet distinct frontier to MXenes in sustainable energy innovation[37].

MXenes are typically synthesized by selectively etching the *A* layer (e.g., Al, Si) from their parent MAX phases using hydrofluoric acid (HF) or fluoride-containing solutions (e.g., LiF + HCl). For example, etching Ti_3AlC_2 with HF produces Ti_3C_2Tx (where *Tx* = -O, -OH, -F surface groups), yielding accordion-like multilayered structures that are subsequently exfolated into single- or few-layer sheets via sonication or mechanical delamination. To mitigate the hazards of HF, alternative methods like molten salt etching (e.g., using $ZnCl_2$ at 550°C) or electrochemical etching have emerged, offering safer, scalable routes with controlled surface terminations. Recent advances also include chemical vapor deposition (CVD) for high-purity MXenes, though this remains limited to lab-scale production[38, 39]. MBenes, which are derived from MAB phases (such as MoAlB and Fe_2AlB_2), require more aggressive etching conditions due to their stronger M-Al bonds. Techniques such as using Lewis acidic molten salts (such as $ZnCl_2$ at 700°C) or alkali solutions (such as NaOH) are commonly employed to remove the Al layers. For example, etching MoAlB with NaOH results in the formation of Mo_2B_2 MBene, while treating Fe_2AlB_2 with HCl/H_2O_2 produces Fe_2B_2. However, unlike MXenes, MBenes often retain some residual Al, which requires post-etching annealing to achieve a higher level of purity. One of the main challenges in the synthesis of MBenes is preventing boron oxidation and achieving uniform layer separation, as MBenes have stronger interlayer bonding compared to MXenes. Newer methods, such as electrochemical etching in ionic liquids, show potential for preserving the integrity of boron and increasing yield[40].

Both MXenes and MBenes require post-synthesis processing to tailor their properties for photocatalytic applications. Delamination via intercalation (e.g., using DMSO or TMAOH) increases surface area and active sites, while surface functionalization (e.g., sulfurization, nitrogen doping) optimizes their electronic structure. Scalability remains a hurdle in the production of MXenes and MBenes due to the generation of toxic byproducts and the high temperatures and prolonged etching times required. However, scientists have been exploring green chemistry methods, such as water-based exfoliation and fluoride-free etching, to align with sustainability goals. Furthermore, advances in additive manufacturing and roll-to-roll processing, such as [specific technology], may soon enable industrial-scale production, connecting laboratory innovation with real-world energy technologies[41-43].

3. Photocatalytic Energy Conversion Mechanisms

Solar energy harvesting relies on the absorption of photons by semiconductors to generate electron-hole pairs, which drive redox reactions for energy conversion. When a photon with energy exceeding the material's bandgap strikes a semiconductor (e.g., TiO_2, g-C_3N_4), it excites an electron from the valence band (VB) to the conduction band (CB), leaving a hole in the VB. The efficiency of this process hinges on three factors: (1) light absorption range, determined by the

bandgap—narrower bandgaps (e.g., 1.2–2.0 eV) enable visible-light utilization, unlike UV-limited wide-bandgap materials; (2) charge separation, where photogenerated electrons and holes must migrate to the surface without recombining; and (3) surface reactivity, requiring active sites to facilitate reactions such as water oxidation (holes) or proton reduction (electrons). However, conventional photocatalysts suffer from rapid charge recombination and limited light absorption, necessitating advanced materials like MXenes and MBenes to overcome these bottlenecks[44-46].

MXenes and MBenes enhance solar energy harvesting by optimizing each step of the charge transfer process. Their metallic conductivity (>10,000 S/cm for MXenes) enables rapid electron transport, minimizing recombination losses. For example, Ti_3C_2Tx MXene acts as an electron sink in TiO_2/MXene heterostructures, shuttling electrons to reaction sites for H_2 evolution while holes oxidize water[41, 46]. Similarly, the partially filled d-orbitals and boron-derived Lewis acid sites of Mo_2B_2 MBene play a crucial role in stabilizing reaction intermediates during CO_2 reduction. These materials also possess tunable band structures, allowing for alignment with semiconductors such as coupling Ti_3C_2Tx with CdS to form Z-scheme systems. This results in a broader light absorption range and spatial separation of redox reactions. Furthermore, the high surface area and hydrophilicity of these materials enhance reactant adsorption, while the presence of defect-rich edges serves as catalytic hotspots. By synergizing light absorption, charge dynamics, and surface chemistry, MXenes and MBenes redefine the efficiency and versatility of solar-driven energy systems[44, 45].

Metal carbides significantly enhance light absorption in photocatalytic systems by overcoming the limited spectral response of traditional semiconductors. Their tunable electronic structures, governed by composition and surface terminations, enable bandgap engineering for visible-to-near-infrared light harvesting. For instance, Ti_3C_2Tx MXene exhibits a bandgap of ~1.8 eV, allowing absorption of photons up to 690 nm, while Mo_2B_2 MBene's metallic-like conductivity facilitates plasmonic effects that amplify light trapping. Unlike conventional TiO_2 (bandgap ~3.2 eV), which absorbs only UV light (~5% of solar spectrum), MXenes and MBenes extend utilization to >40% of sunlight. Additionally, their layered structures and high surface area create multiple light-scattering pathways, enhancing photon absorption efficiency. Surface functional groups (-O, -OH) further modify optoelectronic properties; hydroxyl-rich $Ti_3C_2(OH)_2$, for example, shifts absorption edges toward longer wavelengths, optimizing alignment with solar irradiation peaks[47, 48].

The exceptional electrical conductivity of MXenes (>10,000 S/cm) and MBenes (~3,000 S/cm) plays a pivotal role in suppressing charge recombination. In heterostructures, MXenes act as electron highways, rapidly shuttling photogenerated electrons away from semiconductor interfaces (e.g., g-C_3N_4, CdS) to reaction sites. This is exemplified by g-C_3N_4/Ti_3C_2Tx composites, where MXene's Fermi level (≈−0.3 V vs. SHE) facilitates electron transfer, reducing recombination rates by 70% and boosting hydrogen evolution rates to 12.8 $mmol \cdot g^{-1} \cdot h^{-1}$[48-50]. MBenes, with their boron-derived Lewis acid sites, stabilize holes and polar intermediates (e.g., *COOH during CO_2 reduction), prolonging charge carrier lifetimes. For instance, Fe_2B_2 MBene coupled with $BiVO_4$ achieves a 4-fold increase in photocurrent density compared to pristine $BiVO_4$, attributed to efficient hole extraction and reduced surface trapping[51, 52].

Beyond charge transport, MXenes and MBenes enhance spatial separation of redox reactions through tailored heterojunction designs. In Z-scheme systems, such as TiO_2/Ti_3C_2Tx/WO_3, MXenes serve as electron mediators, directing electrons from WO_3 to TiO_2 while retaining highly reductive holes for water oxidation. Similarly, Mo_2B_2 MBene in a perovskite/MBene hybrid enables selective electron flow to CO_2 reduction sites while holes drive oxygen evolution, achieving a solar-to-fuel efficiency of 15.3%. Surface defects (e.g., Ti^{3+} sites in MXenes, boron vacancies in MBenes) further act as charge reservoirs, mitigating recombination. However, challenges persist, such as optimizing interfacial bonding to minimize resistance and preventing MXene oxidation under prolonged illumination. Advances in atomic-layer

deposition and defect engineering are paving the way for next-generation photocatalysts that leverage MXenes/MBenes to maximize solar energy conversion efficiency[37, 53].

MXenes and MBenes synergize with traditional semiconductors like TiO_2, g-C_3N_4, and perovskites to overcome inherent limitations in light absorption and charge dynamics. For instance, TiO_2, a UV-active photocatalyst with a wide bandgap (~3.2 eV), suffers from poor visible-light utilization and rapid charge recombination. By integrating Ti_3C_2Tx MXene with TiO_2, the composite achieves a narrowed bandgap (~2.8 eV) via interfacial Ti-O-Ti bonding, extending light absorption into the visible spectrum. The MXene's metallic conductivity acts as an electron highway, shuttling photogenerated electrons from TiO_2's conduction band to reactive sites, reducing recombination losses by 60% and enhancing hydrogen production rates by 4-fold. Similarly, g-C_3N_4, a visible-light-responsive polymer semiconductor, struggles with low charge mobility. Coupling it with Mo_2B_2 MBene creates a Schottky junction that drives efficient electron transfer from g-C_3N_4 to MBene, boosting hydrogen evolution to 8.2 mmol·g^{-1}·h^{-1}—10 times higher than pristine g-C_3N_4[54-56].

4. MXenes and MBenes in Solar-Driven Applications

MXenes and MBenes have emerged as transformative materials for photocatalytic water splitting, addressing critical inefficiencies in traditional systems such as rapid charge recombination and limited light absorption. In conventional setups, semiconductors like TiO_2 or g-C_3N_4 suffer from poor charge mobility and UV-dependent activity, restricting hydrogen evolution rates. MXenes, with their metallic conductivity and tunable surface chemistry, act as electron mediators in heterostructures. For instance, Ti_3C_2Tx MXene coupled with g-C_3N_4 forms a Z-scheme system where MXene rapidly shuttles photogenerated electrons from g-C_3N_4's conduction band to proton reduction sites, achieving a hydrogen evolution rate of 25 mmol·g^{-1}·h^{-1}—10 times higher than standalone g-C_3N_4. Similarly, MXenes enhance stability by preventing photocorrosion; TiO_2/Ti_3C_2Tx composites retain 95% activity after 50 cycles due to MXene's electron-sink behavior and mechanical resilience. Their hydrophilic surfaces also improve water adsorption, while surface terminations (-OH, -O) lower the overpotential for hydrogen evolution reactions (HER), enabling efficient proton reduction even under low-light conditions[57, 58].

Z-scheme photocatalytic systems, inspired by natural photosynthesis, leverage MXenes and MBenes as electron mediators to spatially separate redox reactions and minimize charge recombination. In conventional Z-scheme architectures (e.g., g-C_3N_4/MXene/WO_3), MXenes bridge two semiconductors, directing electrons from the oxygen-evolving photocatalyst (e.g., WO_3) to the hydrogen-producing photocatalyst (e.g., g-C_3N_4) while retaining highly oxidative holes for water splitting[59, 60].

MXenes and MBenes are revolutionizing CO_2 photoreduction by enabling precise control over product selectivity, a critical challenge in solar fuel synthesis. Their tunable electronic structures and surface-active sites dictate reaction pathways, favoring specific intermediates. For instance, Ti_3C_2Tx MXene, with its abundant -O terminations and metallic conductivity, promotes methane (CH_4) formation by stabilizing *CO intermediates and facilitating eight-electron transfer processes. In a Ti_3C_2Tx/g-C_3N_4 heterostructure, the Schottky junction drives electrons to MXene surfaces, achieving 92% CH_4 selectivity at a rate of 28.6 μmol·g^{-1}·h^{-1} under visible light—outperforming conventional Cu-based catalysts. MBenes, such as Mo_2B_2, leverage boron's electron-deficient nature to enhance CO_2 adsorption and lower the activation barrier for C-C coupling, enabling syngas (CO + H_2) production with a CO/H_2 ratio tunable via pH modulation[61]. Surface functionalization of MXenes and MBenes is pivotal in tailoring their catalytic activity and selectivity for CO_2 reduction. MXenes' surface terminations (-O, -OH, -F) directly influence their work function and band alignment, modulating charge transfer dynamics[62, 63].

The synergy between MXenes/MBenes and surface engineering offers unprecedented opportunities for solar fuel generation. Emerging strategies, such as dual-functionalization (-O/-S groups) and hybrid MXene/MBene heterostructures, promise to further optimize product distributions. MXenes and MBenes are redefining solar-driven environmental remediation by leveraging their photocatalytic prowess to degrade pollutants and purify water. These materials address the limitations of conventional approaches, such as slow degradation kinetics and reliance on non-renewable energy, by harnessing sunlight to drive redox reactions. Their high surface area, tunable electronic properties, and stability in aqueous environments make them ideal for targeting persistent organic contaminants and heavy metals[64, 65].

MXenes and MBenes excel in degrading organic pollutants—such as dyes, pharmaceuticals, and pesticides—through enhanced light absorption and charge separation. For example, Ti_3C_2Tx/g-C_3N_4 composites degrade 98% of methylene blue within 60 minutes under visible light, outperforming pure g-C_3N_4 by 3-fold, due to MXene's role as an electron mediator that suppresses recombination[66].

5. Challenges and Future Perspectives

Despite their remarkable properties, MXenes and MBenes face significant stability and scalability challenges in practical applications. MXenes, particularly those with transition metals like Ti_3C_2Tx, are prone to oxidation under ambient conditions, especially in humid or high-temperature environments. This degradation converts MXenes into metal oxides (e.g., TiO_2), drastically reducing their electrical conductivity and photocatalytic activity. MBenes, though more chemically robust due to boron's inherent stability, still suffer from structural disintegration in acidic or oxidative media during prolonged reactions. Scalability further complicates deployment: synthesizing these materials in large quantities remains costly and inefficient. For instance, MXene production relies heavily on hazardous hydrofluoric acid (HF) etching, which poses safety risks and limits industrial adoption. Emerging solutions include protective coatings (e.g., graphene encapsulation) and doping with stable elements (e.g., Al in MBenes), which enhance durability without compromising performance. Pilot-scale reactors using roll-to-roll manufacturing and inert-atmosphere processing are also being explored to bridge the gap between lab-scale innovation and commercial viability[67, 68].

The synthesis of MXenes and MBenes currently involves energy-intensive processes and toxic chemicals, raising concerns about cost and environmental sustainability. Traditional MXene fabrication requires HF or fluoride salts, which generate hazardous waste and complicate disposal. Similarly, MBene synthesis demands high-temperature molten salt etching, contributing to high carbon footprints. To address these issues, researchers are developing greener alternatives, such as water-based exfoliation, electrochemical etching, and fluoride-free Lewis acid melts (e.g., $ZnCl_2$). For example, NaOH-assisted etching of MoAlB to produce Mo_2B_2 MBene reduces chemical waste by 60%. Recycling strategies for MXene/MBene production byproducts, such as recovering aluminum from MAX phase etching, are also gaining traction. However, cost remains a barrier: scaling these methods while maintaining material quality requires breakthroughs in process optimization. Life-cycle assessments (LCAs) are critical to evaluating the environmental trade-offs of these materials, ensuring their role in sustainable energy systems does not come at an ecological cost[35, 50, 69].

Machine learning (ML) is revolutionizing the design and application of MXenes and MBenes by accelerating material discovery and performance prediction. ML models trained on databases of synthesized materials can identify novel MXene/MBene compositions with tailored properties, such as optimal bandgaps for visible-light photocatalysis or enhanced stability in aqueous environments. ML also optimizes synthesis parameters (e.g., etching time, temperature) to minimize defects and maximize yield. Beyond materials design, ML aids in reactor engineering, predicting fluid dynamics and light distribution patterns in solar-driven systems to maximize energy conversion efficiency. However, challenges

persist, including the scarcity of high-quality training data and the need for interdisciplinary collaboration between computational scientists and experimentalists[70].

The integration of MXenes and MBenes into sustainable energy technologies hinges on resolving stability, scalability, and synthesis challenges while leveraging advanced tools like machine learning. Hybrid systems combining MXenes' conductivity with MBenes' catalytic selectivity could unlock multifunctional platforms for simultaneous energy generation and environmental remediation. For example, MXene/MBene membranes might enable solar-powered wastewater treatment with integrated hydrogen production. Meanwhile, AI-driven platforms could democratize material innovation, enabling rapid prototyping of next-generation photocatalysts. The journey toward scalable, stable, and sustainable MXene/MBene technologies requires a multidisciplinary approach, merging materials science, computational modeling, and green chemistry. While hurdles remain, the convergence of advanced synthesis techniques, protective engineering, and AI-driven innovation promises to overcome these barriers, positioning MXenes and MBenes as pivotal players in achieving a net-zero future[70-72].

6. Results and discussion

Recent advancements in MXene- and MBene-based photocatalysis have redefined the efficiency and scope of solar energy conversion, offering transformative solutions for both energy generation and environmental remediation. These materials act as electron highways, rapidly shuttling photogenerated charges to reaction sites while suppressing recombination—a critical bottleneck in conventional systems[64, 69]. To effectively translate the successes achieved in the laboratory into real-world impact, it is crucial to have a structured roadmap in place. The first pillar of this roadmap should prioritize scalable synthesis methods. This involves replacing the use of hazardous HF-based MXene etching with more environmentally friendly alternatives, such as molten salt or electrochemical etching. This not only helps to reduce costs, but also minimizes the environmental footprint of the production process. Additionally, efforts should be made to prioritize roll-to-roll manufacturing for MBenes, which will enable industrial-scale production. For example, the use of NaOH-assisted etching in the synthesis of Mo_2B_2 MBenes can reduce chemical waste by 60%, providing a safer and more sustainable pathway for production[73, 74].

Next, hybrid system design will integrate MXenes/MBenes with perovskites and organic semiconductors to create Z-scheme architectures for spatially separated redox reactions. Thus, these systems could enable dual-function solar reactors, such as MXene/MBene membranes that can simultaneously generate green hydrogen through water splitting and remove pollutants from wastewater[75-77]. Stability engineering is crucial in ensuring the longevity and effectiveness of materials. For example, the use of atomic-layer-deposited coatings such as SiO_2 or Al_2O_3 can effectively prevent MXene oxidation in humid conditions[78]. Additionally, incorporating Cr-doped Mo_2B_2 compositions can greatly enhance the corrosion resistance of MBene in acidic industrial effluents[11, 79]. The final pillar encompasses AI-driven optimization and policy collaboration. Machine learning models can predict optimal MXene/MBene heterostructures (e.g., Ti_3C_2Tx-Fe_2B_2) for target reactions, such as CO_2-to-ethanol conversion, accelerating material discovery[80, 81]. Digital twins of solar reactors can simulate performance under variable conditions, guiding large-scale deployment. Concurrently, pilot plants, such as 1 MW solar farms with MXene-coated photocatalytic panels, must validate techno-economic feasibility[82, 83]. Policymakers and industry leaders must collaborate to subsidize green synthesis methods and establish standards for integrating these materials into renewable energy grids. MXenes and MBenes are poised to redefine solar photocatalysis, but their transition from lab-scale curiosities to cornerstone technologies demands coordinated innovation. By

addressing challenges in synthesis scalability, hybrid system design, and stability, while leveraging AI and policy support, these materials could drive the shift from fossil fuels to a solar-powered circular economy. The roadmap outlined here not only bridges scientific advancement with industrial application, but also aligns with global sustainability goals, offering a blueprint for a cleaner, energy-secure future.

7. Conclusion

MXenes and MBenes represent a paradigm shift in the pursuit of sustainable energy solutions, offering a dual promise of decarbonizing energy systems and mitigating environmental degradation. Their unique structural and electronic properties, including metallic conductivity, tunable surface chemistry, and exceptional light absorption, position them as transformative materials for solar photocatalysis. By enabling efficient hydrogen production, selective CO_2 conversion to fuels, and rapid pollutant degradation, these materials address two of humanity's most pressing challenges: energy security and ecological preservation. However, their true potential lies not only in their laboratory performance but also in their ability to bridge the gap between renewable energy generation and circular economy principles, where waste streams are transformed into resources. The journey from lab-scale innovation to global impact hinges on resolving critical challenges. Scalable and eco-friendly synthesis methods must replace hazardous processes, while advanced encapsulation and doping strategies are essential to enhance stability in real-world conditions. Equally vital is the integration of MXenes and MBenes into hybrid systems, such as solar reactors coupling hydrogen production with wastewater treatment, to maximize their multifunctionality. Emerging tools like machine learning and digital twins will accelerate this transition, enabling the predictive design of next-generation photocatalysts tailored for specific industrial applications. However, technical advancements alone are insufficient; interdisciplinary collaboration among scientists, engineers, policymakers, and industry leaders is paramount to standardize protocols, subsidize green technologies, and embed these materials into renewable energy infrastructure.

Ultimately, MXenes and MBenes are more than novel nanomaterials—they are enablers of a systemic transformation. By converting sunlight into storable fuels, detoxifying polluted ecosystems, and reducing reliance on finite resources, they exemplify the convergence of materials science and sustainability. Their success will depend not only on overcoming oxidation or cost barriers but on fostering a global commitment to innovation that prioritizes both planetary health and equitable energy access. As we stand at the crossroads of climate crisis and technological opportunity, MXenes and MBenes illuminate a path toward a resilient, solar-powered future—one where energy systems harmonize with, rather than exploit, the natural world.

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Author contributions

E.F.G. conceptualized the research, analyzed the data (including photocatalytic efficiency and material characterization), and drafted the manuscript. **F.R.** supervised the project, secured funding and resources, and critically revised the manuscript. **M.A.** conceived the original idea, directed the research framework, and finalized the manuscript for submission.

Declaration of competing interest

The datasets generated and analyzed during this study are openly available in public repositories to ensure transparency and reproducibility.

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