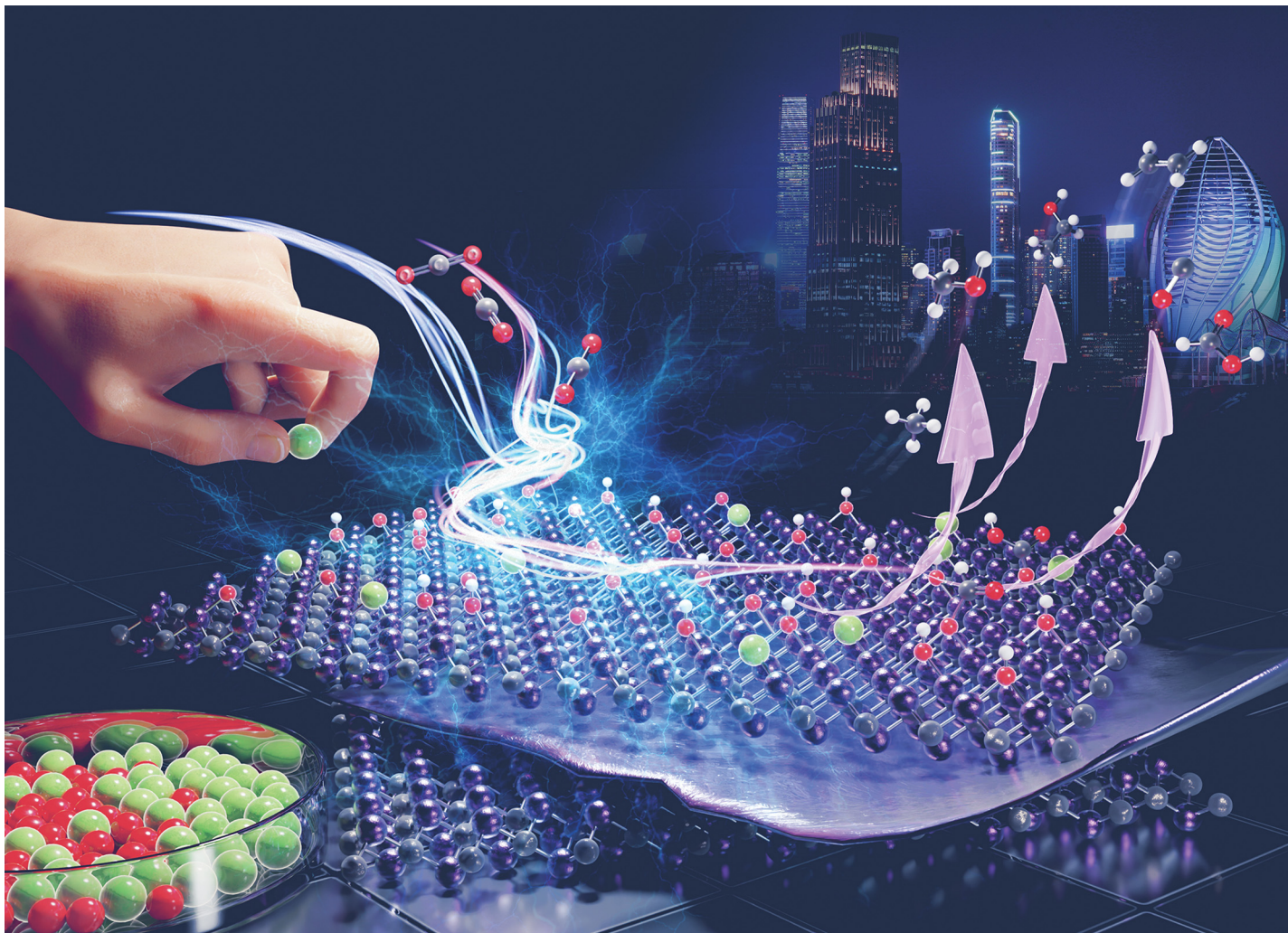




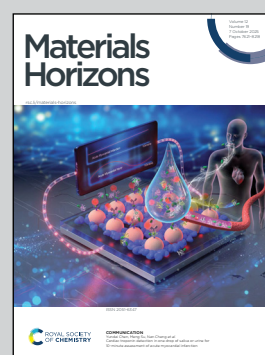
Showcasing a review by Dr Hend Omar Mohamed and Prof. Pedro Castaño, Multiscale Reaction Engineering (MuRE), King Abdullah University of Science and Technology (KAUST), Saudi Arabia.

MXene-based electrocatalysts for CO₂ reduction: advances, challenges, and perspectives

MXene-based electrocatalysts, with tunable surface terminations and abundant active sites, enable efficient CO₂ reduction by facilitating rapid electron transfer and stabilizing key intermediates for high Faradaic efficiencies and enhanced C₂⁺ selectivity. This review provides mechanistic insights and structure-function correlations that guide the rational design of next-generation MXene catalysts for scalable CO₂ valorization and sustainable energy conversion.

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REVIEW

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12, 7648MXene-based electrocatalysts for CO₂ reduction:
advances, challenges, and perspectivesSawsan Abo Talas,^{†a} Pewee D Kolubah,^{†b} Rushana Khairova,^b Manal Alqahtani,^c
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The electrochemical reduction of carbon dioxide (CO₂) is a crucial step toward a sustainable carbon economy, enabling the conversion of greenhouse gases into valuable fuels and chemicals. Among the emerging materials for this transformation, two-dimensional (2D) MXenes comprising transition-metal carbides, nitrides, and carbonitrides are notable due to their tunable surface chemistry and high conductivity. This review comprehensively analyzes recent advancements in MXene-based electrocatalysis for the CO₂ reduction reaction (RR) and explores the unique electronic properties of MXenes that drive their catalytic performance. Composition, surface terminations, defect engineering, and interfacial dynamics dictate activity and selectivity and are analyzed to contextualize the structure–function correlations. This work discusses state-of-the-art strategies to enhance the performance of MXene-based electrocatalysts, including compositional modifications, heteroatom doping, and heterostructure integration. Mechanistic insight into the CO₂RR is examined to pinpoint the advantages and challenges of MXenes in the overall reaction network. Finally, this work presents a forward-looking perspective, outlining challenges and emerging opportunities for MXenes in driving sustainable CO₂ electrocatalytic conversion technology.

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Wider impact

This review discusses key advances in the application of MXene-based materials as electrocatalysts for CO₂ reduction, emphasizing their tunable surface chemistry, high conductivity, and structural robustness. This field has witnessed notable progress in understanding the role of composition, defect engineering, surface terminations, and heterostructure integration in tailoring catalytic performance and selectivity. These developments are of broad significance, as CO₂ electroreduction presents a direct link between greenhouse gas mitigation and renewable energy utilization, enabling the production of value-added chemicals and fuels under mild conditions. The study of MXenes intersects materials science, electrochemistry, and environmental engineering, making it of compelling interest for both fundamental research and industrial applications. As global energy and climate goals intensify, the demand for efficient, scalable, and sustainable catalytic platforms is set to rise. Insights from this review—especially those concerning the molecular-level mechanisms and synthetic strategies—will help guide the rational design of next-generation 2D catalysts with enhanced activity and stability. Ultimately, these contributions will influence the development of modular and deployable CO₂ utilization systems, shaping the future of materials science toward low-carbon technologies and circular economy models.

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1. Introduction

Energy and environmental sustainability is essential for the continuation of life on the planet and has recently risen to the forefront of global concerns.^{1,2} The overutilization of natural resources, combined with unsustainable production and consumption practices such as fossil-fuel combustion, deforestation, and industrial processes, has led to extensive environmental degradation and the emergence of climate change *via* CO₂ emissions.^{3–5}

Global energy consumption is projected to increase by about 80% by 2030, potentially driving CO₂ levels and associated warming even higher without proactive mitigation.⁶ According to the Intergovernmental Panel on Climate Change (IPCC),

anthropogenic greenhouse gas emissions raised average surface temperatures by 1.1 °C above the pre-industrial levels from 2011 to 2020, with more severe impacts to follow without substantial emission reduction.⁷ As shown in Fig. 1A, global temperatures have increased and are expected to continue rising throughout the lifespans of three representative generations born in 1950, 1980, and 2020. Projections indicate that, without proactive mitigation measures, global surface temperatures could rise by up to 4 °C by 2100, underscoring the urgent need for collective action across governments, industry, and society.

CO₂ capture, storage, and utilization (CCSU) strategies aim to mitigate these emissions by capturing CO₂ from major point sources (power plants, gas-processing facilities, and industrial sites) and purifying, compressing, and injecting it into deep

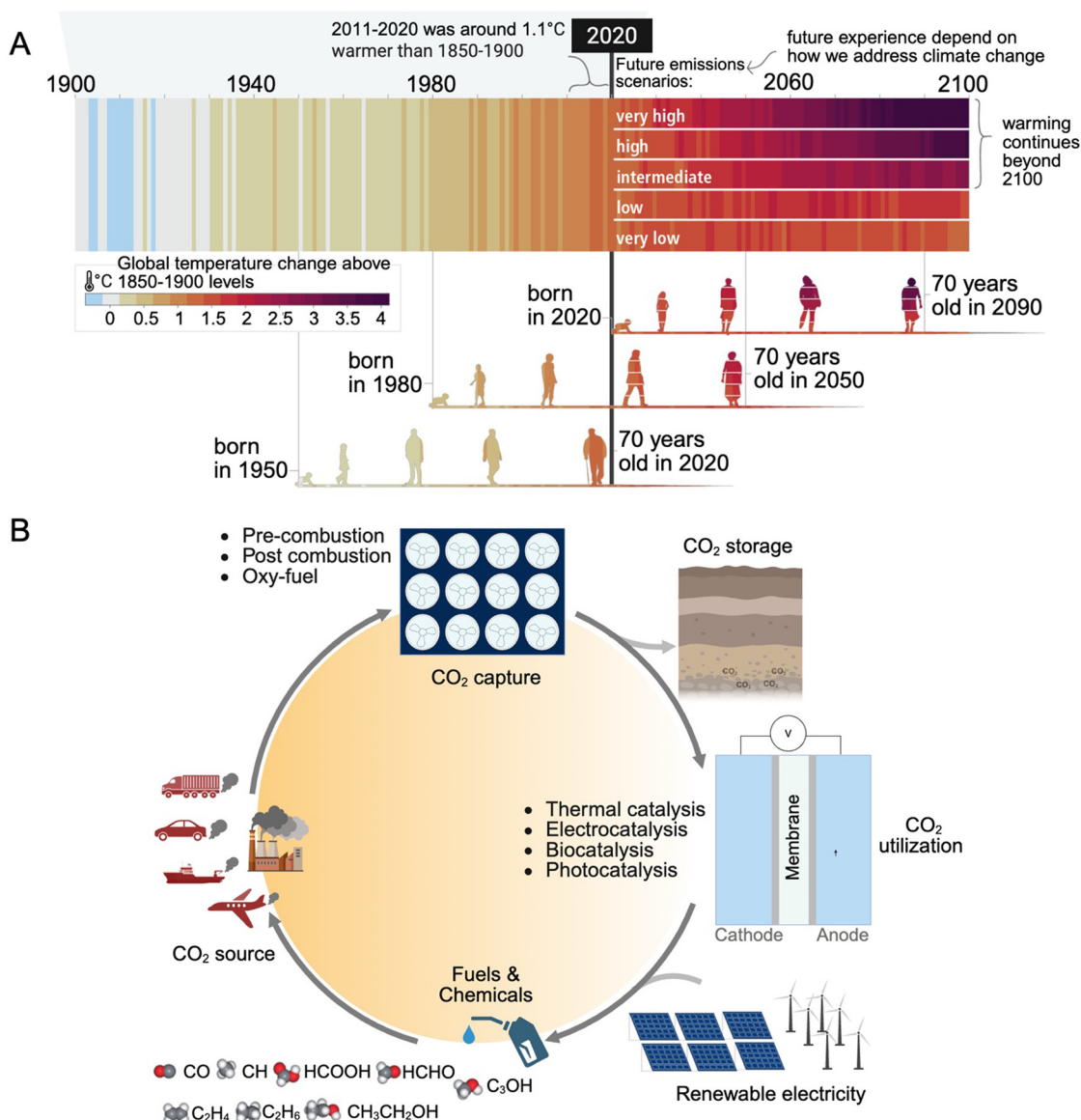


Fig. 1 Circular economy: (A) observed (1900–2020) and projected (2021–2100) changes in global surface temperature (relative to 1850–1900), which are linked to changes in climate conditions and effects, illustrating how the climate has already changed and will change along the lifespan of three representative generations (born in 1950, 1980 and 2020). Reproduced from ref. 7 with permission from IPCC, Copyright [2023]. (B) Schematic of CO₂ capture, storage, and utilization for fuel and chemical production.



geological formations (depleted reservoirs, saline aquifers, and coal seams) for long-term sequestration. The choice of capture method (pre-combustion, post-combustion, or oxy-fuel combustion) depends on the CO₂ concentration, required purity, and pressure of the emission stream. Those strategies are considered vital tools to reduce global CO₂ emissions by up to 32% by 2050 (Fig. 1B).^{8–15} The CCS provides the CO₂ feedstock for utilization pathways, enhanced oil recovery, construction materials, chemical and fuel synthesis, and agricultural applications, creating value and supporting a circular-carbon economy.¹⁶ However, the thermodynamic stability of CO₂ requires high energy input for the chemical activation and conversion of the O=C=O molecule into hydrocarbons, alcohols, or oxygenates.

Four primary catalytic approaches have been explored for CO₂ conversion: thermal, electrochemical, photocatalytic, and photothermal catalysis. In thermal catalysis, CO₂ is converted through high-temperature reactions such as hydrogenation and dry reforming with methane (CH₄), typically conducted at elevated pressures and under above-atmospheric conditions.¹⁷ Photocatalysis mimics natural photosynthesis, using solar energy to generate electron-hole pairs that migrate to the catalyst surface and drive redox reactions with adsorbed CO₂ species.¹⁸ Photothermal catalysis combines photochemical and thermochemical pathways to enhance reaction rates. This approach operates at lower temperatures than conventional thermal methods by harnessing the synergistic effects of semiconductor excitation and localized heating induced by plasmonic or nonplasmonic nanostructures.^{19,20}

Among these approaches, electrocatalysis offers a uniquely advantageous route for CO₂ utilization by directly coupling with renewable electricity. Unlike thermal processes that depend on externally produced H₂ (e.g., *via* water electrolysis), the electrochemical CO₂ reduction reaction (CO₂RR) proceeds *via* a proton-coupled electron transfer (PCET) mechanism. This enables CO₂ conversion under mild operating conditions, typically at room or moderately elevated temperatures (<100 °C) and ambient pressure, making it energy-efficient and scalable.²¹ The CO₂RR can generate a wide range of high-value products, including carbon monoxide (CO), formic acid (HCOOH), ethylene (C₂H₄), ethanol (C₂H₆O), and propanol (C₃H₈O).²² However, the competing hydrogen evolution reaction (HER), which reduces product selectivity by diverting electrons toward H₂ production, remains a key challenge.

Most of the CO₂RR products possess commercial relevance, and their selectivity can be tailored through rational design of the reaction environment, which involves optimizing electrolyte composition and reactor configuration, and, most critically, catalyst engineering.^{23,24} By tuning catalyst morphology, elemental composition, exposed crystal facets, and defect structures, researchers aim to enhance catalytic activity, boost selectivity for specific products, and improve long-term durability.²⁵

Despite rapid progress in the electrocatalytic CO₂RR, many conventional catalyst systems, such as transition metals, metal oxides, and carbides, suffer from low selectivity, poor product formation rates, and rapid deactivation.²⁶ As a result, significant

research has focused on engineering more effective catalytic architectures, including alloy catalysts, metal-support hybrids, and heterostructures, that enhance CO₂ activation, suppress the competing HER, and improve stability.^{27–29}

Recent years have seen a few breakthrough studies that define the current performance frontier for the CO₂RR. For instance, Wang *et al.*³⁰ developed a fluorine-modified copper (Cu) catalyst integrated into a flow-cell reactor, achieving an unprecedented current density of 1.6 A cm^{−2}, >80% C₂⁺ faradaic efficiency (FE), and 16.5% single-pass yield under ambient conditions. The fluorine surface functionalization was shown to enhance water activation and stabilize key CHO intermediates, thus promoting C–C coupling and boosting multicarbon product selectivity. Sargent *et al.*³¹ demonstrated that pairing a strong-acid electrolyte with an atomically sputtered planar Cu catalyst yields >90% C₂⁺ FE, 78% single-pass CO₂ utilization, and 30% energy efficiency for C₂⁺ products, with an exceptionally low energy cost of 249 GJ t^{−1} for ethanol production. While promising, the synthesis approach is complex and cost-intensive, posing scalability challenges. Yang *et al.*³² achieved 97% CO selectivity at −0.5 V vs. RHE and a specific current of 350 A g^{−1} using nickel (Ni) single atoms supported on N, S-co-doped graphene. A 100 h durability test confirmed long-term operational stability, and DFT calculations revealed that the non-centrosymmetric ligand environment around Ni(I) significantly enhanced adsorption strength for CO₂ and key intermediates. These breakthroughs illustrate how combining precise atomic-level design, reactor integration, and advanced surface engineering can collectively overcome longstanding CO₂RR challenges. Yet despite such advances, broader challenges remain in scalability, cost, and long-term performance, motivating exploration of new catalyst platforms.

Among the most promising emerging materials are two-dimensional (2D) systems, including graphene, transition-metal dichalcogenides (TMDs), layered double hydroxides (LDHs),²³ and the newest class—MXenes. MXenes are a family of 2D transition-metal carbides, nitrides, or carbonitrides, known for their high electrical conductivity, tunable surface chemistry, excellent mechanical integrity, and abundant redox-active sites, making them particularly attractive for CO₂RR applications.^{25,33–40} For instance, their metallic conductivity facilitates electron transport for complex proton-coupled electron transfer (PCET) steps. Surface terminations (e.g., −O, −OH, and −F) can be engineered to steer intermediate adsorption and reaction pathways, while their robustness supports long-term operation under electrochemical conditions. However, despite these promising features, most experimental MXene-based CO₂RR studies focus on Ti₃C₂T_x, due to the ease of synthesis and well-established chemistry.⁴¹ This field remains in its early stages: over 80% of reported studies are theoretical, relying on quantum mechanical calculations to evaluate CO₂ binding, activation energies, and selectivity trends.⁴² Experimental progress lags due to synthesis challenges, such as controlling etching, delamination, defect density, and surface terminations, affecting catalytic performance and reproducibility.

This review provides a comprehensive overview of recent progress in MXene-based catalysts for the CO₂RR. A brief



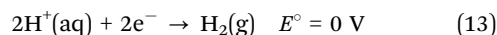
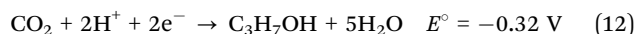
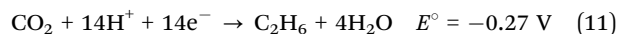
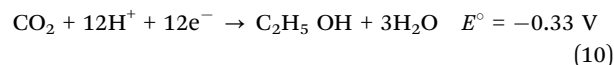
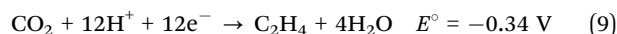
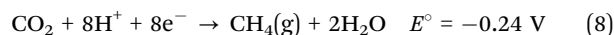
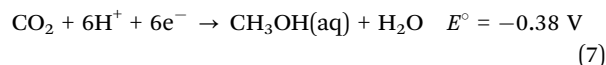
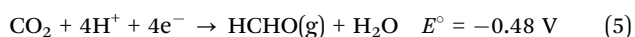
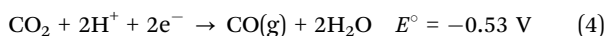
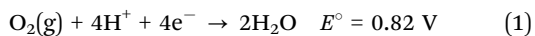
overview of the CO₂RR covers general reaction mechanisms, pathways for various product groups (*e.g.*, hydrocarbons, alcohol, and oxygenates), critical intermediates governing product formation, and the internal and external factors influencing the overall system architecture. Next, this work explores the distinctive chemical and structural properties of MXenes that enhance their catalytic potential for the CO₂RR, highlighting how they differ from conventional CO₂RR catalysts.

A critical assessment of recent developments in catalyst design and modification strategies follows, particularly on progress in operational parameters that significantly affect catalytic activity and selectivity. Then, this work explores the electrocatalytic mechanisms of the CO₂RR using MXene-based catalysts, highlighting how these mechanisms can be tailored to enhance CO₂ conversion efficiency and steer product selectivity, underscoring the novelty and promise of MXene-based catalysts. Additionally, critical factors affecting CO₂RR performance, including electronic properties, surface chemistry, and electrolyte interactions, are reviewed. Finally, this work provides a forward-looking perspective, emphasizing the necessity of a systematic approach to developing cost effective MXene-based catalysts for practical applications.

2. Fundamentals of CO₂ reduction

In a CO₂ electrolyzer, the anode and cathode reactions occur in separate chambers, divided by an ion-conducting membrane. The CO₂RR electrolyzers have distinct configurations, including H-cells, membrane electrode assembly (MEA), and microfluidic cells.⁴³ These reactor configurations have an anode and a cathode. At the anode, water is oxidized to produce molecular oxygen (O₂; eqn (1)), whereas at the cathode, CO₂ is reduced into C-containing species (Fig. 2a). An external energy input is required to drive the overall reaction. From a thermodynamic perspective, the potential required to drive the one-electron reduction of CO₂ to the CO radical is -1.9 V vs. the standard Hydrogen electrode (SHE) (eqn (2)), making the reaction highly energy-intensive and thermodynamically unfavorable in the absence of an appropriate catalyst.⁴⁴ The formation of CO₂RR products is influenced by the PCET process involving electron transfer ranging from 2 to 18 e[−] per CO₂ molecule (eqn (3)–(12)).^{45–47}

Although the proton-assisted process enables the formation of a wide range of products, achieving the selective production of the desired compounds remains a significant challenge due to the similar redox potentials of competing reaction pathways. Selectivity limitations are exacerbated in aqueous electrolyte-based CO₂ electrolyzers, where the HER occurs at a comparable potential (eqn (13)), directly competing with the CO₂RR:



Depending on the available catalyst surface during the reaction, O₂ is activated and converted into intermediates. These intermediates transform into final products *via* distinct mechanistic pathways (Fig. 2B).⁴⁹ The paths are classified into C₁ products (CO, HCOOH, methanol (CH₃OH), and CH₄), C₂ products (C₂H₄ and C₂H₆O), and a C₃ product (C₃H₈O).^{46,50,51} For instance, HCOOH formation includes the creation of an *OCHO intermediate *via* the activation and reduction of CO₂.⁵² This step requires catalysts with high O affinity, such as p-block metals (*e.g.*, tin [Sn], bismuth [Bi], indium [In], and lead [Pb]), facilitating the reduction of *OCHO to form HCOOH.^{53–57}

In contrast, producing CO involves two proton–electron steps that generate a *COOH intermediate. Catalysts (*e.g.*, gold [Au], silver [Ag], and zinc [Zn]) known for their lower affinities for O and H reduce *COOH to CO.⁴⁶ The selectivity of the overhead product in the aqueous CO₂RR can be explained by the ability of various catalyst surfaces to bind reaction intermediates, in which catalyst surface properties play a critical role in determining the reaction pathway and product selectivity (Fig. 2C).⁵⁸ Moreover, CO serves as a crucial intermediate for higher hydrocarbons and oxygenates, including formaldehyde (HCHO), CH₃OH, and CH₄, involving four, six, and eight electron transfer, respectively.⁴⁶ In addition, CO is widely considered an intermediate for forming C₂H₄ and C₂H₅OH. Table 1 shows the classification of value-added products and significant intermediates.

The formation of these C₂₊ products involves the dimerization of two CO molecules or the combination of CO with *CHO. Copper (Cu)-based catalysts are effective in these reactions because they facilitate C–C coupling, achieving high selectivity and activity for C₂₊ products.⁵⁹ In addition, Cu-based materials are among the most promising catalysts for CO₂ reduction because they exhibit relatively low activity toward the HER while demonstrating unique intrinsic catalytic activity for the CO₂RR, forming a wide range of hydrocarbons, alcohols, and oxygenates. Although the elemental composition of the CO₂RR catalyst is crucial in determining reaction pathways, the overall reaction mechanism is considerably influenced by several factors, including operating conditions, such as electrolyte pH and concentration, cation/anion size, applied potential, cell configuration, and catalyst surface characteristics (*e.g.*, facets,



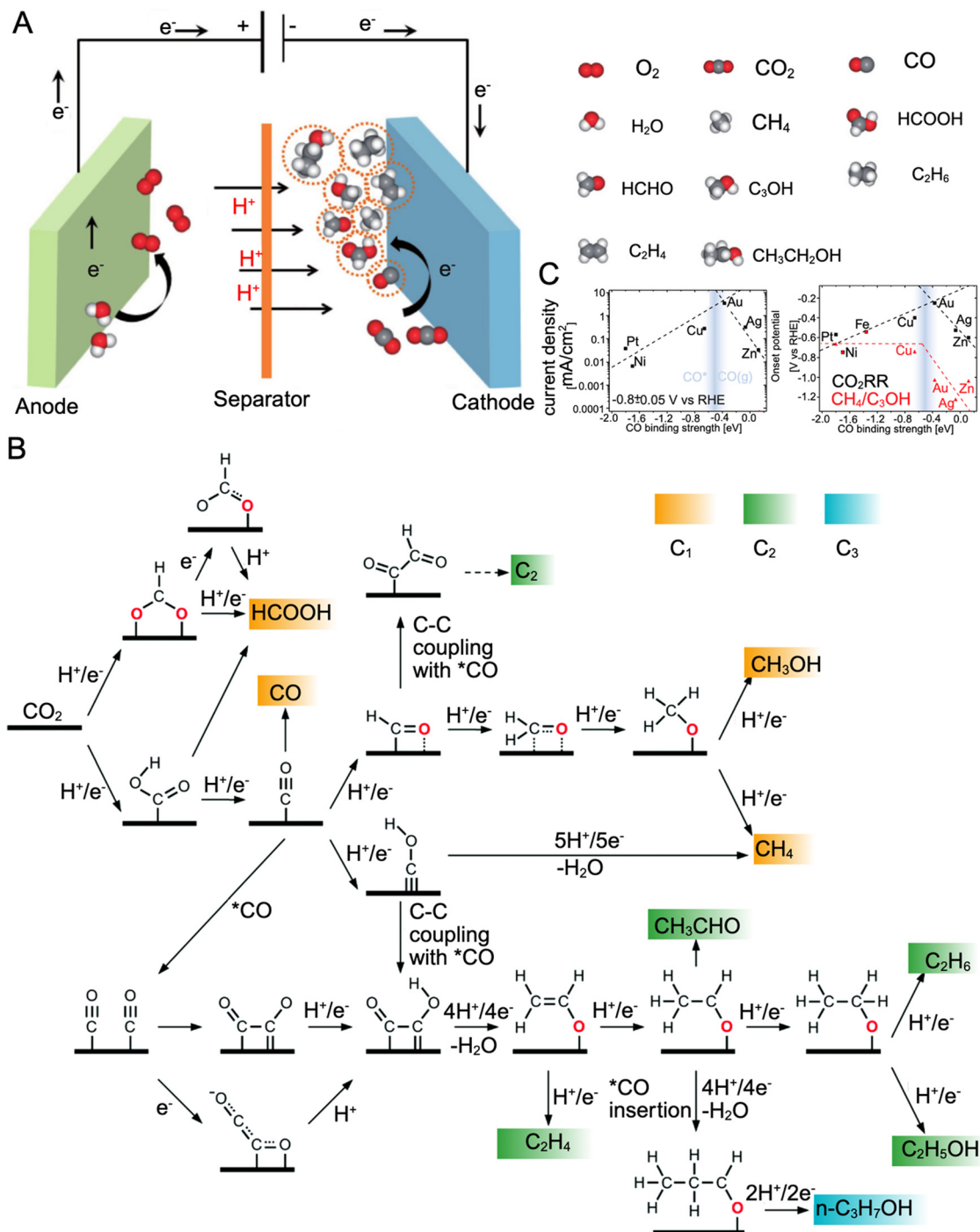


Fig. 2 (A) Schematic of the electrochemical CO₂ reduction reaction system. Reproduced from ref. 47, with permission from John Wiley and Sons, copyright [2017]. (B) Reaction mechanism, product distribution from CO₂ reduction (C1–C3). Reproduced from ref. 48, with permission from Royal Society of Chemistry, Copyright [2021]. (C) Left: volcano plot of the partial current density for the CO₂RR at 0.8 V vs. the CO binding strength. Right: two onset potentials plotted vs. CO binding energy, the overall CO₂RR, and the conversion of CO₂ to methane or methanol (Reprinted with permission from *Am. Chem. Soc.* 2014, 136, 40, 14107–14113. Copyright [2014] American Chemical Society).

defects, structure, morphology, and surface adsorbates).^{60–63} These physical and chemical parameters strongly influence the thermodynamic adsorption energies of critical intermediates and the kinetic barriers of the reactions, leading to alternative reaction pathways. The following section examines the crucial factors influencing the CO₂RR mechanism in greater detail.

2.1. Factors affecting the CO₂ electroreduction process

The efficiency of the CO₂RR is governed by the interrelation of internal and external factors in the overall system architecture (Fig. 3A). Internal factors include the electrode configuration and electrolyte characteristics, whereas external factors include the applied potential and electrolyzer design. Significant

Table 1 Classification of value-added products and significant intermediates.⁴⁸

	Products	Critical intermediates
Two-electron products	Formate (HCOO^-), formic acid (HCOOH)	$^*\text{OCHO}/\text{HCOO}^*$
Deeply reduced C1 products	Carbon monoxide (CO)	$^*\text{COOH}$
	Methane (CH_4)	CH_3O^* , $^*\text{OH}$
	Methanol (CH_3OH)	CH_3O^* , $^*\text{OH}$
Multicarbon products	Ethylene (C_2H_4)	CH_2CHO^*
	Acetaldehyde (CH_3CHO)	CH_2CHO^*
	Ethanol ($\text{C}_2\text{H}_5\text{OH}$)	CH_2CHO^* , CH_3CHO^* , $\text{CH}_3\text{CH}_2\text{O}^*$
	Ethane (C_2H_6)	$\text{CH}_3\text{CH}_2\text{O}^*$
	<i>n</i> -Propanol ($n\text{-C}_3\text{H}_7\text{OH}$)	CH_3CHO^* , $\text{CH}_3\text{CH}_2\text{O}^*$

research has been focused on computational modeling and the experimental analysis of the electrode/electrolyte (E/E) interface to clarify electrochemical processes, such as reaction dynamics, product selectivity, and overall electrochemical performance.^{64–66} The E/E interface is influenced by the constant potential during CO_2RR processes, inducing negative surface charges and promoting the formation of the electrical double layer (EDL),^{67–69} as depicted in Fig. 3B.

The EDL comprises charged species and oriented dipoles, organized into three distinct layers: the inner Helmholtz plane (IHP), the outer Helmholtz plane, and the diffuse layer.⁶⁸ The IHP is closest to the electrode surface where the electrochemical reaction occurs, whereas cations gather in the outer Helmholtz plane region in response to the applied potential. According to the classical Gouy–Chapman–Stern model, the EDL and bulk electrolytes have a distinctly different composition. Therefore, they are considered two distinct phases separated by the diffuse layer.⁷⁰ Ions form the diffuse layer due to electrostatic repulsion and thermodynamic diffusion. The concentration of the diffuse

layer decreases progressively outward toward the bulk electrolyte. In the electrochemical system, the species in the EDL are widely accepted to be in equilibrium with the bulk electrolyte in the absence of any faradaic processes.⁶⁷

The CO_2RR is an inner-sphere process in the IHP involving adsorption and bond rearrangement of CO_2 and intermediates. When the CO_2 molecule adsorbs onto the electrode surface, it binds through chemisorption, a process involving electron redistribution and chemical bond formation.⁷¹ The CO_2 binding process at the surface is influenced by the highest occupied and lowest unoccupied molecular orbitals. The orientation of these orbitals relative to the surface determines the nature of the binding. Such a CO_2 -binding process on MXenes is expected to be effective due to the tunable surface chemistry. According to the computational investigations, their surface chemistry influences the diffusion and adsorption of species and metal ions on MXene surfaces.⁷² Therefore, understanding the molecular-level interaction between CO_2 and MXenes at the E/E interface is crucial to evaluating intermediates' adsorption/

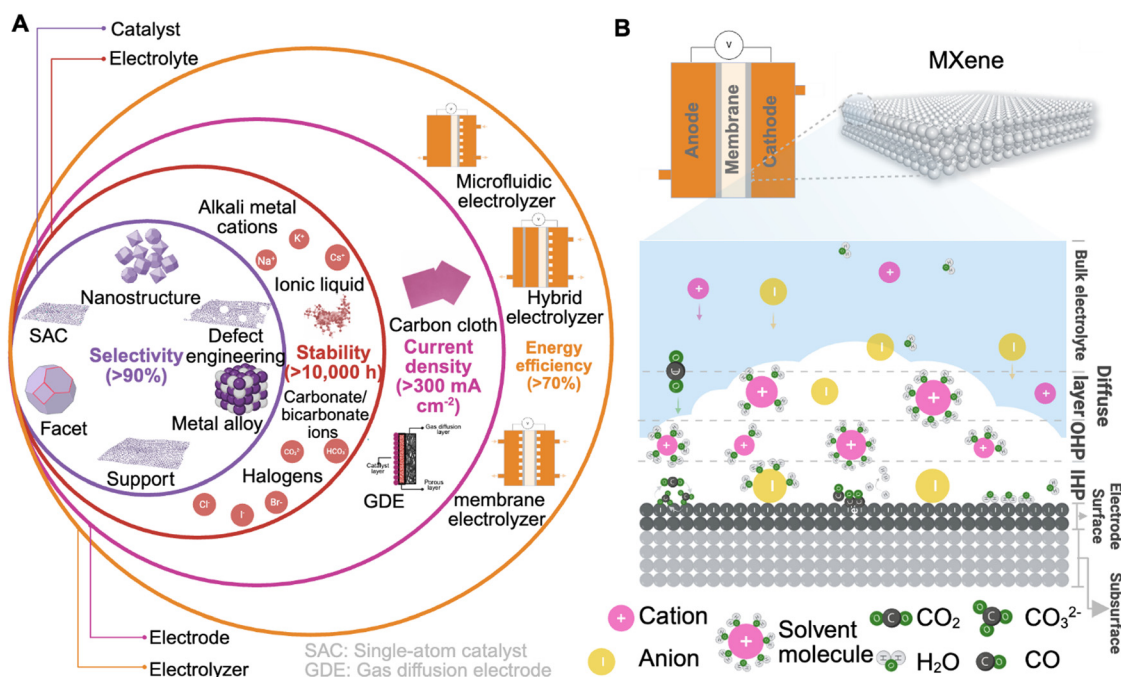


Fig. 3 (A) Factors affecting the CO_2 electroreduction process. (B) Schematic of the electrode–electrolyte interface for the CO_2RR , accounting for the electric double layer and bulk electrolyte.



desorption process, reaction kinetics, and dynamic behavior and designing highly active, selective, and durable catalysts.

Harris *et al.*⁷³ employed multinuclear magnetic resonance experiments to elucidate the strong H-bonded water molecule to the terminal hydroxyl (–OH) group on the MXene surface, providing key insights for estimating Gibbs free energy profiles and the reaction-limiting potential (U_L) of spontaneous electrochemical reactions.

Later, Cheng *et al.*⁷⁴ employed the density functional theory (DFT) to model EDL properties and proposed an intermediate electronic structure and reaction pathways of the CO₂RR on modified Nb₂CO₂ surfaces while considering the effect of water. The results indicated that pure Nb₂CO₂ is unsuitable as a catalyst for the CO₂RR; nonmetal-doped MXenes can lower the U_L of the CO₂RR and does not significantly change the reaction products. In contrast, MXene surface modification with TMs reduced the U_L of the CO₂RR and altered the reaction products. The V-modified Nb₂CO₂ system was identified as the most effective CO₂RR catalyst, favoring HCOOH as the primary product with a U_L of –0.11 V (Fig. 4A). The presence of d-levels in TMs provides a diverse range of electronic configurations, which can participate in bonding with CO₂ molecules, enhancing the electron transfer processes essential for the CO₂RR. The interaction between the d-levels of the metal and the π^* orbitals of CO₂ can lead to a more efficient electron transfer, which is crucial for breaking strong C=O bonds in CO₂.^{75,76}

The EDL properties of MXenes modified by TMs as single-atom catalysts (SACs) have been extensively explored.^{79–82} Li *et al.*⁷⁷ investigated the Mo₃C₂ MXene modified with a series of Group IVB, VB, and VIB TMs and explored the mechanism behind the breaking of linear scaling relationships between TMs and the adsorption energies of critical intermediates OCH₂O* and HOCH₂O* (Fig. 4B). Their findings revealed that substituting TMs on the MXene surface induces an upshift in the d-band center of the molybdenum (Mo) layer surface, selectively tuning the adsorption strength of OCH₂O* and HOCH₂O*, further lowering U_L from –0.651 V for Mo₃C₂ to –0.350 V for Mo₂TiC₂ (Fig. 4C). The electron localization function analysis indicated the strong localization of lone electrons on the surface Mo layer upon TM substitution, enhancing its chemical activity due to electronic coupling between the valence states of adsorbates and the TM states, resulting in splitting the bonding and antibonding states (Fig. 4D). In addition, Mo₂TiC₂ demonstrated the highest conversion performance of CO₂ to CH₄ among the studied MXenes.

Although electrode properties play a crucial role, the E/E interface is significantly influenced by the electrolyte medium. Aqueous solutions, organic solvents, and ionic liquids (ILs) can stabilize the solid–electrolyte interphase, enhance CO₂ solubility, and facilitate efficient ionic transport, all essential for optimizing electrochemical reactions. Among these, aqueous KHCO₃ solutions (0.1 to 0.5 M) are widely employed to evaluate the performance of MXene-based catalysts due to their cost-effectiveness, nontoxicity, and buffering capacity, making them the preferred medium for CO₂RR investigations. A recent

experimental study⁸³ demonstrated that the performance of Ti₃C₂T_x on a glassy carbon electrode improved for mono- and multicarbon products, achieving selectivity toward CO (42.2%), CH₃OH (23.6%), C₂H₆O (20.1%), and acetone (10.1%) as the KHCO₃ concentration in the electrolyte increased from 0.1 to 0.5 M. The authors attributed this performance to the enhanced CO₂ adsorption capacity of 0.16 mmol g^{–1}, facilitating a higher current density.

Otgonbayar *et al.*⁸⁴ demonstrated enhanced selectivity toward alcohols, such as CH₃OH and C₂H₆O, using a 2D MXene coupled with cuprous oxide (Cu₂O)/magnetite (Fe₃O₄) nanocomposites using various electrolytes, including sodium carbonate (Na₂CO₃), potassium carbonate (K₂CO₃), potassium chloride (KCl), and sodium chloride (NaCl). A strong interaction between the catalyst surface and the electrolyte, particularly with alkali metals and halide ions (chlorine [Cl[–]]), enabled faster adsorption/desorption dynamics, influencing their ability to donate or retain a negative charge. This interaction generated a dipole moment, modified the local surface environment, and enhanced the catalytic activity.

Qu *et al.*⁸⁵ demonstrated CO₂ electrolysis using seawater as the cost-effective electrolyte. This strategy achieved 92% faradaic efficiency (FE) for CO production using synthesized nitrogen (N)-doped Ti₃C₂ MXene nanosheets with abundant V_{Ti} defects. Mechanistic studies have revealed that N dopants and V_{Ti} synergistically modulate the electronic structure of the active titanium (Ti) site, significantly lowering the free energy barriers for *COOH formation and *CO desorption.

Notably, pH is pivotal in influencing aspects of PCET processes in the CO₂RR. The local pH at the E/E interface can change during the CO₂RR, significantly affecting the selectivity and activity of the catalyst.^{86,87} For example, Varela *et al.*⁸⁸ investigated the influence of the electrolyte concentration and the importance of local pH in controlling the selectivity of the CO₂RR on Cu. The study demonstrated that the buffer capacity of the electrolyte is critical in influencing catalytic activity and product selectivity. In dilute KHCO₃, the lower proton concentration near the electrode surface suppresses the formation of H₂ and CH₄, whereas the production rates of CO and C₂H₄ remain largely unaffected.

Xie *et al.*⁷⁸ employed lateral-type *in situ* surface-enhanced Raman spectroscopy combined with computational simulations using COMSOL to investigate the effect of local pH variations at the E/E interface on CO₂RR selectivity and activity (Fig. 4E). The study revealed that, in the diffusion layer, the local pH gradually decreases as the distance from the catalyst surface increases, with a sharp pH drop indicating limited proton mass transport (Fig. 4F–H). As reported, these local pH variations are influenced by the buffering capacity of the electrolyte and can have a considerable influence on the selectivity of C₂⁺ products during the CO₂RR (Fig. 4I).⁸⁹

The pH dependence of CO₂ activation differs from that of the competing HER. For example, previous work has demonstrated that the overall product selectivity of graphite-immobilized coproporphyrin is highly pH sensitive. At a pH of 1, H₂ is the dominant product, whereas at a pH of 3, CO



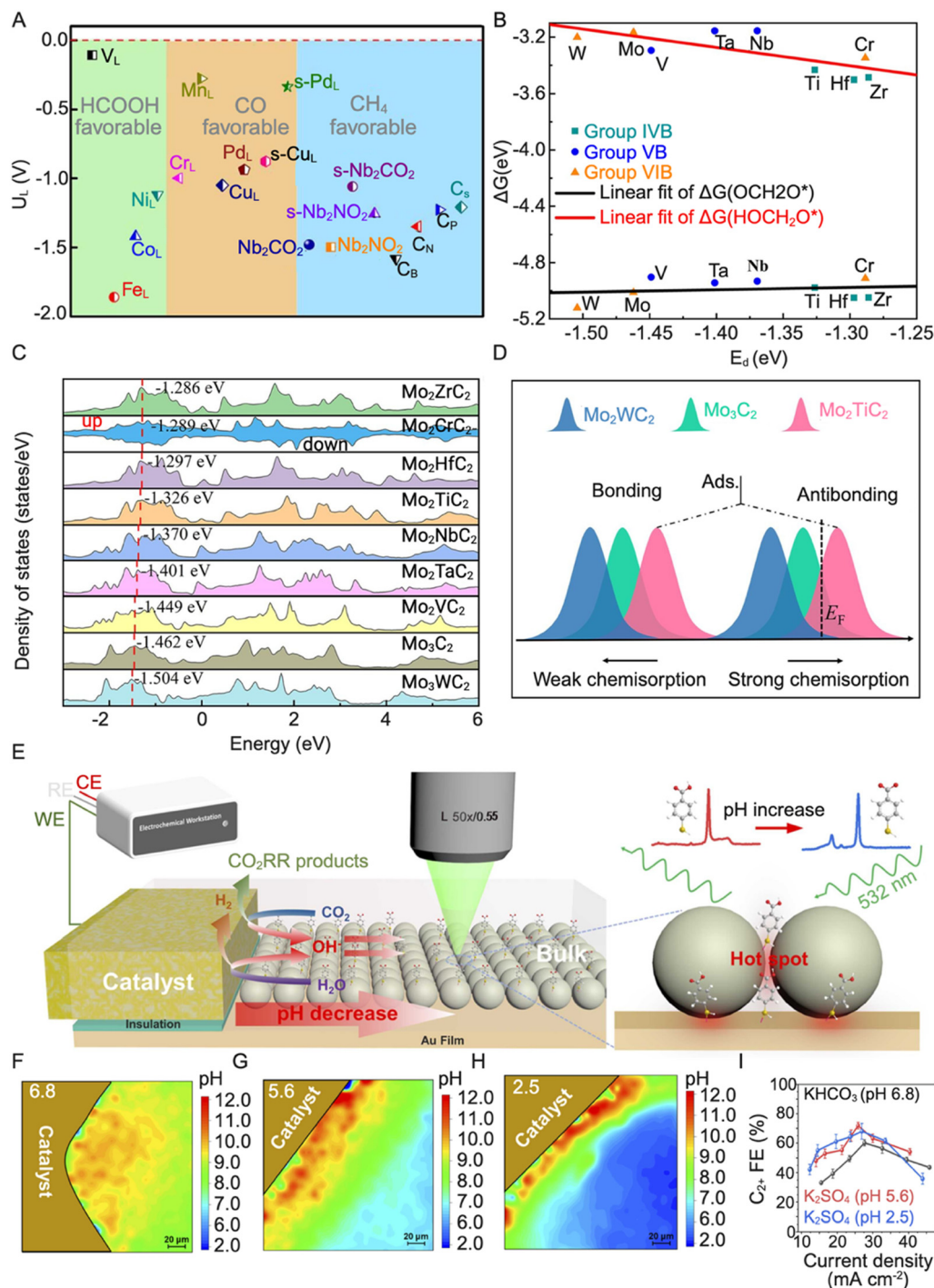


Fig. 4 (A) Potential limiting the U_L of NbCO₂ and modified Nb₂CO₂. Reproduced from ref. 74, with permission from Elsevier, Copyright [2021]. (B) Linear relation of adsorption free energy $\Delta G(\text{OCH}_2\text{O}^*)$ and $\Delta G(\text{HOCH}_2\text{O}^*)$ vs. the d-band center E_d . (C) Projected density of state plots for the d orbital of surface Mo atoms in MXenes, in which the Fermi level was set to 0, and the calculated d-band centers are denoted by dashed vertical red lines. (D) Schematic of the bond formation between the adsorbate (Ads.) and reaction surface of MXenes, represented by Mo₂WC₂, Mo₃C₂, and Mo₂TiC₂. (E) Schematic of the L-SERS system for *in situ* local pH measurement and illustration of pH-sensitive molecules (4-MBA) in the SERS. (F)–(H) Local pH images around the catalyst surface in CO₂-saturated electrolytes of (F) KHCO₃ (pH 6.8), (G) K₂SO₄ (pH 5.6), (H) K₂SO₄ (pH 2.5) with the applied current density of 10 mA cm⁻², and (I) C₂+ faradaic efficiency influenced by pH. (E)–(I), Reproduced from ref. 78 with permission from Elsevier, Copyright [2024].

becomes the primary product, illustrating the strong influence of pH on reaction pathways.⁹⁰ The DFT calculations indicate that the critical intermediate is anionic hydride, which

undergoes a nucleophilic attack on CO₂ to yield HCOO⁻. The reaction is facilitated by potential-induced changes in the oxidation state of the catalyst, with the hydride typically

residing on the ligand for In and Sn porphyrins. The stability of the resulting species is vital for reactions leading to CO or HCOOH/HCOO[−] formation.

Pourbaix diagrams, analogous to standard pressure–volume phase diagrams, offer insight into the thermodynamic equilibrium surface structure under varying pH and applied potential (*U*) conditions. According to the Pourbaix diagram of MXenes with various surface termination groups (Fig. 5),⁹¹ MXenes do not exhibit a bare surface at any pH–*U* conditions in an aqueous environment. At a *U* value below −0.6 V, the MXene surface is fully hydrogenated, with all reaction sites occupied by H*. As *U* increases, the surface undergoes progressive oxidation, with OH* gradually replacing H*, highlighting the strong *U* sensitivity of the process. The intricate relationship between *U* and MXene functionalization, as demonstrated for other electrochemical reactions, such as the HER⁹² and N reduction reaction,⁹³ is significant because it directly influences catalytic activity. This understanding can guide the design of MXene-based catalysts for the CO₂RR, facilitating the selection of optimal surface terminations for enhanced performance. Future studies should develop Pourbaix diagrams for MXene compositions under CO₂RR-relevant pH and *U* conditions, offering deeper insight into their electrochemical stability and reactivity.

The electrolyte's metal cation/anion composition is another critical factor influencing the product distribution of the CO₂RR. Alkaline-metal cations facilitate CO₂ adsorption in aqueous solutions and stabilize critical intermediates, such as COOH*, via noncovalent interactions with adsorbed species or a field effect.⁹⁴ For instance, Hori *et al.*⁹⁵ observed that C₂H₄ formation increased relative to CH₄ as the cation size increased (lithium [Li⁺] < sodium [Na⁺] < potassium [K⁺] < cesium [Cs⁺]).⁹⁶ This variation in hydrocarbon selectivity was attributed to differences in specific adsorption or the preferential hydrolysis of various cations. Among anions, halide ions (F[−], Cl[−], bromine [Br[−]], and iodine [I[−]]) could modulate the geometry and electronic structure of metal-based electrocatalysts, stabilize active species, regulate the adsorption and desorption of reaction intermediates, and reduce the overpotential to enhance the selectivity and activity of the CO₂RR for multi-carbon products.^{97–99} This finding is attributed to halide ions donating electrons to the empty orbitals of CO₂.¹⁰⁰

Ni *et al.*¹⁰¹ synthesized fluorine (F)-doped caged porous C, achieving an FE of 88.3% for CO production at −1.0 V vs. RHE, with a corresponding current density of −37.5 mA cm^{−2}. The microporous structure of the F-doped C shells, particularly at edge positions, induces localized high electric fields, lowering the thermodynamic energy barrier for CO₂ reduction. Similarly,

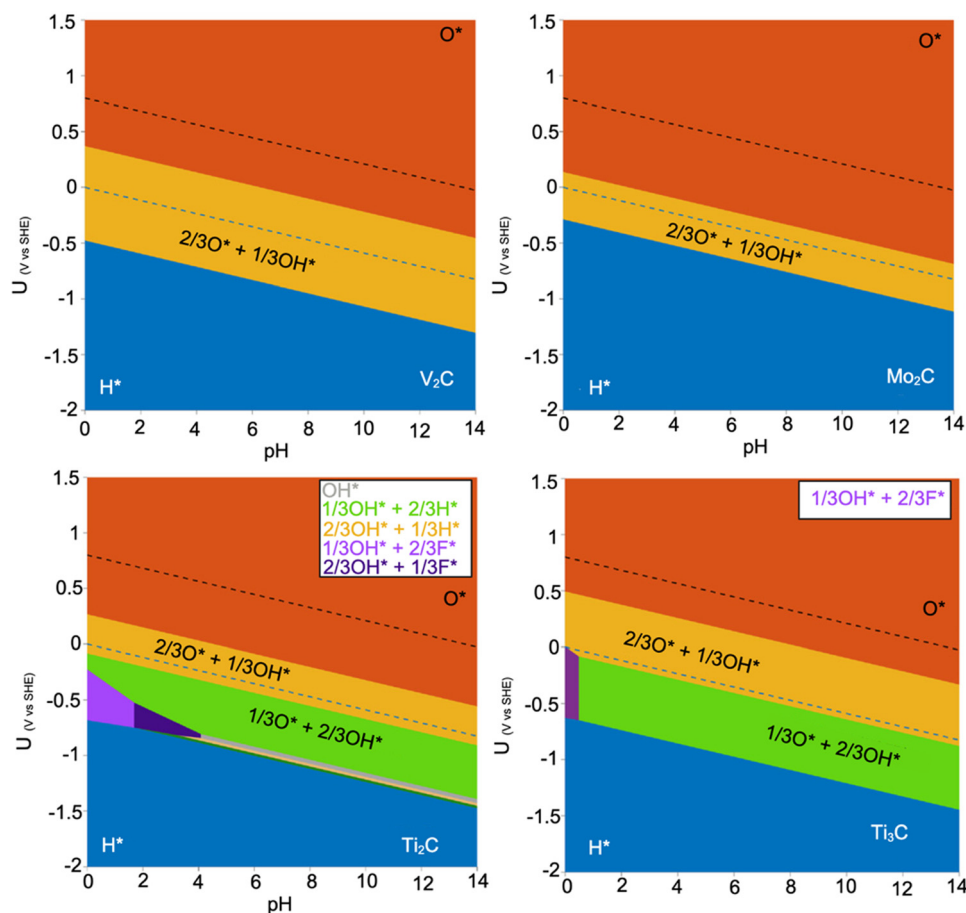


Fig. 5 Pourbaix diagrams of Mo₂C, V₂C, Ti₂C, and Ti₃C₂. Reproduced from ref. 91 with permission from Wiley and Sons, Copyright [2022].



Gao *et al.*¹⁰² demonstrated that O₂-plasma-activated Cu catalysts, combined with electrolyte design, exhibited enhanced CO₂RR activity and selectivity toward multicarbon hydrocarbons and alcohols, achieving a FE of ~69% and a partial current density of -45.5 mA cm^{-2} for C₂₊ products at -1.0 V vs. RHE. Their findings indicated that larger alkali-metal cations and subsurface O species promoted cation adsorption, facilitating C–C coupling on CuO_x electrodes. Furthermore, using an electrolyte containing Cs⁺ and I[−] induced a significant reorganization of the CuO_x surface, forming well-defined Cu species, and enhanced the intermediate stabilization and C₂₊ product selectivity.

Considering the well-documented positive influence of halide ions on CO₂RR performance, MXenes, with abundant halide surface terminations, present a promising platform for enhancing the selectivity of multicarbon products. Halogen-based etching using molecular Cl, Br, or I can introduce halide terminations onto MXene surfaces, potentially modulating active species and regulating the adsorption–desorption dynamics of reaction intermediates during the CO₂RR.^{103–105} For instance, a Cu-immobilized Ti₃C₂Cl_x MXene demonstrated over 58% selectivity for CH₃OH, with dominant Cl functional groups residing on the outermost Ti layers.¹⁰⁶ Synchrotron-based X-ray absorption spectroscopy and DFT calculations attributed the exceptional performance of the catalyst to single-atom Cu species with an unsaturated electronic structure (Cu^{δ+}, $0 < \delta < 2$), facilitating a low-energy-barrier conversion from HCOOH* to the CHO* intermediate.

However, despite confirming the abundant Cl terminations, the study did not explicitly address their role in the activity and selectivity of the catalyst. Given the widely accepted understanding that halide ions influence reaction mechanisms by modulating intermediate adsorption and desorption, further investigation of the Cu-immobilized Ti₃C₂Cl_x catalyst is necessary to clarify the role of Cl termination groups. Future research should systematically explore the effects of $-\text{Cl}$, $-\text{Br}$, $-\text{F}$, and $-\text{I}$ terminations on MXene-based catalysts, offering deeper insight into their influence on CO₂RR performance and product distribution.

The electrolyte employed during the CO₂RR can also influence product distribution and overall performance. Despite being the most applied electrolyte systems in the CO₂RR, aqueous solutions have limited CO₂ solubility (about 0.034 M), constraining their application in the H-cell. Research efforts have been directed toward using dipolar aprotic solvents, such as acetonitrile (about 0.27 M)¹⁰⁷ and ILs, which can serve as mediators that prevent the HER and as cocatalysts that form complexes with CO₂ molecules to overcome this problem and improve CO₂ solubility. In one of the earliest studies on MXenes using ILs, Handoko *et al.*¹⁰⁸ combined experimental and theoretical approaches to investigate Ti- and Mo-based MXenes for HCOOH production, achieving a 56% FE in an electrolyte system containing IL 3-butyl-1-methyl-1*H*-imidazol-3-ium tetrafluoroborate dissolved in an acetonitrile–water solution. This work highlighted the crucial role of $-\text{O}$ surface termination groups in suppressing the HER while revealing the limitations of

acetonitrile as an electrolyte due to its volatility, causing fluctuations in HCOOH selectivity.

Attanayake *et al.*¹⁰⁹ suppressed the competing HER using the IL 1-ethyl-2-methylimidazolium tetrafluoroborate as an electrolyte in acetonitrile. Under these conditions, Ti₃C₂ and Mo₂C demonstrated a remarkable FE of 90% for CO production. Despite the favorable solubility of CO₂ in ILs, their relatively high viscosity compared to conventional solvents poses challenges, including a lower CO₂ adsorption rate and increased pumping costs in industrial applications. Cosolvents, such as water or CH₃OH, can be introduced to reduce viscosity while maintaining CO₂ solubility to mitigate viscosity-related limitations.¹¹⁰

Previous studies on energy storage devices have demonstrated strong synergy between surface terminations of MXenes and IL functional groups, significantly influencing supercapacitor performance.^{111–114} Applying insight from MXene-IL interactions in energy storage devices to the CO₂RR could enhance interfacial interactions, improving product selectivity and addressing stability challenges. This approach presents a promising strategy for applying the complementary properties of MXenes and ILs to enable efficient and scalable CO₂ conversion into a diverse range of valuable products.

The catalyst structure can also affect the activity and selectivity of the CO₂RR. A Cu-based catalyst is highly capable of producing multicarbon products. However, selectivity toward a specific product is challenging. Nanostructured Cu, including nanoparticles, nanowires, and hierarchical structures with varying compositions, sizes, morphologies, and crystal orientations, has gained considerable research attention due to its ability to enhance the selectivity of the CO₂RR.^{115,116} The exposed crystal facets of the nanostructured Cu play a crucial role in determining the reaction pathway and controlling product distribution. Adjusting the exposed facet on the Cu crystals can change the specific atom arrangements, reaction intermediate affinity, and surface energy, influencing the CO₂RR pathway and product distribution.¹¹⁷

Luo *et al.*¹¹⁸ investigated the facet-dependent selectivity of Cu₂O nanocrystals, demonstrating that tailoring the exposed facets enhanced selectivity toward C₂H₄. Star-shaped Cu₂O nanocrystals with (332) facets achieved over 74% selectivity for C₂H₄. This high selectivity was attributed to a reduction in Gibbs free energy, with the (332) facets exhibiting the lowest energy barrier (0.13 eV) in the initial step of gaseous CO₂ hydrogenation, compared to (111) at 0.20 eV and (100) at 0.22 eV. Furthermore, the *in situ* Raman spectroscopy of star-shaped Cu₂O (332) nanocrystals revealed the presence of *COOH and *CHO intermediates, indicative of C–C coupling, facilitating C₂H₄ formation.

The nanocrystal structure influences the facet dependence of the selectivity of Cu nanocrystals in the CO₂RR. An investigation of Cu single crystals in an H-cell has revealed that (100) is suitable for C₂H₄ formation, whereas (111) favors CH₄ formation. For example, Gregorio *et al.*¹¹⁹ developed a colloidal method to synthesize Cu cubes, spheres, and octahedral nanocrystals and tested them for the CO₂RR in flow cells. The study



revealed that the Cu octahedral nanocrystals dominantly produced CH_4 , in line with the presence of the exposed (111) facets. In contrast, the Cu cubes with dominant (100) facets exhibited much higher selectivity (55%) toward C_2H_4 . These studies demonstrated the facet-structure dependence of the selectivity of Cu-based nanocrystals. The influence of external factors, such as temperature and applied voltage (constant and pulse/dynamic), remains underexplored in optimizing MXene performance for the CO_2RR . Most studies have focused on ambient temperature conditions,¹²⁰ either *via* DFT predictions or experimental investigations, aiming to maintain temperature as a constant parameter to ensure catalyst stability and durability. Conversely, the applied potential is a dynamic factor essential for activating the catalyst surface and forming an E/E interface. Changes in applied voltage alter the charge density on the MXene surface, affecting the organization of ions and solvent molecules in the EDL and affecting CO_2 adsorption and intermediate stabilization. Moreover, potential variations can modify the oxidation state of the catalyst, changing its electronic structure and overall surface properties and influencing reaction pathways and product selectivity.

For example, Han *et al.*¹²¹ used *in situ* X-ray analysis to monitor changes in Sn species' oxidation states and the local chemical environment in the $\text{SnO}_2/\text{MXene}$ catalyst under various applied potentials ranging from -0.6 to -1.2 V *vs.* RHE. The authors observed a gradual shift toward lower energy on Sn K-edge X-ray absorption near-edge structure (XANES) profiles with a more negative applied potential. They reported a progressive reduction in the oxidation valence state in the CO_2RR . The excellent performance and selectivity of the CO_2RR to

HCOOH in a 0.1 M KHCO_3 aqueous solution reached a maximum of 94% at -0.8 V, attributed to the intermediate/mixed Sn oxidation state between metallic Sn^0 and Sn^{4+} .

Furthermore, Govindan *et al.*¹²² highlighted the influence of the applied potential on MXene-based catalysts, where tuning the cell potential enabled a palladium (Pd)-MXene nanocomposite to achieve a FE of 67.8% for CH_3OH at -0.5 V *vs.* RHE. Moreover, CO and H_2 became the dominant products at higher potentials, attributed to CO serving as a crucial intermediate in CH_3OH formation. However, as the potential increased, CO desorption from the catalyst surface intensified, restricting its further conversion to CH_3OH and shifting the selectivity toward CO and H_2 evolution. This observation highlights the vital role of the applied potential in determining product selectivity and reaction pathways. However, despite its importance, no studies have investigated using a pulsed potential for MXenes in the CO_2RR , highlighting a notable research gap for future investigation.

The system configuration is a critical factor in determining the overall catalytic performance of MXene-based electrocatalysts in the CO_2RR . This configuration encompasses electrode type (*e.g.*, carbon paper, glassy carbon, and gas diffusion electrodes) and reactor design (*e.g.*, H-cells, microfluidic cells, and membrane electrode assemblies, MEAs). Each component plays a distinct role in controlling mass transport behavior, product selectivity, energy efficiency, and scalability (Fig. 6).

While H-cells are the most widely used reactors for fundamental CO_2RR studies, they frequently underrepresent real-world performance due to low CO_2 solubility (~ 34 mM), mass transport limitations, and high ohmic resistance from large

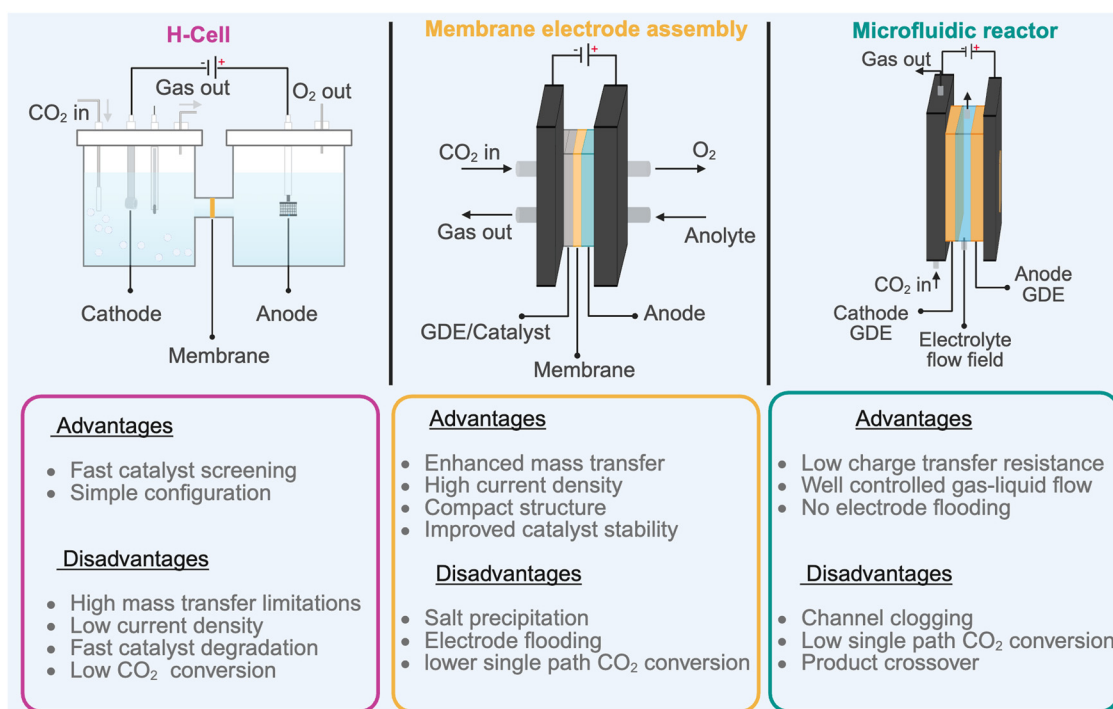


Fig. 6 Schematic of the typical electrochemical flow cells for CO_2 reduction.



inter-electrode spacing (>2 cm). As a result, H-cells typically achieve modest current densities (<50 mA cm $^{-2}$) and produce faradaic efficiencies that are difficult to reproduce under industrial conditions.^{123,124} In contrast, flow-cell reactors, particularly those employing gas diffusion electrodes (GDEs), directly expose the catalyst to a continuous CO $_2$ gas stream, dramatically improving CO $_2$ mass transport and achieving reliable partial current densities between 50 and 300 mA cm $^{-2}$. For instance, a SnO $_2$ quantum dot/MXene composite attained 57.8 mA cm $^{-2}$ with 94% faradaic efficiency for formate in a flow-cell GDE/MEA configuration, significantly outperforming the H-cell benchmark. Similarly, an FePc/MXene composite tested in a flow cell demonstrated $\sim 98\%$ FE for CO with stability over 24 h, highlighting improved mass transport and HER suppression compared to the H-cell configuration.¹²⁵

MEA-based reactors integrate solid-state ion-exchange membranes, enabling compact reactor designs, ion-specific transport control, and minimal reactant/product crossover. A Bi $_2$ O $_3$ /MXene composite demonstrated continuous operation at 300 mA cm $^{-2}$ with $>90\%$ formate selectivity over 60 h in an MEA.¹²⁶

Abdinejad *et al.*¹²⁷ evaluated a Cu–Pd/MXene composite catalyst using both configurations. In an H-cell, the catalyst achieved a CO $_2$ -to-formate conversion with a FE of 79% at -0.5 V vs. RHE. In contrast, when tested in a zero-gap MEA reactor, the same catalyst achieved an enhanced FE of 93% at -2.8 V and a full-cell energy efficiency of 47%, showcasing the MEA's ability to sustain higher current densities and reduce resistance. These comparisons underscore that while H-cells are valuable for mechanistic insights, they are limited in reflecting the behavior of MXene catalysts under realistic, high-throughput conditions. MEAs offer enhanced gas transport, stable interfaces, and minimized side reactions, allowing MXenes to achieve higher selectivity, greater stability, and industrially relevant current densities. This reinforces the need to assess MXene catalysts under MEA configurations to realize and report their catalytic potential. Table 2 shows comparison of MXene catalyst performance across different reactor configurations.

3. MXene fabrication, structure, and characteristics

3.1. MAX phase synthesis and etching

The MAX phase is a layered carbide, nitride, or carbonitride with the formula M $_{n+1}$ AX $_n$. The A layers (group 11 to 16 elements) are

weakly bonded to the M layers *via* metallic bonds, making them selectively etchable, whereas strong covalent bonds hold together the M and X layers. Fig. 7A presents the chemical composition of MAX phase precursors and their MXene derivatives. Since MXenes were first discovered, over 150 MAX phases have been predicted *via* computational investigations.¹²⁹ The diversity of MAX phases is presented through the possible MAX chemical compositions and the ability to form various *n* structures, including MAX precursors (M $_2$ AX, M $_3$ AX $_2$, M $_4$ AX $_3$, and M $_5$ AX $_4$).¹³⁰ Recently, out-of-plane (M $_2$ M'AX $_2$ and M $_2$ M' $_2$ AC $_3$) and in-plane (*e.g.*, (M $_2$ /M' $_3$) $_2$ AlC) ordered structure MXenes have been reported.¹³¹

The MAX phases are synthesized at elevated temperatures (800 °C to 1800 °C) in an inert atmosphere. The process involves mixing elemental powders (M and A) or carbide/nitride mixtures, followed by sintering. The precursor selection, stoichiometry, and heating rate strongly influence the properties and purity of the MAX phase. Since the discovery of MXenes, extensive research has focused on optimizing MAX phase synthesis, refining etching protocols and improving delamination methods. The addition of excess Ti and aluminum (Al) beyond the stoichiometric ratio during the reactive sintering of Ti $_3$ AlC $_2$ enhances the stability and conductivity of the resulting MXene.^{134,135} This improvement is attributed to the excess Al, which reacts with O in the system, promoting the formation of more stoichiometric Ti $_3$ AlC $_2$ with fewer defects, including O substitution in the C sublattice.

Recently, Michałowski *et al.*¹³⁶ employed atomic-resolution ultralow-energy secondary-ion mass spectrometry to detect O incorporation in the C sublattice. The study revealed that when a stoichiometric Ti:Al:C ratio is used, Ti $_3$ AlC $_2$ can contain up to 30% O in the C sublattice, forming an oxycarbide MXene upon etching. In contrast, using excess metals in synthesis led to Ti $_3$ AlC $_2$ with no detectable O. Excessive A-layer content during the MAX phase synthesis reduces O substitution and C vacancies, improving MXene stability and electronic properties.¹³⁴ Similarly, the composition of X in the MAX phase can influence MXene properties.

For example, Shuck *et al.*¹³⁷ used three C sources, graphite, TiC, and C lampblack, to synthesize the MAX phase. The produced MXene exhibited distinct stability and conductivity depending on the composition and morphology. Therefore, choosing elemental precursors, mixing ratios, and sintering conditions is crucial to achieving desirable MAX phase characteristics for

Table 2 Comparative performance of MXene-based electrocatalysts in H-cell, flow-cell, and MEA configurations, showing the same material under different reactor designs, associated current densities, product selectivities, and literature references

MXene catalyst	Cell configuration	Current density (mA cm $^{-2}$)	Product & FE (%)	Ref.
Au/Ti $_3$ C $_2$ T $_x$ MXene	H-cell	17.3	CO (48.3%), H $_2$ (25.6%)	128
Cu–Pd/MXene aerogel	H-cell	~ 20	Formate ($\sim 79\%$)	127
Cu–Pd/MXene aerogel	MEA	150	Formate ($>90\%$)	127
FePc/MXene composite	Flow-cell	>100 – $200+$	CO ($\sim 98\%$) stable	125
FePc/MXene composite	MEA	200+	CO ($\sim 98\%$), 96% stability	125
Pd–Ti $_3$ C $_2$ T $_x$ MXene	H-cell	~ 10 – 20	CO ($\sim 48\%$), H $_2$ ($\sim 26\%$)	122
SnO $_2$ QD/MXene composite	H-cell	<30	Formate ($<70\%$)	121
SnO $_2$ QD/MXene composite	Flow-cell	57.8	Formate ($\sim 94\%$)	121



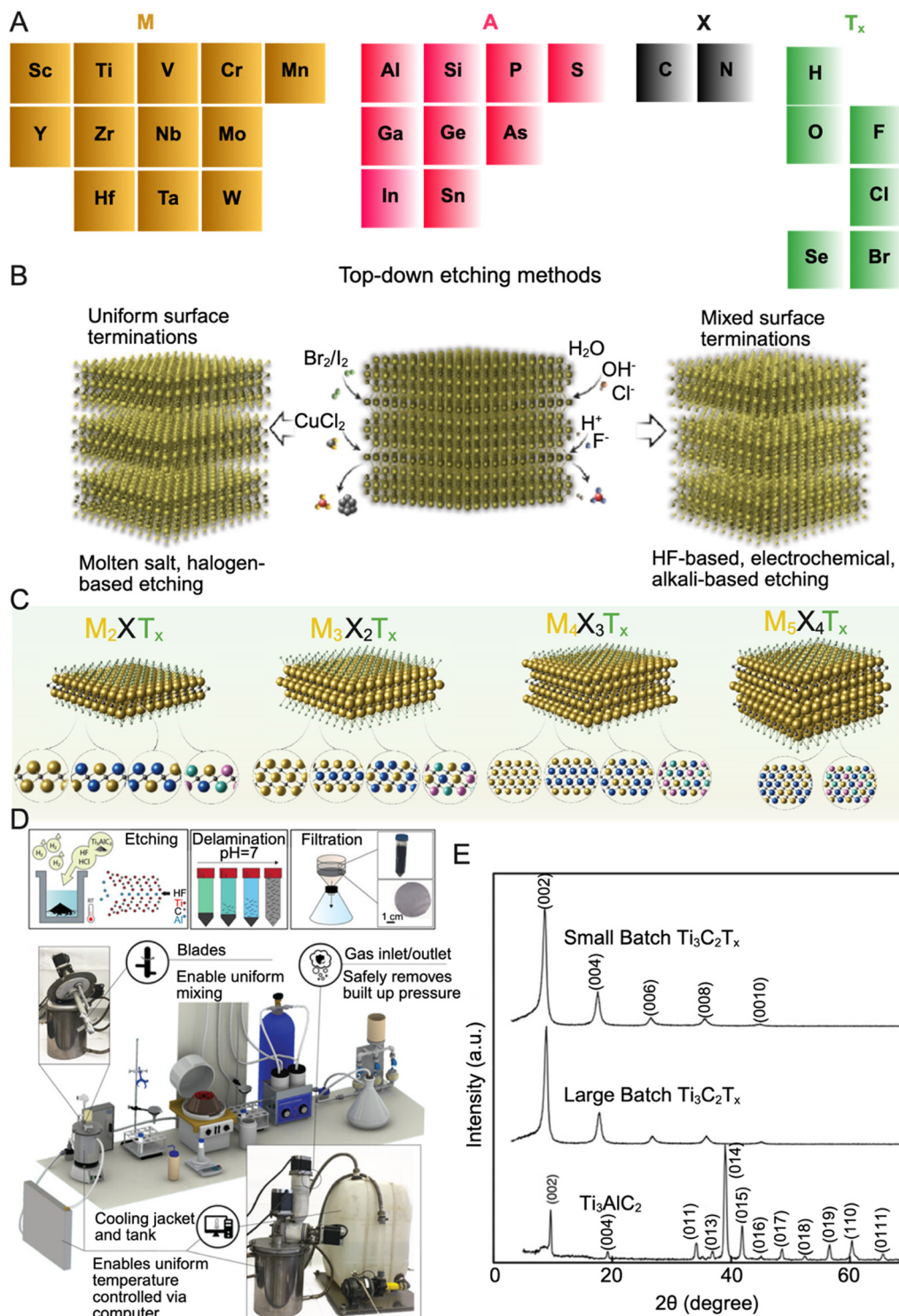


Fig. 7 (A) Periodic tables presenting MAX phase and MXene compositions. (B) Top-down etching methods for MXene synthesis. (C) MXene forms synthesized using top-down etching methods. (B) and (C) Reproduced from ref. 132 with permission from Springer Nature, Copyright [2025]. (D) Schematic demonstrating the large-scale synthesis of MXenes using the HCl:HF:H₂O etching method. (E) X-ray diffraction pattern of MXenes synthesized via a large-scale process and a small batch. No notable change in structure is observed. (D) and (E) Reproduced from ref. 133 with permission from Wiley and Sons, Copyright [2020].

CO₂RR applications. Future research should explore the influence of these factors, particularly the M, A, and X compositions, on the electrocatalytic performance of MXenes.

MXene synthesis involves the removal of the A layer from the MAX phase to form multilayered MXenes, with the reaction's Gibbs free energy determining the etching effectiveness. This



approach is called the top-down approach for MXene synthesis (Fig. 7B). MXenes produced using this approach come in M_2XT_x , $M_3X_2T_x$, $M_4X_3T_x$, and $M_5X_4T_x$ forms (Fig. 7C). Naguib *et al.*¹³⁸ synthesized the first MXene by etching Ti_3AlC_2 with concentrated hydrofluoric acid (HF), selectively weakening Ti–Al bonds while preserving Ti–C bonds. During etching, the initial adsorption of H and F atoms onto Ti atoms selectively weakens the less stable Ti–Al bonds, leaving the stronger Ti–C bonds intact. This process creates interlayer spacing, facilitating the intercalation of HF and H_2O for sequential layer-by-layer etching.¹³⁹ This process exposed undercoordinated Ti metallic surfaces, which were saturated with termination groups, such as –O, –OH, and –F, denoted as T_x .^{140,141} Since the first reported synthesis of MXenes, significant efforts have been directed toward optimizing synthesis protocols and minimizing the use of hazardous HF. Therefore, numerous alternative methods have been developed, including low HF etching, electrochemical, alkaline, molten salt, and halogen etching approaches.

Low concentrations or reduced quantities of HF yield high-quality MXenes with fewer defects. Acid mixtures have been explored as alternative etching solutions to minimize HF usage while maintaining efficient MAX-phase etching. For example, a comparative study evaluated HF/HCl and HF/ H_2SO_4 etching systems to remove the Al layer from Ti_3AlC_2 and reported that MXenes synthesized *via* HF/HCl displayed larger interlayer spacing and higher structural water compared to HF and HF/ H_2SO_4 , which might be due to the –Cl termination.¹⁴² Recently, an optimized HCl:HF: H_2O etching solution has gained widespread adoption due to its reduced HF content and ability to produce high-quality MXene sheets. This approach uses a 6:1:3 ratio of HCl, HF, and H_2O per gram of MAX powder.¹⁴³

Shuck *et al.*¹³³ applied the HCl:HF: H_2O etching method for the scalable synthesis of up to 50 g of $Ti_3C_2T_x$ MXene (Fig. 7D). Notably, the large-batch synthesized MXene exhibited identical structural and chemical characteristics to small-batch samples, demonstrating that this approach enables scaling up without compromising material quality (Fig. 7E), making it a promising route for commercialization.

In a three-electrode configuration, the electrochemical etching method selectively removes the A atomic layer by applying a potential while using the MAX phase as an electrode. The applied potential disrupts the M–A bond using electrolyte solutions, such as NaCl, HCl, or HF.¹⁴⁴ Effective control over the etching potential and time ensures selective A atom removal, enabling precise control over MXene synthesis. An uncontrollable increase in the applied potential can eliminate the M-layer, yielding amorphous C materials.^{145,146}

Chen *et al.*¹⁴⁷ synthesized $Ti_3C_2T_x$ *via* electrochemical etching in a mixed lithium hydroxide (LiOH) and lithium chloride (LiCl) aqueous solution, achieving over 90% etching efficiency. The synthesis was performed at 5.5 V for 5 h, using two identical Ti_3AlC_2 blocks as symmetric electrodes. As the etching progressed, the Ti_3AlC_2 cathode remained intact, whereas the Ti_3AlC_2 anode was partially consumed. The presence of Li^+ ions in the etching solution facilitated the etching process by

intercalating into the layers and promoting the delamination of the MXene with –Cl surface termination.

Similarly, Shen *et al.*¹⁴⁸ prepared an F-free $Ti_3C_2Cl_2$ MXene using a molten-salt-assisted electrochemical etching technique. During the electrochemical etching process, the surface termination was modified from –Cl to –O and sulfur (–S), considerably shortening the modification steps and enriching the variety of surface terminations.

Electrochemical etching is a green and safe synthesis method with low energy consumption. However, challenges remain, including forming an amorphous C layer under uncontrolled etching conditions and the relatively low yield of the MXene. Although the MAX phase electrode can be reused multiple times, the typical etching process results in limited MXene production, making it unsuitable for large-scale synthesis. Despite these limitations, this approach can potentially prepare MXenes for the CO_2RR .

Alkaline etching is a nonacid etching method for synthesizing MXenes with functional groups, such as –OH and –O, making it hydrophilic and suitable for fabricating electrodes for aqueous applications, such as the CO_2RR . Despite the limited toxicity of this method, MXene synthesis using this approach is challenging because the reaction is spontaneous at elevated temperatures, making it difficult to control oxidation at elevated temperatures and low concentrations. The fast oxidation is attributed to –OH termination groups that oxidize MXenes quickly.

For example, Li *et al.*¹⁴⁹ successfully prepared $Ti_3C_2(OH)_2$ MXenes using KOH in a hydrothermal reactor. Replacing the Al atoms with –OH groups allows the formation of 2D $Ti_3C_2(OH)_2$. Similarly, NaOH-assisted hydrothermal alkali etching at 270 °C yielded $Ti_3C_2T_x$ with a yield of 92% and improved interlayer spacing.¹⁵⁰ The primary reaction pathway involves converting Al into Al(oxide) hydroxides, followed by their dissolution in an alkaline medium. Elevated reaction temperatures and concentrated NaOH facilitate the rapid dissolution of Al(oxide) hydroxides, forming F-free MXenes with abundant –OH and –O surface terminations. The abundant –OH terminations on MXenes synthesized using this method may enhance C_2 product formation.

Literature reports indicate that the presence of –OH terminations on Cu catalysts can lower the binding energy of CO and improve the charge equilibrium between C atoms in the adsorbed OCCO intermediate. This interaction reduces the energy barrier for C_2H_4 formation by facilitating CO dimerization.^{151–153}

Molten salt etching can be divided into fluoride-containing and fluoride-free molten salt etching.¹⁵⁴ The fluoride-containing approach allows the *in situ* formation of HF during synthesis. By combining a strong acid (*e.g.*, HCl or H_2SO_4) and fluoride salts (*e.g.*, LiF, NaF, KF, NH_4F , and FeF_3) or using bifluoride salts (*e.g.*, NH_4HF_2 , $NaHF_2$, and KHF_2), HF can be formed *in situ* during the etching process.^{154,155} During synthesis, metal cations (Li^+ , Na^+ , and K^+) enter negatively charged MXene layers and increase interlayer spacing, eliminating the need for an extra intercalation step. The etching temperature



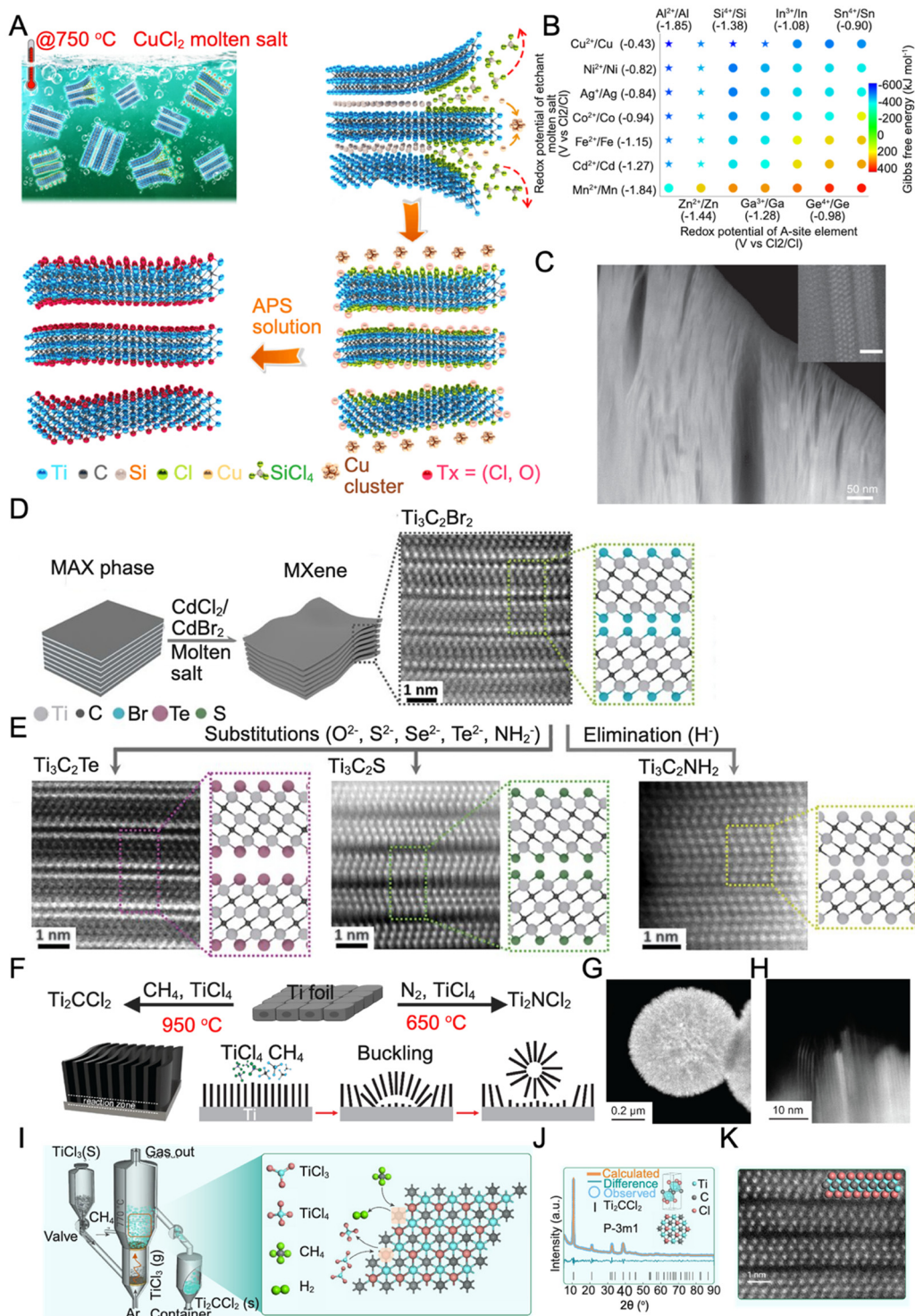


Fig. 8 (A) Schematic of Ti₃C₂Cl₂ synthesis via the Lewis acid etching route. (B) Gibbs free energy mapping (700 °C) guiding the selection of Lewis acid Cl salts based on the electrochemical redox potential. (C) High-resolution transmission electron microscopy imaging of an MXene. (A)–(C) Reproduced from ref. 158 with permission from Springer Nature, Copyright [2020]. (D) Etching MAX phases in Lewis acidic molten salts and atomic-resolution high-angle annular dark-field (HAADF) image of Ti₃C₂Br₂. (E) HAADF images of Ti₃C₂Te, Ti₃C₂S, and Ti₃C₂NH₂ MXenes. (B) and (E) Reproduced from ref. 159 with permission from American Association for the Advancement of Science, Copyright [2020]. (F) Schematic of the reaction zone and proposed mechanisms of CVD-Ti₂CCl₂. (G) Scanning transmission electron microscopy (STEM) images of spherical MXenes. (H) High-resolution image of spherical MXenes. (F)–(H) Reproduced from ref. 160 with permission from American Association for the Advancement of Science, copyright [2023]. (I) Schematic of a fluidized reactor bed for the CVD process. (J) X-ray diffraction pattern of Ti₂CCl₂ obtained using FBR-CVD before delamination. (K) Cross-sectional HAADF-STEM image of the (0001) plane of Ti₂CCl₂ flakes. (I)–(K) Reproduced from ref. 161 with permission from Elsevier, Copyright [2024].



and concentration of the acid and fluoride salt can significantly affect the quality of MXene sheets.

Wang *et al.*¹⁵⁶ reported the synthesis of an MXene with an accordion-like structure by introducing LiF into a NaCl–KCl molten salt etchant with CuCl₂. The reaction was kept for 5 h at 750 °C, and monolayer flakes of MXene nanosheets were synthesized by incorporating the prepared MXene into a tetrabutylammonium hydroxide (TBAOH) solution during agitation, achieving an MXene yield of ≈ 15% to 20%.

The Lewis acidic molten salt etching approach is proposed to prepare fluoride-free MXenes by adjusting MAX precursors with various Lewis acid salts at elevated temperatures. For example, Li *et al.*¹⁵⁷ used an element replacement approach that replaces the A-layer atom in the MAX phase with Zn atoms in molten ZnCl₂. This approach synthesizes and etches several MAX phases, including Ti₃ZnC₂, Ti₂ZnC, Ti₂ZnN, and V₂ZnC, to achieve their respective MXene derivatives. The MXene synthesis was achieved by the MXene Al-MAX with ZnCl₂ in a 1 : 6 molar ratio and heating at 550 °C for 5 h to achieve pure Cl-terminated MXene sheets.

Li *et al.*¹⁰⁵ expanded this approach using Lewis acidic etching to synthesize MXenes from the MAX phase precursors containing A elements, such as Si, Zn, and gallium (Ga; Fig. 8A). As illustrated in Fig. 8B, this approach can prepare MXenes with other types of A-layer atoms. By tuning the chemistry of the MAX precursor and the composition of the Lewis acid melt, a direct redox interaction between the A element and the cation of the Lewis acid molten salt enables the prediction of MAX phase reactivity in the molten salt, facilitating MXene synthesis. For instance, Ti₃SiC₂ was immersed in molten CuCl₂ at 750 °C. During the reaction, the exposed Si atoms, which are weakly bonded to Ti in the Ti₃C₂ sublayers, were oxidized to silicon (Si⁴⁺) cations using Lewis acid Cu²⁺, forming volatile SiCl₄ and the concomitant reduction of Cu²⁺ to metallic Cu. The metallic Cu was removed by immersing the Ti₃C₂Cl₂ product in an ammonium persulfate solution. High-resolution scanning transmission electron microscopy (STEM) revealed that the resulting MXene exhibited a lamellar microstructure similar to that of the MXene synthesized using the HF etching approach (Fig. 8C). Considering the high activity of Cu for the CO₂RR, this research should optimize this approach to preserve Cu metallic particles in the resulting MXene structure and test it for the CO₂RR.

Kamysbayev *et al.*¹⁵⁹ employed substitution and elimination reactions in molten organic salts to synthesize MXenes with varied surface termination groups using CdCl₂ or CdBr₂ molten salts (Fig. 8D). The study demonstrated that Cl[−] or Br[−] terminated MXenes can actively participate in surface reactions, where halide ion exchange enables precise control over the surface chemistry and properties of MXene sheets. The surface terminations of the synthesized MXenes were further modified by dispersing them in molten alkali-metal halides, such as Li₂Te, Li₂S, Li₂Se, Li₂O, and NaNH₂ (Fig. 8E), allowing for tailored functionalization and enhanced material properties.

Recently, Liu *et al.*¹⁶² prepared Ti₃C₂T_x (T_x: Cl[−] and O[−]) *via* a molten-salt-etching route in acetonitrile-based electrolyte.

Moreover, CuCl₂ was applied as the main molten salt etching, and NaCl/KCl was employed as a supporting electrolyte. The synthesis was performed at 680 °C for 24 h in an argon (Ar)-filled furnace. The obtained MXene displayed enhanced electrochemical stability.

The literature has reported several new top-down MXene synthesis approaches, including hydrothermal-assisted HCl etching¹⁶³ and microwave-assisted molten salt etching.^{164–166} These methods are still in their early stages and require more investigation to optimize them to produce high-quality MXenes.

Most studies on MXene synthesis are based on a top-down approach. Three bottom-up synthesis approaches, chemical vapor deposition (CVD), the template method, and plasma-enhanced pulsed laser deposition, have been reported for synthesizing MXenes. The CVD method allows the growth of ultrathin MXene sheets at elevated temperatures and a non-terminated surface.

Xu *et al.*¹⁶⁷ produced defect-free molybdenum carbide (Mo₂C), tungsten carbide (WC), and tantalum carbide (TaC) thin films using CVD at elevated temperatures (1085 °C). Recently, Wang *et al.*¹⁶⁰ synthesized Ti₂CCl₂ using CVD. The reaction of CH₄ and TiCl₄ on a Ti surface enables direct CVD growth at 950 °C of Ti₂CCl₂ carpets and complex spherulite-like morphologies that form *via* buckling and the release of the MXene carpet to expose a fresh surface for further reactions (Fig. 8F). Scanning electron microscopy imaging revealed that the synthesized MXene evolved from bulges into spherical MXene vesicles (Fig. 8G) with sheets radiating from the center and oriented normally to the surface (Fig. 8H). The template method uses 2D TM oxide (TMO) nanosheets as templates. During the synthesis, the TMO nanosheets are carbonized or nitrified to form a carbide or nitride MXene, respectively.¹⁶⁸

For example, Xiao *et al.*¹⁶⁹ produced molybdenum nitride (MoN) using 2D molybdenum trioxide (MoO₃) nanosheets as templates. MoN was synthesized by annealing the MoO₃ cover with NaCl at 280 °C for 2 h. MoN exhibited very uniform nanosheets with a thickness of about 0.71 nm. The 2D tungsten nitride and vanadium nitride nanosheets were also synthesized using this method. Plasma-enhanced CVD and pulse laser deposition can be combined to prepare 2D MXenes.

Zhang *et al.*¹⁷⁰ prepared an ultrathin large-area Mo₂C film on sapphire by combining plasma-enhanced CVD and pulse laser deposition. The sapphire substrate was heated to 700 °C for depositing the high-quality Mo₂C film using CH₄ plasma as the C source.

Xiang *et al.*¹⁶¹ reported a scalable gas-phase technology for synthesizing Cl-terminated Ti₂CCl₂. The synthesis was conducted in a fluidized bed CVD reactor, where TiCl₃ was introduced into the reactor at 770 °C and was rapidly sublimated to form a gaseous precursor for nucleation (Fig. 8I). The gaseous precursors were transported by Ar gas to react with CH₄ in the upper region of the fluidized reactor bed, forming TiCCl₂ powders. The process yielded about 0.1 kg per batch, underscoring the high efficiency of the synthesis method. X-ray diffraction (Fig. 8J) and atomically resolved high-angle annular



dark-field (HAADF)-STEM images (Fig. 8K) revealed the typical characteristics of $\text{Ti}_3\text{C}_2\text{Cl}_2$.

3.1.1. Intercalation and delamination. Top-down approaches for MXene synthesis typically yield multilayer MXenes, requiring intercalation and delamination to obtain monolayer MXene sheets, which have enhanced physical and chemical properties compared to their multilayer counterparts. Due to strong interlayer interactions in multilayer MXenes, the insertion of organic molecules or inorganic ions can weaken these interactions and increase interlayer spacing, facilitating delamination.¹⁷¹ Common organic intercalants include dimethyl sulfoxide (DMSO), *N*-methyl-2-pyrrolidone, tetramethylammonium hydroxide (TMAOH), TBAOH, hydrazine monohydrate, *N,N*-dimethylformamide, and urea, whereas LiCl is widely used as an inorganic intercalant.¹⁷²

Following the initial discovery of MXenes in 2011, Mashtalir *et al.*¹⁷³ demonstrated in 2013 that multilayer MXenes could be delaminated into monolayer MXene nanosheets *via* DMSO intercalation. After delamination, the X-ray diffraction analysis revealed that the interlayer spacing of the $\text{Ti}_3\text{C}_2\text{T}_x$ MXene increased from 1.95 to 3.50 nm, reducing van der Waals interactions and promoting exfoliation *via* ultrasonication. Delamination into the monolayer MXene increases surface terminations and enhances the hydrophilicity and the negatively charged surface of MXene nanosheets, facilitating their dispersion and the formation of stable colloidal solutions. Although DMSO has promising results as an intercalation molecule for $\text{Ti}_3\text{C}_2\text{T}_x$, it is not effective for delaminating other MXene types.

Hydrazine monohydrate, *N,N*-dimethylformamide, and urea have been explored as intercalation agents to exfoliate multilayer $\text{Ti}_3\text{C}_2\text{T}_x$ into a monolayer $\text{Ti}_3\text{C}_2\text{T}_x$ MXene.¹⁷³ However, these methods have demonstrated limited efficiency due to the aggregation of monolayers, resulting in thicker flakes (20 to 50 nm). Naguib *et al.*¹⁷⁴ demonstrated that TBAOH, hydroxyl choline, and *n*-butylamine could facilitate the delamination of V_2C_x and Ti_3CNT_x from their multilayered structures into single layers *via* simple handshaking in water. Following intercalation and delamination, the interlayer spacing increased from 2.14 to 3.86 nm for Ti_3CNT_x and from 1.99 to 3.86 nm for V_2CT_x . The similarity in interlayer spacing for both MXenes highlights the crucial role of intercalating molecules in determining the final interlayer spacing of delaminated MXenes.

Han *et al.*¹⁷⁵ demonstrated that hydrothermal-assisted intercalation of TMAOH can efficiently intercalate multilayer $\text{Ti}_3\text{C}_2\text{T}_x$, increasing the monolayer $\text{Ti}_3\text{C}_2\text{T}_x$ MXene yield to over 73% while achieving a thickness of 1.7 nm. The hydrothermal-assisted intercalation process facilitates diffusion and incorporation of TMAOH between layers. Ascorbic acid was introduced as a mild reductant to prevent the oxidation of the MXene at elevated temperatures.

With the continuous expansion of the 2D MXene family, alternative delamination solvents have been explored for various MXene compositions. Montazeri *et al.*¹⁷⁶ applied NaOH to intercalate Na^+ ions into Nb_2CT_x and $\text{Mo}_2\text{Ti}_2\text{C}_3\text{T}_x$ multilayers following a washing step with TBAOH. The resulting delaminated MXenes exhibited increased *d*-spacing values of 1.6 and

1.5 nm for Nb_2CT_x and $\text{Mo}_2\text{Ti}_2\text{C}_3\text{T}_x$, respectively. In addition to assisting with delamination, NaOH also reduced the surface oxidation of the flakes. Similarly, Mashtalir *et al.*¹⁷⁷ reported amine-assisted delamination of the Nb_2C MXene, where the intercalation of isopropylamine between the Nb_2CT_x layers followed by mild sonication in water for 18 h at room temperature led to successful exfoliation. X-ray diffraction analysis of the delaminated Nb_2CT_x revealed an increased interlayer spacing of 1.23 nm, which is sufficiently large to accommodate more than one isopropylamine molecule and water between layers.

In addition, LiCl can be employed as an intercalator for multilayer MXenes to enlarge their interlayer spacing by inserting Li^+ .¹⁴³ Zhang *et al.*¹⁷⁸ applied LiCl as an etchant to delaminate $\text{Ti}_3\text{C}_2\text{Cl}_2$, synthesized *via* Lewis acid molten salt etching. A primary challenge associated with Lewis acid molten salt etching is the difficulty of achieving monolayer nanosheets due to the hydrophobic nature and strong interlayer interactions of halogen-terminated MXenes. Delamination was accomplished using a LiCl-assisted DMSO intercalation approach, where the sample was treated for 24 h followed by centrifugation. As $\text{Ti}_3\text{C}_2\text{Cl}_2$ is hydrophobic, hydrated cations struggle to intercalate between layers. The experiment was conducted in a moisture-free environment to avoid forming a hydration shell around Li^+ , which could hinder intercalation.¹⁷⁹

Notably, the HCl/LiF molten salt etching approach eliminates the need for additional intercalation because MXenes synthesized *via* this method can be directly delaminated. This result is attributed to the spontaneous insertion of Li^+ into interlayers, expanding and weakening interlayer interactions, facilitating separation into monolayers *via* ultrasonication or simple shaking by hand.¹⁸⁰

Song *et al.*¹⁸¹ proposed a freeze-sonication delamination strategy for exfoliating a multilayer MXene into a monolayer MXene with the yield exceeding 74%. This approach applies the synergistic effect of ultrasonic treatment and ionic intercalation, facilitating the penetration of numerous water molecules into the interlayer space. The volume expansion, followed by ultrasonic treatment in a frozen state, forms the monolayer MXene. The delaminated MXene demonstrated an excellent gravimetric capacitance of 261.1 F g^{-1} and satisfactory cycling stability. Many of the reported delamination approaches produced MXenes with smaller flakes, limiting their application for large MXene flakes.

3.1.2. Scalability and defect minimization. Large-scale synthesis of various MXenes, beyond the commonly reported Ti_3C_2 , is essential to broaden their practical use in catalytic applications such as CO_2 reduction. Conventional top-down synthesis methods, particularly HF-based etching (including HF, HCl/HF/ H_2O , and LiF/HCl mixtures), are widely adopted for MXene production due to their simplicity and relatively high throughput. However, these approaches suffer from significant limitations when applied to large-batch synthesis. Challenges include the toxicity of etchants, poor control over surface terminations (typically resulting in F-rich terminations), and considerable variability in flake morphology and chemistry,





Table 3 Comparative overview of top-down MXene synthesis methods

Method	Scalability and throughput	Termination control	Advantages	Industrial suitability	Key limitations
HF etching ¹⁴¹	High (tens of grams per batch)	Poor (–F dominated)	Simple, fast, widely adopted	Mature, used in academic and lab-scale work	Highly toxic; uncontrolled terminations; defect formation
HCl–HF–H ₂ O/ LiF–HCl ^{105,133}	Moderate (~5–15 g per batch)	Moderate (mixed –F/–OH)	Safer than pure HF; better delamination via Li ⁺	Feasible at lab and pilot scales (~50 g)	Involves fluoride; sensitive to processing parameters
Electrochemical etching ¹⁴⁷	Low (batch); moderate (flow reactors: ~10 g h ^{–1})	High (tunable –O, –Cl)	Fluoride-free; selective and tunable; potential-controlled	Promising for industrial translation	Lower yield; possible defect formation; scaling challenges
Alkaline etching ^{149,150}	Moderate (gram-scale hydrothermal setups)	Good (–O, –OH rich)	Fluoride-free; environmentally benign; improved hydrophilicity	Feasible for specific MAX phases	Limited to few MAX phases; low efficiency
Molten salt etching ^{162,184}	Moderate to high (up to tens of grams per run)	Moderate (–Cl, –O, –S possible)	Fluoride-free; high crystallinity; controlled terminations	Pilot studies reported	Requires >600 °C; substrate dependent
Halogen etching ^{159,161}	Moderate-high (~0.1 kg per batch via a CVD or halide vapor route)	Tunable (–Cl, –Br, –I)	Unique terminations; dry etching; scalable in CVD setups	Emerging technique	Toxic gases; process maturity is low

including thickness, lateral dimensions, and termination groups, all of which adversely impact catalytic performance and batch-to-batch reproducibility.^{182,183} Alternative etching techniques have emerged, including low-HF protocols, electrochemical etching, alkaline (e.g., NaOH/KOH) etching, molten salt, and halogen-based etching. Each offers different trade-offs regarding yield, safety, termination control, and structural preservation.¹⁸⁴ For instance, molten salt etching provides better control over surface terminations (e.g., –Cl and –O) without hazardous liquid acids, though it requires high temperatures (>600 °C).¹⁸⁴ Electrochemical etching in flow reactors enables tunable, fluoride-free synthesis under ambient pressure, but is limited by relatively low yields and the risk of defect formation from overpotential exposure.¹⁸² These methods are summarized in Table 3, which compares key parameters including scalability, termination control, industrial suitability, and limitations.

As MXene synthesis scales toward industrial production, reducing structural defects and chemical impurities becomes vital for preserving material performance and enabling application-specific functionality.¹³³ Several complementary strategies have been proposed to mitigate these challenges throughout the synthesis workflow. Continuous-flow etching systems offer more homogeneous reaction environments than static batch processing, ensuring consistent exposure of MAX phases to etchants and minimizing local concentration gradients that can induce uneven etching.¹⁸⁵ This leads to improved uniformity in layer thickness and flake size.^{133,185} Additionally, precursor engineering, such as stoichiometric optimization of MAX phases with slight excess of Ti or Al, can suppress intrinsic carbon vacancies and oxygen substitutions that degrade the final MXene quality.^{134,137} The choice of etching media significantly affects structural integrity and termination control. Mixed-acid systems, such as the commonly used 6:1:3 HCl:HF:H₂O ratio, offer safer and more reproducible etching than pure HF, reducing structural collapse and enhancing monolayer yield.¹⁸⁶ Shuck *et al.*¹⁸⁷ demonstrated that this protocol could be scaled to synthesize up to 50 g of Ti₃C₂T_x MXene per batch, while maintaining flake morphology and surface chemistry similar to those obtained in small-scale syntheses. Among the emerging approaches, soft delamination has shown significant promise.^{188,189} This method eliminates ultrasonication, shaking, or centrifugation while separating MXene sheets. Instead, the intercalated MXene mixture is left undisturbed for ~30 minutes, allowing gravity-assisted flake separation and the formation of a dark colloidal suspension. Although this method tends to yield more bi- and tri-layered flakes and is relatively slow, it produces large, low-defect flakes ideal for catalytic applications where surface integrity is critical.^{188,189}

Finally, storage and environmental stability must be considered, as freshly synthesized MXenes are highly susceptible to oxidation and hydrolysis when exposed to air or moisture. Best practices include storing MXenes under inert atmospheres (e.g., Ar or N₂), applying freeze-drying techniques to avoid hydrolysis, or using protective encapsulation (e.g., polymer or carbon coatings) to retain surface activity before electrochemical

deployment.^{190,191} Collectively, these defect-mitigation strategies, spanning reactor design, etchant optimization, purification, delamination, and post-synthesis stabilization, are critical for producing high-quality, scalable MXenes suitable for the industrial CO₂RR and other energy applications.

3.2. MXene properties

MXenes possess a unique combination of physicochemical properties, making them promising materials for the CO₂RR. Their compositional diversity, derived from various transition metals (M), carbon or nitrogen X layers, and surface terminations, grants them exceptional tunability of electronic structure,¹⁸⁶ metallic electronic conductivity,¹⁷¹ and mechanical robustness.¹⁹² Pristine MXenes such as Ti₃C₂ are metallic, with reported conductivities as high as 24 000 S cm⁻¹,^{171,193,194} which facilitates rapid electron transfer kinetics critical for electrocatalysis.¹³² Their surface termination groups (e.g., -O, -OH, -F, and -Cl) play a central role in modulating reactivity by stabilizing key intermediates (*COOH and *HCOO) and adjusting binding energies, thereby influencing product selectivity. These terminations also impart hydrophilic behavior,¹⁹⁵ enhance electrolyte accessibility, and affect mechanical properties, such as Young's modulus, which ranges from ~0.33 to 0.50 TPa depending on surface chemistry, synthesis route, and defect density.^{196,197} MXenes also demonstrate thermal stability under inert conditions (up to ≥ 500 °C)¹⁹⁸ and are structurally robust in acid electrolytes or under electrochemical cycling when surface terminations are well controlled. However, their susceptibility to oxidation and hydrolysis in ambient or aqueous environments is a well-documented challenge. Therefore, maintaining MXene stability during the CO₂RR requires appropriate synthesis methods, surface passivation, and environmental control. Several studies have explored strategies to mitigate this degradation, demonstrating long-term cycling stability and preserved morphology in a controlled environment. For example, Xie *et al.*¹⁹⁹ performed a comprehensive DFT analysis showing that Ti₂C and Ti₃C₂ MXenes retain their structural integrity and electronic conductivity during multivalent ion intercalation. Their findings suggest that MXenes can exhibit structural and electrochemical stability under conditions relevant to energy storage, provided that surface terminations and operating environments are carefully controlled. Also, Ghidui *et al.*¹⁵⁴ demonstrated long-term electrochemical stability of Ti₃C₂T_x synthesized *via* a LiF-HCl route, maintaining performance over thousands of cycles in 1 M H₂SO₄. This suggests that MXenes can exhibit high structural stability under specific aqueous electrochemical conditions. In contrast, Cao *et al.*¹⁹⁰ highlighted degradation pathways and proposed mitigation strategies including (i) defect-controlled synthesis, (ii) post-treatment (e.g., annealing or reduction), (iii) encapsulation with carbon or polymer coatings, and (iv) controlled storage under inert, low-moisture conditions. Soomro *et al.*²⁰⁰ further reported that low-temperature, deoxygenated storage extended the stability of aqueous Ti₃C₂T_x dispersions up to 60 days. Post-treatment techniques such as thermal annealing under an inert gas or chemical functionalization can be employed to remove labile terminations or introduce more stable groups, thereby improving MXene's catalytic performance. Ultimately,

the catalytic behavior of MXenes for the CO₂RR depends not only on their inherent properties but also on how they are processed and stabilized. Post-reaction and operando characterization (e.g., XPS, XRD, Raman, and XAS) will be crucial to track structural evolution and guide the rational design of durable, selective MXene-based electrocatalysts. Despite their known advantages, current understanding of MXenes in the CO₂RR remains largely based on computational studies. Experimental efforts are urgently needed to validate theoretical predictions, tune surface chemistry, enhance electrode-electrolyte interactions, and achieve long-term stability and selectivity under realistic reaction conditions.

4. Effect of surface chemistry

The surface chemistry of MXenes plays a pivotal role in governing CO₂ adsorption behavior, stabilization of key reaction intermediates, and product selectivity during electrochemical reduction. Computational investigations, especially density functional theory (DFT) studies, have demonstrated that specific surface terminations, such as -O and -OH, significantly lower the Gibbs free energy barriers for the formation of intermediates like *COOH and *HCOO, thereby favoring the production of CO and formic acid (HCOOH). In contrast, -F terminations typically exhibit weak binding with *CO₂ and *CO, leading to reduced catalytic activity but may promote *CHO intermediate formation, thereby shifting selectivity toward CH₃OH or CH₄ under specific conditions. More recently, halogen terminations (e.g., -Cl), introduced *via* molten salt or halogen etching, have been shown to alter surface charge distribution and electronic structure, potentially influencing intermediate adsorption and desorption dynamics. However, their direct influence on CO₂RR performance remains insufficiently explored and warrants further studies.

DFT calculations further indicate that CO₂ interacts with MXene surfaces *via* physisorption, driven by noncovalent interactions, or chemisorption, involving covalent bonds with surface metal sites. The computed Gibbs free energy (ΔG) for chemisorption varies substantially depending on the MXene composition, ranging from -3.19 to -1.29 eV, as summarized in Table 4. These energetic variations, combined with the electronic effects introduced by different surface terminations, underscore the importance of functional group engineering in tuning MXene-based catalyst activity and selectivity toward the targeted CO₂RR products.^{120,201} These energetic variations and the electronic effects introduced by different surface terminations underscore the critical importance of tailoring MXene functional groups to direct specific CO₂RR pathways. Table 5 compares the effects of MXene surface terminations on CO₂RR intermediates and product selectivity.

Among TM-based MXenes, Group IV (e.g., Ti₃C₂, Zr₃C₂, and Hf₃C₂) exhibits a stronger binding affinity for CO₂ compared to Group V (e.g., V₂C and Nb₂C) or VI (e.g., Mo₃C₂ and Cr₃C₂).¹²⁰ This trend can be attributed to the 'TM atoms' electronic configuration and d-band center, influencing the overlap between metal orbitals and CO₂ antibonding orbitals.^{202,211,212} For example, Mo₃C₂ and Cr₃C₂ MXenes preferentially interact



Table 4 Gibbs free energy of reaction (in eV) for CO₂RR intermediates calculated from the density functional theory²⁰²

Species/M ₃ C ₂	Group IV Ti ₃ C ₂	Group V Zr ₃ C ₂	Group VI Hf ₃ C ₂	V ₃ C ₂	Nb ₃ C ₂	Ta ₃ C ₂	Cr ₃ C ₂	Mo ₃ C ₂
*CO ₂	−0.59	0.17	0.18	0.29	0.35		0.25	0.15
**CO ₂	−3.01	−3.19	−3.05	−1.47	−1.60	−2.30	−1.29	−2.11
**OCHO	−2.04	−2.25	−2.89	−1.40	−1.71	−1.58	−1.61	−1.74
**HOCO	−2.06	−2.49	−2.79	−1.41	−1.54	−1.92	−1.74	−1.91
**OCH ₂ O	−3.51	−4.08	−4.31	−1.93	−2.22	−2.86	−1.60	−1.64
**HCOOH	−1.01	−2.19	−2.47	−0.15	−0.12	−0.32	0.01	−0.78
**CO	−1.18	−1.11	−1.54	−1.45	−1.39	−1.80	−2.00	−2.27
**HOCH ₂ O	−2.47	−2.82	−3.11	−1.59	−1.88	−2.56	−1.85	−2.15
**HOCH ₂ OH	−1.09	−1.07	−3.56	−0.61	−0.68	−1.10	−0.69	−0.90
**H ₂ CO	−2.43	−3.21	−3.31	−1.81	−2.16	−2.39	−1.78	−1.86
**C ₂ OH	−1.58	−2.05	−1.89	−1.26	−1.36	−1.94	−1.51	−1.64
**CH ₃ O	−2.93	−3.12	−3.33	−2.20	−2.36	−2.98	−2.12	−2.53
**CH ₂	−1.81	−1.88	−1.21	−0.97	−1.47	−2.33	−1.65	−2.11
**CH ₃ OH	0.06	0.07	0.01	0.33	0.08	0.22	0.33	0.17
**O	−4.80	−5.24	−5.23	−3.45	−3.95	−4.27	−3.53	−3.57
**CH ₃	−2.04	−2.37	−2.86	−2.26	−2.47	−3.27	−2.52	−2.98
**OH	−4.59	−4.65	−4.80	−3.70	−3.90	−4.35	−3.73	−3.91
**CH ₄	−1.18	−0.70	−0.94	−2.15	−0.77	−0.82	−0.55	−0.70
**H ₂ O	−3.03	−2.96	−3.04	−2.46	−2.37	−2.64	−2.55	−2.88

with CO₂ over H₂O, making them highly promising for the CO₂RR in aqueous environments. The mechanistic pathway for CH₄ formation on Mo₃C₂ involves successive hydrogenation steps of intermediates, such as OCHO*, *OCH₂O*, and HOCH₂O*, yielding CH₃O* and CH₄ as products (Fig. 9A). The DFT calculations suggest that CH₃O* is thermodynamically favored over H₂COH* during the fifth H⁺/e[−] addition, directing the reaction away from CH₃OH and toward CH₄ formation.

Moreover, M₂C MXenes, such as V₂C and Cr₂C, have demonstrated potential for HCOOH production, as evidenced by a volcano-type relationship between the adsorption strength and catalytic activity (Fig. 9B). This relationship suggests that intermediate adsorption strengths facilitate efficient CO₂-to-HCOOH conversion. Excessively strong adsorption impedes intermediate desorption, whereas weak adsorption hinders activation, demonstrating the critical role of adsorption energy in catalytic performance.^{121,214–216}

The surface functionalization of MXenes significantly enhances their catalytic performance by modifying electronic properties, adsorption energies, and reaction pathways.^{217,218} Oxygen-terminated MXenes (e.g., Ti₂CO₂ and V₂CO₂) are effective for the CO₂RR because the pathway to *HCOOH is preferred over the *CO pathway due to the stabilizing effect of −O groups on reaction intermediates (Fig. 9C).²¹¹ Oxygen vacancies, forming during the reaction, further improve selectivity by

stabilizing transition states and creating active sites for intermediate binding. For instance, O-terminated MXenes have been reported to preferentially catalyze CO₂ to HCOOH with reduced overpotentials, applying the accessibility of H-coordinated mechanisms over C-coordinated pathways.²¹⁹ In addition, Sc₂C(OH)₂ and Y₂C(OH)₂ are promising candidates for CH₄ production due to the reactive H atom in the −OH group. This reactive H atom facilitates stable intermediate formation, lowering overpotentials and enhancing selectivity for CH₄ formation.²⁰⁵ Fluoride-containing terminations influence product pathways differently. Furthermore, Ti₃C₂ MXenes with −F terminations tend to favor a path involving formaldehyde intermediates, forming CH₃OH. In contrast, −F-free MXenes follow a distinct mechanism, producing HCOOH and methylene glycol, decomposing into CH₃OH and water.²²⁰

Sun *et al.*²¹³ used DFT to evaluate the activity and selectivity of a dual-atom-modified MXene catalyst for the CO₂RR to C₂H₆O. They demonstrated that the Co–Co dual-atom catalyst, with its asymmetric C–C coupling mechanism, achieves high catalytic activity due to its moderate d-band center, optimally balancing electron occupancy in antibonding orbitals, ensuring efficient adsorption of reaction intermediates. The d-band analysis revealed that vanadium (V)–V and chromium (Cr)–Cr dual-atom catalysts, characterized by higher d-band centers, exhibit stronger adsorption of intermediates (*CH₃CH₂O and

Table 5 Effects of MXene surface terminations on CO₂RR pathways and intermediates

Termination	Representative MXenes	Key intermediaries	Favored product(s)	Mechanistic insight
−O ^{203,204}	Ti ₃ C ₂ O ₂ , Ti ₂ CO ₂	*COOH, *HCOO	CO, HCOOH	Strong binding of O-bound species; promotes proton-coupled electron transfer
−OH ^{120,205,206}	Ti ₃ C ₂ (OH) ₂	*COOH	CO	Increases local proton availability; improves surface hydrophilicity
−F ^{207–210}	Ti ₃ C ₂ F _x	*CHO, weak *CO ₂	CH ₃ OH, CH ₄ (low rate)	Weakens CO ₂ adsorption; shifts path to *CHO; often lowers activity
−Cl ²⁰⁹	Ti ₃ C ₂ Cl ₂	Not fully studied; charge effects	(under study)	Alters electronic distribution; stabilizes some adsorbates; promising but immature



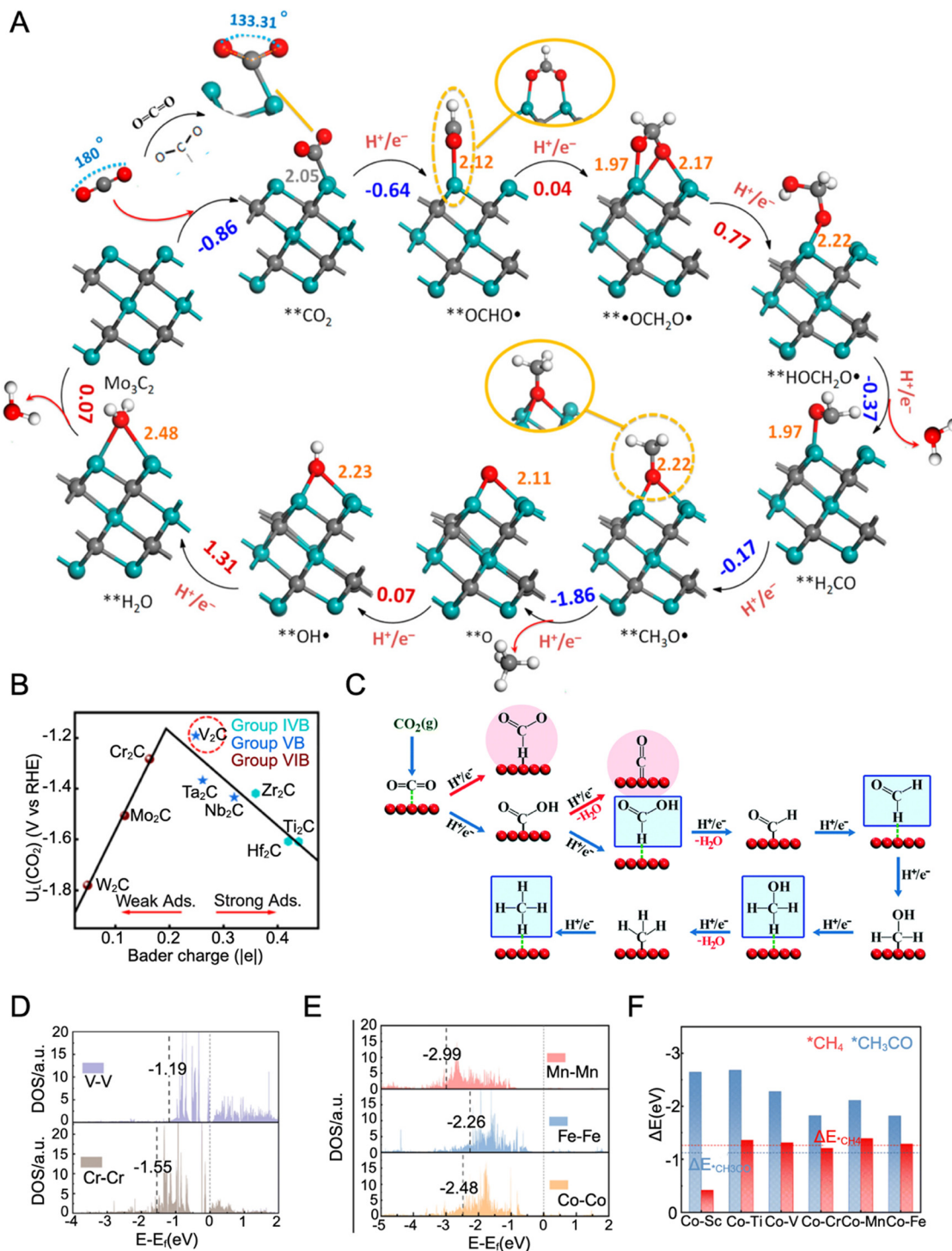


Fig. 9 (A) CO₂ conversion mechanism into $^{*}\text{CH}_4$ and $^{*}\text{H}_2\text{O}$ catalyzed by Mo₃C₂ (Reprinted with permission from ACS Nano 2017, 11, 11, 10825–10833. Copyright [2017] American Chemical Society). (B) Volcano-type relationship between U_L and the Bader charge of $^{*}\text{HCOOH}$ on M₂C (Reprinted with permission from Ind. Eng. Chem. Res. 2023, 62, 48, 20716–20726. Copyright [2023] American Chemical Society). (C) Reaction mechanism of electrochemical reduction of CO₂ on O-terminated MXenes (Reproduced from ref. 211 with permission from Royal Society of Chemistry. Copyright [2022]). (D) and (E) Density of states (DOS) corresponding to d-orbitals of the adsorbed dual-atom, where the d-band center is denoted by dashed lines. (F) Adsorption energy of $^{*}\text{CH}_3\text{CO}$ and $^{*}\text{CH}_4$ intermediates on dual-atom catalysts/Ti₂CO₂. (D)–(F) Reproduced from ref. 213 with permission from Royal Society of Chemistry, Copyright [2025]).

$^{*}\text{CH}_2\text{OHCH}_2\text{O}$), making hydrogenation steps energetically demanding, with energy barriers of 0.81 and 0.93 eV, respectively (Fig. 9D). In contrast, manganese (Mn)–Mn, iron (Fe)–Fe, and cobalt (Co)–Co dual-atom catalysts have d-band

Table 6 Summary of CO₂RR results using MXene-based electrocatalysts

Electrocatalyst	Potential	Current density (mA/cm ²)	Electrolyte	Faradaic efficiency (%)	Prod.	Ref.
Pd-MXene	0.5 V	17	CO ₂ -saturated 1.0 M KHCO ₃	67.8	CH ₃ OH	122
SA-Cu-MXene	−1.4 V <i>vs.</i> RHE	−21.3	0.1 M KHCO ₃	59.1	CH ₃ OH	106
CdS/Ti ₃ C ₂	−1.0 V _{RHE}	~6.4	0.1 M KHCO ₃	94	CO	222
VS-CdS/Ti ₃ C ₂	−1.0 V _{RHE}	~−6	0.1 M KHCO ₃	96	CO	
M _x O _y /MAX hybrid	−0.4 to −0.6 V	2.4	0.5 M NaHCO ₃	67	CO	223
Ag-ZnO/Ti ₃ C ₂ T _x	−0.87 V _{RHE}	22.5	0.5 M KHCO ₃	98	CO	224
d-Ti ₃ C ₂ T _x	−2.2 V <i>vs.</i> SCE	−1.5	Acetonitrile, 1 ethyl-3 methylimidazolium tetrafluoroborate EMIMBF ₄	65	CO	108
d-Mo ₂ CT _x	−2.2 V <i>vs.</i> SCE	−2.5	Acetonitrile, 1 ethyl-3 methylimidazolium tetrafluoroborate EMIMBF ₄	90	CO	108
Cu-Pd/MXene	−2.8 V	150	0.1 m KHCO ₃	93	Formate	127
SnO ₂ /MXene	1.1 V	−57.8	CO ₂ -saturated 0.1 M KHCO ₃	94	Formate	121
ZnO-Fe-MXene	1.0 V	18.745	0.5 M NaOH	—	Formate	225
Cu-/Ti ₃ C ₂ T _x	−1.5 V <i>vs.</i> Ag/AgCl	−1.08	0.1 M NaHCO ₃	58.1	HCOOH	76
MXene (Ti ₃ C ₂ T _x) modified with boron-doped diamond	−1.3 V <i>vs.</i> Ag/AgCl		0.5 M KOH	97	HCOOH	226

centers positioned farther from the Fermi level (Fig. 9E), allowing antibonding orbitals to be more readily occupied by electrons. This positioning weakens the adsorption of intermediates (Fig. 9F), facilitating smoother reaction pathways without excessive energy barriers and increasing chemical reactivity.²²¹

Table 6 presents innovative MXene-based electrocatalysts, their electrocatalytic activities, working electrolytes, performance, and CO₂RR products, further driving innovation in MXene-based electrocatalysts toward the CO₂RR.

5. Structural engineering

MXene-based catalysts are emerging as promising electrocatalysts for the CO₂RR due to their excellent electronic conductivity, large surface area, tunable surface chemistries, and structural robustness.^{227,228} Their surface termination groups can effectively stabilize critical reaction intermediates, facilitating efficient proton-coupled electron transfers essential for CO₂ activation and subsequent reduction pathways. Despite these beneficial properties, the presence of specific surface functionalities, particularly hydrogen-affinity groups (such as −OH or −F), can unintentionally promote the competing hydrogen evolution reaction.^{229,230} Specifically, the high density of reactive sites and negatively charged surfaces of MXenes can readily adsorb protons from aqueous electrolytes, thereby enhancing HER activity.²³¹ This unintended promotion of the HER poses a significant challenge by diverting electrons and protons from CO₂ reduction, thereby reducing selectivity toward valuable carbon products. To address this intrinsic limitation, various structural engineering approaches have been developed. These strategies include controlled surface termination modification, defect and vacancy engineering, single-atom or heteroatom doping, formation of MXene-based heterostructures, and hybrid composite catalysts. These engineering methods are crucial to selectively suppress HER activity while enhancing MXene-based catalysts' performance and selectivity toward desired CO₂RR products.^{127,128,232–234}

5.1. Surface termination engineering

The catalytic selectivity of MXenes toward the CO₂RR strongly depends on surface termination groups (*e.g.*, −O, −OH, −F, and −Cl).²³⁵ Table 5 compares the effects of MXene surface terminations on CO₂RR intermediates and product selectivity. For instance, oxygen-terminated MXenes (−O) strongly stabilize key reaction intermediates such as *COOH and *HCOO, reducing the energy barriers for CO₂ conversion reactions and selectively suppressing the HER.²⁰⁷ Computational studies conducted by Albertus *et al.*²³⁶ demonstrated that oxygen terminations on Ti and Mo-based MXenes significantly enhance CO₂ adsorption and intermediate stabilization, promoting selective CO₂RR towards formic acid.²⁰⁹ In contrast, MXenes with abundant fluorine (−F) terminations generally exhibit weaker CO₂ adsorption and lower selectivity for carbon-based products due to increased HER activity. Meng *et al.* explicitly found that fluorinated Ti₃C₂ MXenes exhibit a higher HER overpotential (~0.58 V), indicating their stronger proton affinity and subsequent HER promotion. Additionally, recent studies have explored halogen-terminated MXenes (*e.g.*, −Cl, −Br, and −I), synthesized *via* molten salt or halogen etching methods, that offer potential avenues to adjust the electronic structure of MXenes and weaken proton adsorption, which may reduce HER activity.²³⁷ However, comprehensive experimental validation of HER suppression in halogen-terminated MXenes remains limited and warrants further investigation.

5.2. Defect engineering and heteroatom doping

Engineering defects and doping MXenes with heteroatoms have proven effective strategies for improving CO₂RR selectivity and suppressing the HER by altering electronic structures, modifying intermediate adsorption energies, and enhancing active-site densities.^{238–241} Introducing controlled oxygen vacancies, metal vacancies, or edge defects can significantly boost MXene catalytic performance by selectively stabilizing CO₂-derived intermediates. For example, Qian *et al.*³⁴ employed DFT to investigate dual-oxygen vacancies in Mo₂TiC₂O₂ MXenes, revealing enhanced catalytic activity and C–C coupling due to enriched



adsorption of reaction intermediates. Furthermore, heteroatom doping (such as N, P, S, or transition metals) provides another powerful route to tune MXene catalytic properties. Three distinct doping strategies have been identified: The lattice substitution, functional substitution, and surface adsorption. Lattice substitution involves replacing atoms in MXene lattices to alter their electronic structures significantly.²⁴² Functional substitution adjusts surface-functional groups to improve catalytic selectivity. Surface adsorption involves anchoring active dopants on MXene surfaces, stabilizing CO₂RR intermediates, and selectively inhibiting the HER. For instance, nitrogen-doped MXenes exhibited enhanced electronic modulation, reducing HER selectivity and promoting carbon-based products such as CO and formic acid.²⁴³

5.3. Hybrids and heterostructures

Forming MXene-based heterostructures or hybrids by integrating MXenes with other 2D materials or active components effectively combines their intrinsic properties, mitigates individual limitations, and significantly enhances CO₂RR selectivity and HER suppression.²⁴⁴ Heterostructure formation typically involves the *in situ* growth of complementary 2D materials onto MXene surfaces, facilitated by electrostatic interactions or covalent bonding.^{245,246}

Liu *et al.*²⁴⁷ demonstrated the synthesis of MXene/metal-organic framework (MOF) heterostructures through electrostatic attraction, where the surface terminations of the Ti₃C₂T_x MXene strongly interacted with MOF precursors, forming well-integrated composites that effectively enhanced CO₂ adsorption and catalytic selectivity. Similarly, a covalent organic framework (COF)-Ti₃C₂ heterostructure achieved >90% CO selectivity at −0.6 V vs. RHE due to the synergistic effect of the MXene's large exposed surface area and the COF's catalytic functionalities, substantially suppressing the HER.²⁴⁸ This significant performance was primarily attributed to the large, exposed surface of the MXene, which effectively disperses the COF, endows the heterojunction with more active sites, and facilitates efficient transport channels. The 3D MXene/graphene oxide/perylenediimide aerogel heterostructure was synthesized *via* impregnation and freeze-drying for the photocatalytic CO₂RR.²³³ The resulting heterostructure featured a large surface area, an enhanced photogenerated carrier, and an electron transfer network facilitated by π - π stacking *via* electrostatic attraction. This structural configuration, interconnecting the faces of the heterostructure, promotes the efficient transfer of photogenerated electron-hole pairs, enabling rapid carrier movement and separation. Additionally, perylenediimide functions as an electron donor, activating catalytic sites for enhanced photocatalytic CO₂RR.

5.4. Single-atom catalysts

The size of metal particles in metal-based heterogeneous catalysis is intricately linked to catalytic activity.²⁴⁹ Catalytic activity increases as the size of metal nanoparticles decreases until they reach an optimal size. Understanding this fundamental concept has played a significant role in advancing SACs,

which display high catalytic activity and maximize metal utilization due to the significantly larger surface area and quantum size effects of metal nanoparticles compared to their bulk counterparts.^{250–252} Based on this well-established principle, extensive studies have demonstrated that controlling the structure and size of metal nanoparticles at the atomic level maximizes metal utilization and enhances electrocatalytic performance.²⁵³ The choice of support material for dispersing single metal atoms plays a crucial role in determining the activity and stability of single atoms under reaction conditions. Therefore, strong metal-support interactions are essential for maintaining catalyst performance.²⁵⁴

Computational and experimental studies have highlighted the potential of MXenes as promising support materials for facilitating strong metal-support interactions in CO₂RR catalysts. The abundant surface-functional groups and metal vacancy defects in MXenes serve as ideal anchoring sites for single metal atoms, primarily due to the high surface energy, adjustable electronic structure, and uniform atomic arrangement of MXenes.^{214,255–257} The synthesis of MXene-based SACs can be achieved using three strategies: surface adsorption, metal vacancy anchoring, and anchoring at surface-functional group vacancies.²⁵⁸ According to a computational study, the adsorption of single metal atoms is possible on the top, hollow (hcp and fcc), and bridge sites.

Chen *et al.*²⁵⁹ employed electrostatic adsorption and *in situ* reduction to synthesize a Co-Ti₃C₂T_x SAC for photocatalytic CO₂ reduction. Co-cations are initially adsorbed onto the negatively charged functional groups on the MXene surface during synthesis, forming ionic bonds facilitated by electrostatic attraction. The ionic bond formation is followed by reducing Co cations on the MXene, leading to covalent bonds between the metal atoms and surface-functional groups (−F and −O). Sodium borohydride was employed as a reducing agent for Co²⁺ ions and as an oxidation inhibitor of MXenes to overcome its fast oxidation.

Zhou *et al.*²⁴⁸ designed and synthesized the MXene@Por-COF-Co heterostructure. The dispersed COF structures and exposed MXene nanosheets offer more accessible reactive sites and quicker ion transfer channels to the heterostructure because the covalent interactions between the aldehyde groups in the COF structures and the amino groups of MXene can facilitate the *in situ* formation of COFs on the surface of amino-functionalized MXene nanosheets. TEM images of MXene@Por-COF-Co-7 reveal a homogeneous distribution of COF nanosheets across the surface of the MXene nanosheets. Furthermore, MXene@Por-COF-Co-7 exhibits a remarkable CO FE of 97.28% at −0.6 V, significantly higher than that of Por-COF-Co (0%) at the same potential. In addition, MXene@Por-COF-Co-7 also maintains a high FE in the potential range of −0.5 to −1 V vs. RHE, suggesting its good selectivity for CO formation. The bias current density of CO increased with a rise in voltage.

Zhao *et al.*²⁶⁰ employed self-reduction stabilization to anchor platinum (Pt) single atoms onto Ti vacancies of Ti₃C₂ for CO₂ activation with amines and silane, producing formamides. The single Pt atoms on the Ti_{3−x}C₂T_y support exhibited



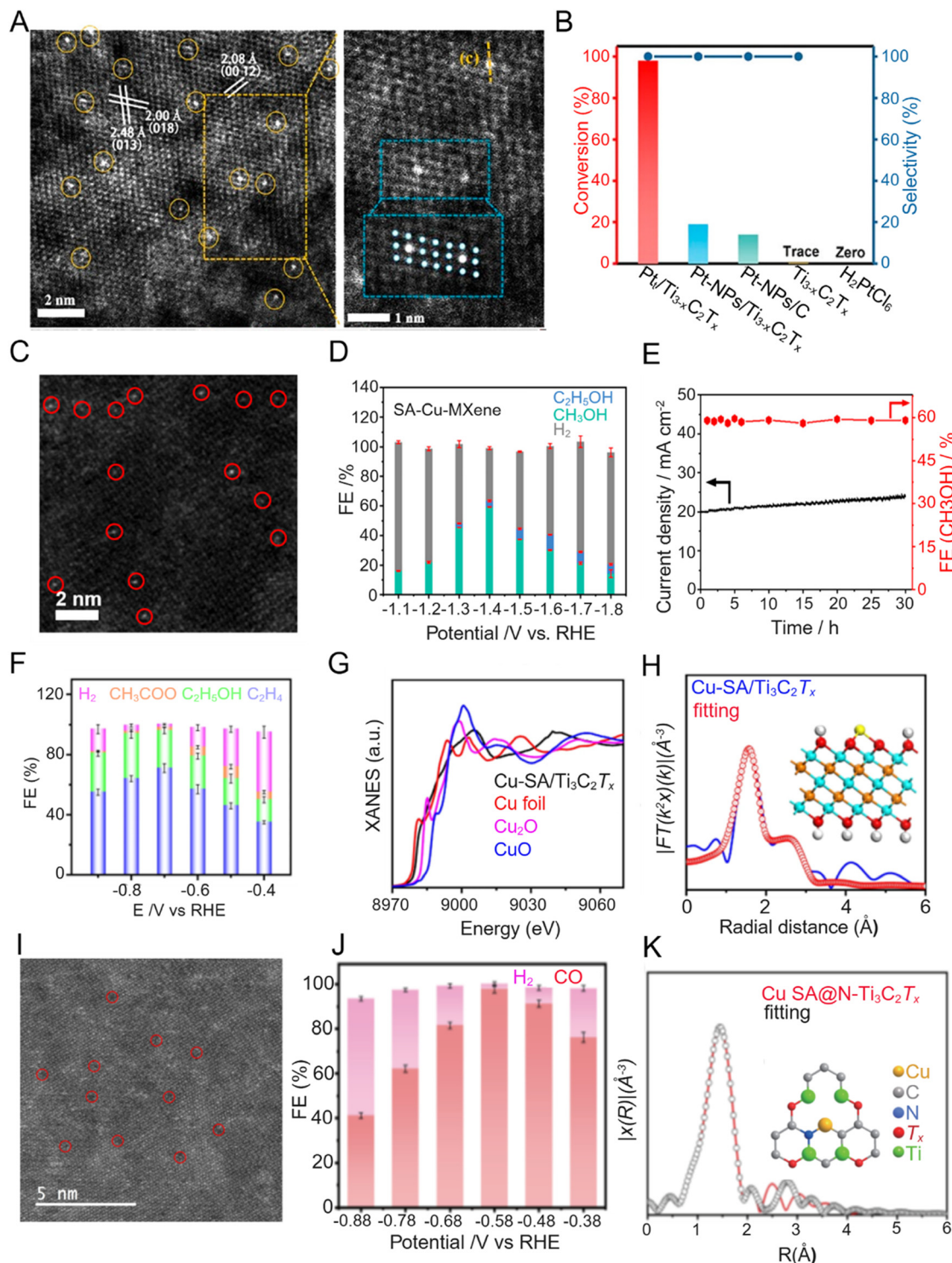


Fig. 10 (A) High-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) image of Pt/Ti_{3-x}C₂T_x. (B) Catalytic performance of catalyst systems. (A) and (B) Reprinted with permission from *J. Am. Chem. Soc.* 2019, 141, 9, 4086–4093. Copyright [2019] American Chemical Society. (C) Aberration-corrected (AC) HAADF-STEM image of the SA-Cu-MXene. (D) Faradaic efficiency (FE) of product formation on the SA-Cu-MXene. (E) Current stability and corresponding FE for CH₃OH formation on the SA-Cu-MXene. (C)–(E) Reprinted with permission from *ACS Nano* 2021, 15, 3, 4927–4936. Copyright [2021] American Chemical Society. (F) FE of Cu-SA-Ti₃C₂T_x. (G) X-ray absorption near-edge structure spectra at the Cu K-edge with CuO, Cu₂O, and Cu foil as a reference. (H) Extended X-ray absorption fine structure (EXAFS) fitting curve of Cu-SA/Ti₃C₂T_x; inset illustrates the Cu-SA-Ti₃C₂T_x structure. Yellow, blue, dark yellow, red, and white balls represent Cu, Ti, C, O, and H, respectively. (F)–(H) Reproduced from ref. 261 with permission from Springer Nature, Copyright [2021]. (I) AC HAADF-STEM of Ti₃C₂T_x demonstrating Ti vacancies.²⁶² (J) Potential-dependent FE of H₂ and CO on Cu SA@N-Ti₃C₂T_x at applied potentials. (K) EXAFS fitting of Cu SA@N-Ti₃C₂T_x; inset presents the atomic interface structure model. (I)–(K) Reproduced from ref. 262 with permission from Springer Nature, Copyright [2024].

partial positive charges and atomic dispersion. Adsorbing and reducing Pt^{4+} simultaneously were successful without adding a reductant. Moreover, HAADF imaging revealed that the Pt single atoms were anchored at the Ti site in Ti_3C_2 rather than at the lattice gap (Fig. 10A). These Ti vacancies strongly correlate with the etching conditions during MXene synthesis, especially the etchant. Fig. 10B reveals that $\text{Pt}_1/\text{Ti}_{3-x}\text{C}_2\text{T}_x$ SAC displayed superior catalytic performance for converting CO_2 compared to that of Pt nanoparticles (NPs).

Zhao *et al.*¹⁰⁶ developed single-atom Cu loaded on MXene layers by selectively etching Al layers from quaternary MAX phases $[\text{Ti}_3(\text{Al}_{1-x}\text{Cu}_x)\text{C}_2]$ for CH_3OH synthesis, applying easy sublimation of AlCl_3 and leaving unreacted Cu on the MXene. The improved selectivity for CH_3OH arises from the capacity of atomically dispersed Cu sites to impede the C–C coupling of $^*\text{CO}$, facilitating the formation of CH_3OH (Fig. 10C). This coordination lowers the energy barrier for converting HCOOH^* into an absorbed CHO^* intermediate, enhancing electrocatalytic activity for CO_2 conversion. The SA-Cu-MXene catalyst exhibited an increased FE of 59.1% for CH_3OH production with high stability and a low energy barrier for the rate-determining step (HCOOH^* to CHO^* ; Fig. 10D and E).

Bao *et al.*²⁶¹ synthesized a Cu SAC anchored on $\text{Ti}_3\text{C}_2\text{T}_x$ nanosheets *via* chemical reduction, followed by freeze-drying. The resulting Cu-NP/ $\text{Ti}_3\text{C}_2\text{T}_x$ SAC reduced CO well, achieving over 98% selectivity toward C_{2+} products with a high C_2H_4 selectivity of 71% (Fig. 10F). The catalyst promotes the formation of the $^*\text{CO}$ – CHO intermediate, facilitating C–C coupling. The XANES analysis revealed that the Cu valence state in the Cu-NP/ $\text{Ti}_3\text{C}_2\text{T}_x$ SAC lies between that of metallic Cu and Cu^+ , indicating the presence of O coordination and formation of Cu–O₃ species (Fig. 10G and H).

Similarly, Liu *et al.*²⁶² reported a monoatomic Cu catalyst featuring Cu–N₁C₁ coordination anchored on the N-doped $\text{Ti}_3\text{C}_2\text{T}_x$ MXene for the efficient CO_2 reduction to CO. This catalyst achieved over 97% selectivity toward CO at an applied potential of -0.58 V *vs.* RHE (Fig. 10J). The excellent performance was attributed to a potential-dependent valence transition of the Cu species. Aberration-corrected HAADF imaging indicated a high density of Ti vacancies in the MXene lattice, serving as preferential anchoring sites for immobilizing isolated Cu atoms (Fig. 10I). The XANES analysis revealed a negative shift in the Cu absorption edge relative to the pristine $\text{Ti}_3\text{C}_2\text{T}_x$, which is indicative of strong electronic interactions between Cu single atoms and the MXene support (Fig. 10K).

In developing SACs, a primary consideration is their stability because several factors, such as decomposition, dissolution, and atom migration, can promote cluster formation and morphological degradation. The high surface energy and mobility of isolated atoms drive these transformations.²⁶³ Instability of SACs often results in diminished current density and FE.^{264,265} Although many studies on MXene-based SACs for the CO_2RR have emphasized activity and selectivity, the stability of the single atoms under reaction conditions remains underexplored.

Future investigations should prioritize evaluating catalyst stability by conducting detailed post-reaction analyses. Such

efforts could provide crucial insight into the structural and chemical evolution of catalysts, facilitating the rational design of MXene–single-atom interactions for enhanced catalytic activity, durability, and selectivity.

DFT has been pivotal in advancing 2D material-based electrocatalysis by predicting performance under several atomic configurations.^{82,266,267} This theory has been critical in developing SAC-supported 2D material-based electrocatalysts. Numerous studies have employed the DFT to design SAC-MXene-based catalysts for the CO_2RR . For instance, Li *et al.*²⁵⁸ demonstrated the high catalytic activity of single-atom scandium (Sc), Ti, and V-supported Ti_2CN_2 to produce CO with a low overpotential of 0.37, 0.27, and 0.23 eV, respectively. In contrast, Mn and Fe supported on Ti_2CN_2 primarily produce HCOOH with a low overpotential of 0.32 and 0.43 eV. The high catalytic activity of single atoms on Ti_2CN_2 can be attributed to N-functionalization, stabilizing SACs effectively by anchoring TM atoms. This functionalization also lowers the energy barrier for CO_2 reduction and improves catalytic selectivity. These SACs on Ti_2CN_2 exhibit high catalytic activity with much lower overpotentials.

Similarly, Athawale *et al.*²³⁴ explored the feasibility of MXenes serving as an anchoring site for isolating TM SACs for the CO_2RR . Several SAC systems containing 3d (Sc, Ti, V, Cr, and Mn), 4d (yttrium [Y], zirconium [Zr], niobium [Nb], and Mo), and 5d (hafnium [Hf]) transition metals, supported on an O-terminated MXene ($\text{TM}@\text{Ti}_2\text{CO}_2$), were designed using DFT calculations. The findings indicate that TMs anchored on top of the C atom of Ti_2CO_2 (hollow-C site) present the most stable configuration. The hollow-C site, primarily for Nb, Mo, Zr, V, Cr, and Ti atoms, exhibits the most negative E_b values, indicating higher stability and better suitability for the CO_2RR .

5.5. MXene–metal/metal-oxide hybrids

Metal and metal oxide (MMO) catalysts have demonstrated notable potential in the CO_2RR ; however, their application is often limited by intrinsic drawbacks such as low electrical conductivity, poor long-term stability, and limited product selectivity.^{268–270} To overcome these challenges, use of hybrid electrocatalysts that integrate MMOs with conductive and chemically tunable materials, such as MXenes, have emerged as an effective strategy.^{271–273} MXenes offer high electrical conductivity, a two-dimensional architecture, and versatile surface terminations, collectively making them ideal supports for enhancing the performance of MMO-based systems. The integration of MMOs with MXenes generates synergistic interfacial interactions that modulate the electronic structure of active sites, improve charge transport, and promote favorable binding of CO_2RR intermediates. Specifically, the surface terminations of MXenes (*e.g.*, $-\text{O}$, $-\text{OH}$, and $-\text{F}$) can attract metal cations from the MMO phase and facilitate oxygen vacancy formation at the interface, enhancing catalytic activity and electron transfer efficiency.^{224,234,274} These vacancies serve as additional active sites and improve the adsorption and activation of CO_2 molecules. For example, Wu *et al.*²³² developed an $\text{Fe}_2\text{O}_3@\text{MXene}$ hybrid photocatalyst in which the introduction of $\text{Ti}_3\text{C}_2\text{T}_x$ increased oxygen vacancy concentration and formed Fe–O–Ti



bonds at the interface. These interfacial sites enhanced *COOH intermediate formation and improved CO production. Although this system was used for photocatalytic CO₂ reduction, the findings highlighted the general importance of MXene–MMO synergy, which is also transferable to electrocatalytic applications.^{41,232,275}

In the electrocatalytic domain, Liu *et al.*²⁷⁶ reported a hybrid composed of TiO₂ and SnO₂ nanowires self-assembled onto the Ti₃C₂ MXene *via* van der Waals interactions. The MXene suppressed MMO aggregation provided efficient electron

pathways and improved structural integrity. This integration enhanced CO₂ adsorption and activation, significantly improving CO₂RR activity.²⁷⁷

Hao *et al.*²²⁴ fabricated an Ag–ZnO/Ti₃C₂T_x hybrid catalyst *via* a cation exchange and self-assembly method—the MXene-regulated interface featured undercoordinated sites and mesoporous nanostructures. The catalyst achieved nearly 100% CO FE and a partial current density of 22.59 mA cm^{−2} at −0.87 V vs. RHE (Fig. 11A). DFT calculations confirmed that MXene addition shifted the d-band center, enhanced *COOH binding, and

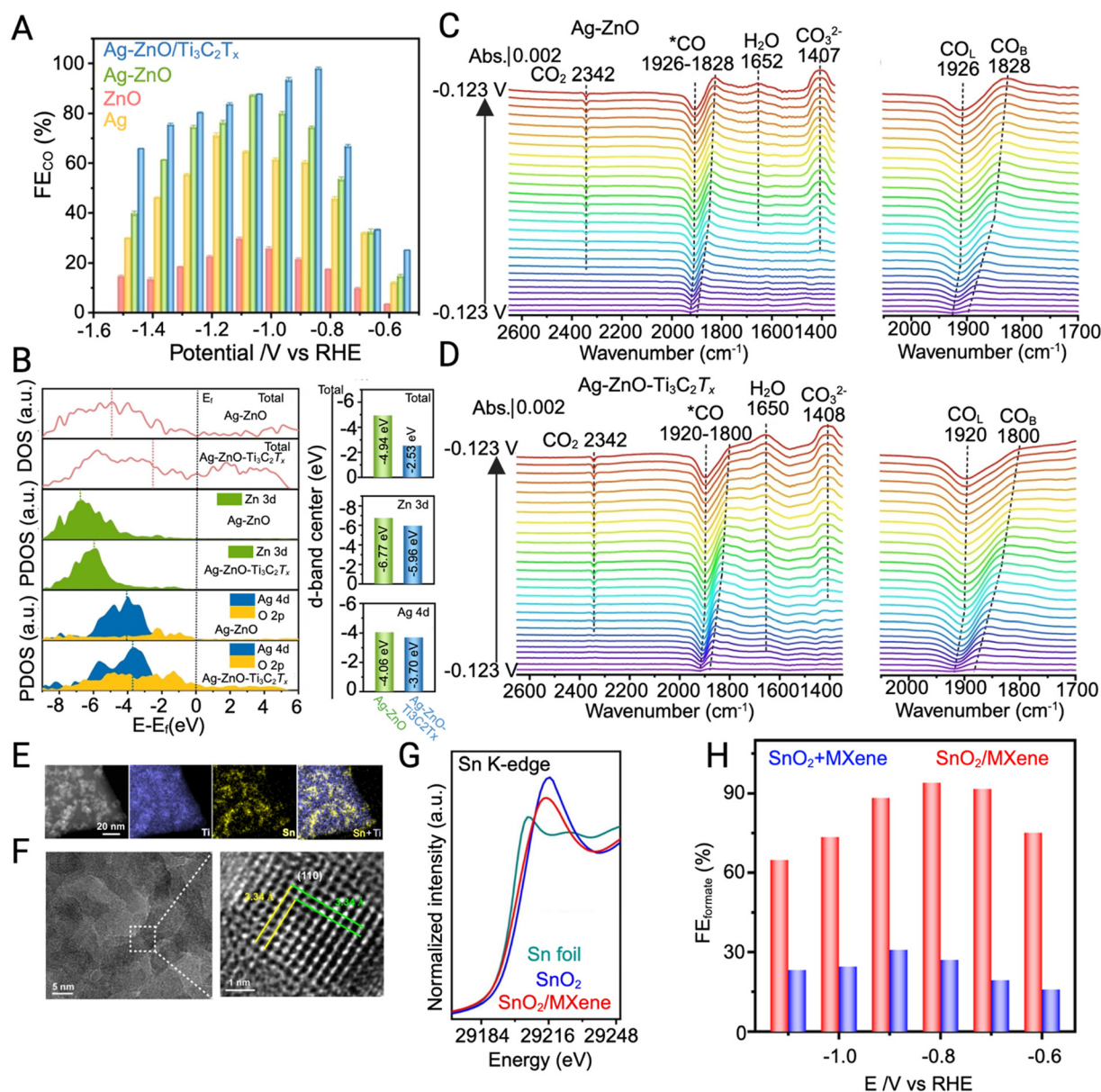


Fig. 11 (A) Faradaic efficiency (FE) of CO on Ag–ZnO–Ti₃C₂T_x. (B) Density of states (DOS) for Zn 3d, Ag 4d, and O 2p orbitals of Ag–ZnO and Ag–ZnO/Ti₃C₂T_x (left pane) and the corresponding d-band center (right pane). (C) and (D) *In situ* attenuated total reflectance infrared spectra while stepping the potential from −0.123 to −1.423 V on (C) Ag–ZnO and (D) Ag–ZnO/Ti₃C₂T_x. (A)–(D) Reproduced from ref. 224 with permission from Wiley and Sons, Copyright [2023]. (E) Low-magnification high-angle annular dark-field scanning transmission electron microscopy image and corresponding electron-dispersive spectroscopy element maps of SnO₂/MXene. (F) High-resolution transmission electron microscopy image and lattice plane. (G) Sn K-edge X-ray absorption near-edge structure spectra of the SnO₂/MXene catalyst, Sn foil, and SnO₂ references. (H) Potential-dependent FE of formate. (E)–(H) Reproduced from ref. 121 with permission from PNAS, Copyright [2022].

lowered the energy barrier for intermediate formation (Fig. 11B). *In situ* attenuated total reflectance infrared spectroscopy offered valuable insight into the reaction intermediates, elucidating the origin of CO selectivity (Fig. 11C and D). Within the applied potential window of -0.123 to -1.423 V, the attenuated total reflectance infrared spectra revealed characteristic signals corresponding to CO_2 , CO_3^{2-} , and adsorbed $^*\text{CO}$ species. The $^*\text{CO}$ bands exhibited a bipolar profile, indicative of Fano line shape modulation. For the $\text{Ag-ZnO}/\text{Ti}_3\text{C}_2\text{T}_x$ catalyst, the inverted band observed at 1920 cm^{-1} was attributed to linearly bonded CO (CO_L), whereas the positive band at 1800 cm^{-1} was assigned to bridge-bonded CO (CO_B). These observations suggest that forming $^*\text{CO}$ intermediates from CO_2 is more favorable on $\text{Ag-ZnO}/\text{Ti}_3\text{C}_2\text{T}_x$ than on Ag-ZnO . DFT revealed that adding the MXene facilitated stronger binding abilities of $^*\text{COOH}$ compared to Ag-ZnO . Moreover, the MXene regulated the Ag-ZnO interface by reducing the electron filling of anti-binding sites and optimizing the electronic structure by lowering the formation energy barrier of the intermediate.

Similarly, Cao *et al.*²³² reported a $\text{ZnO}/\text{N-Ti}_3\text{C}_2\text{T}_x$ catalyst that achieved an FE exceeding 96% for CO production. ZnO provided the primary active sites for CO_2 conversion, while the N-doped MXene improved textural properties and conductivity, facilitating PCET. Similarly, SnO_2 quantum dots grown on ultrathin $\text{Ti}_3\text{C}_2\text{T}_x$ MXene sheets (*via* hydrothermal synthesis) delivered a 94% FE and a partial current density of 57.8 mA cm^{-2} for formate production. *In situ* XANES measurements revealed that SnO_2 was partially reduced to metallic Sn during operation, which acted as the true catalytic site. Coordination environment changes observed *via* EXAFS confirmed strong Sn-Ti interfacial coupling unique to the MXene-based hybrid (Fig. 11F-H).¹²¹ In addition, the absorption edge position of the Sn K-edge XANES spectrum of the $\text{SnO}_2/\text{MXene}$ is situated between that of metallic Sn foil (Sn^0) and SnO_2 (Sn^{4+} ; Fig. 11G). The extended X-ray absorption fine structure spectra of $\text{SnO}_2/\text{MXene}$ in the *R*-space and *K*-space differ from those of pure SnO_2 , suggesting that the local coordination environment of Sn in $\text{SnO}_2/\text{MXene}$ is unlike that in pristine SnO_2 .

In a similar study, Yu *et al.*²¹⁰ synthesized a $\text{TiO}_2/\text{Ti}_3\text{C}_2\text{T}_x$ MXene photocatalyst *via* thermal calcination. By adjusting the temperature (350 – 650°C), TiO_2 nanoparticle loading was modulated, influencing CH_4 production. Though photocatalysis, this system again underscores the broader relevance of MXene–MMO interactions across catalytic modalities.

Recently, a $\text{Cu}_2\text{O}/\text{MXene}$ 0D/2D hybrid catalyst demonstrated excellent selectivity for propane (C_3H_8) production at -1.3 V vs. RHE .²⁷⁸ The interface between Cu_2O and the MXene created cooperative binding sites; the MXene favored $^*\text{CO}$ adsorption while Cu_2O stabilized $^*\text{C}_2$ intermediates, facilitating C–C–C coupling and efficient hydrogenation to C_3 products. This hybrid highlights the unique potential of MXene–MMO heterostructures in enabling multicarbon product formation, which is rarely achieved using either component alone. These examples illustrate how electronic coupling, vacancy engineering, and interfacial coordination at the MXene–MMO boundary promote enhanced CO_2 adsorption, intermediate stabilization

(*e.g.*, $^*\text{COOH}$ and $^*\text{CHO}$), and improved selectivity. Moreover, MXenes can help suppress competing hydrogen evolution reactions due to their hydrophilicity and binding site modulation, thereby further enhancing CO_2RR selectivity. Future work should focus on understanding how the oxidation states, vacancy density, and structural morphology of MXenes and MMOs evolve under electrochemical operating conditions, and how these changes influence catalytic stability and product distribution. In particular, quantifying the role of MXenes in HER suppression and tailoring interfaces for selective multi-electron/multicarbon pathways are promising directions for designing next-generation MXene-based hybrid electrocatalysts.

6. Challenges and outlook

MXene-based electrocatalysts show exceptional promise for the electrochemical reduction of CO_2 due to their high conductivity, tunable surface chemistry, and structural versatility. Despite significant progress, several interconnected challenges must be addressed to transition these materials from fundamental research to practical, large-scale implementation. A key challenge is balancing catalytic activity, selectivity, and energy efficiency, particularly the selective formation of higher-value multicarbon products such as ethylene, ethanol, and propanol. Currently, MXenes predominantly yield simpler products like CO and formate due to limitations in intermediate stabilization and the competing HER. Future strategies involving advanced surface engineering, controlled doping, and precise defect management are essential to overcome these scaling limitations and direct reaction pathways toward desired multicarbon products.

Beyond intrinsic catalyst design, the practical implementation of MXene-based electrocatalysts is significantly influenced by reactor-level constraints inherent to industrial electrolyzer systems (as discussed in Section 2.1). Industrial electrolyzers require operation under stringent conditions, including continuous high current densities ($>200\text{ mA cm}^{-2}$), efficient heat and water management, effective control of CO_2 crossover, and stable long-term performance. Traditional laboratory-scale H-cell reactors, which dominate fundamental studies, fail to replicate these conditions due to inherent limitations such as low CO_2 solubility ($\sim 34\text{ mM}$), diffusion-controlled mass transport, large electrode spacing, and dilute electrolytes, resulting in low achievable current densities ($<100\text{ mA cm}^{-2}$). Consequently, performance metrics derived from H-cells rarely translate effectively to industrial-scale systems. These reactor designs significantly enhance CO_2 transport through direct gas-phase delivery, minimize ohmic losses, control reaction interfaces more effectively, and offer improved electrolyte management, addressing many limitations of conventional H-cell setups.

Nevertheless, a lack of standardized evaluation protocols hinders widespread adoption and advancement in the MXene-based CO_2RR . Variations in cell designs, electrode materials, electrolyte compositions, gas flow conditions, and performance metrics currently impede meaningful comparison between



studies. Establishing community-wide benchmarking guidelines and uniform testing standards will enhance performance evaluation reproducibility, transparency, and reliability.

Moreover, the catalytic performance of MXenes remains closely tied to their synthesis routes, which influence structural characteristics such as flake size, surface termination chemistry ($-O$, $-OH$, $-F$), and defect density. Oxygen-terminated MXenes have demonstrated promising catalytic properties by lowering reaction barriers and stabilizing critical reaction intermediates. However, achieving reproducible and controlled termination profiles is challenging. To address this, scalable, cost-effective, and precisely controllable synthesis methods must be developed. Additionally, defect engineering and doping offer strategic routes to optimize the catalytic properties of MXenes. Introducing oxygen vacancies or doping with heteroatoms (N, P, or transition metals) can modify the electronic structure, enhance active site densities, and tune intermediate binding energies. However, excessive defects may negatively affect structural stability and induce undesired side reactions. Therefore, careful optimization and systematic evaluation of doping strategies under realistic electrochemical conditions are necessary.

Significant gaps remain between computational predictions and experimental outcomes. Many theoretical studies utilize idealized MXene structures without realistic surface heterogeneities and defects. Experimentally synthesized MXenes typically feature mixed terminations, variable flake sizes, and structural imperfections. Future theoretical efforts should incorporate realistic structural models that account for these variations to enhance predictive accuracy, thereby more effectively guiding experimental development.

Currently, most experimental CO_2RR studies focus on $Ti_3C_2T_x$ MXenes. Exploring under-investigated MXene compositions such as Mo_2CT_x , Nb_2CT_x , and V_2CT_x could uncover unique catalytic properties, improved stability, and enhanced activity. Leveraging machine learning and high-throughput computational screening methods may accelerate the discovery of promising MXene candidates and guide targeted experimental validation.

The operational stability of MXenes under realistic electrochemical conditions remains relatively unexplored. Prolonged exposure to negative potentials, variable pH environments, and continuous gas flow can induce oxidation, structural deformation, and changes in surface termination composition. To address this, *in situ* and operando characterization techniques such as transmission electron microscopy (TEM), X-ray absorption spectroscopy (XAS), and Raman spectroscopy should be employed to monitor catalyst evolution under reaction conditions. Such insights are crucial for designing MXenes with enhanced durability and reliable long-term performance. Finally, emerging fabrication technologies, particularly additive manufacturing and 3D printing, offer novel opportunities for transitioning MXene catalysts into practical, scalable electrode architectures. Printable MXene inks, already successfully demonstrated in energy storage and electronics, could facilitate customized, high-surface-area electrode designs, enhancing

mass transport and reaction interface stability. Combining MXenes with complementary materials through advanced printing techniques further opens new possibilities for scalable integration into commercial CO_2RR systems. In summary, the successful industrial deployment of MXene-based electrocatalysts for the CO_2RR demands a comprehensive approach that integrates advanced material synthesis and surface engineering, optimized reactor design, standardized evaluation methods, and scalable fabrication techniques.

6.1. Economic viability and cost reduction

While MXenes offer significant advantages of catalytic performance, tunability, and selectivity, their current production costs remain a nontrivial challenge for commercial adoption. Laboratory-scale synthesis protocols, often involving high-purity MAX-phase precursors, hazardous etching agents (e.g., HF or LiF/HCl), and multi-step purification, contribute to relatively high per-gram costs, often ranging from 100 to 1000 USD, depending on scale and quality. However, recent advances in scalable and safer synthesis actively address this limitation. Alternative fluoride-free etching strategies, including electrochemical, alkaline, and molten-salt routes, eliminate the need for hazardous chemicals while improving yield and environmental safety. Continuous-flow production methods have demonstrated multi-gram scale fabrication with excellent reproducibility and are being increasingly optimized for cost-effectiveness. For example, Anasori *et al.*⁴¹ conducted a life-cycle analysis demonstrating reduced environmental and financial costs when replacing HF-based synthesis with alternative etching processes. Another critical factor in cost reduction lies in material efficiency. Due to their high intrinsic conductivity and activity, MXenes often require lower loadings to achieve catalytic performance than conventional catalysts. In hybrid systems, such as MXene-metal oxide composites or single-atom-doped MXenes, the synergy between active sites allows for minimized MXene usage while maintaining or enhancing selectivity and stability. Long-term durability further enhances economic feasibility. Stable MXene-based catalysts reduce the need for frequent replacement, lowering operational expenses over extended use cycles. Moreover, enhanced selectivity for high-value CO_2RR products, such as C_{2+} compounds, increases the overall value of the catalytic process. As interest grows, industrial integration and shared manufacturing infrastructure (e.g., with battery or supercapacitor industries) may further lower precursor costs and streamline production. Techno-economic assessments of MXene-based membrane electrode assemblies (MEAs) and gas-diffusion electrodes (GDEs) are beginning to demonstrate promising cost-performance trade-offs at the device level. Finally, it's worth mentioning that while $Ti_3C_2T_x$ MXenes currently cost approximately 20–100 USD per g, this is still considerably lower than that of noble-metal catalysts (e.g., Pt/C at ~ 156 USD per g) besides, MXenes offer additional value through superior tunability, conductivity, and durability. In conclusion, although MXenes are currently more expensive than traditional transition-metal-based electrocatalysts, ongoing innovations in synthesis, material design, and system



integration are rapidly closing the gap. With continued improvements in low-cost, scalable production methods, reduced catalyst loading requirements, and enhanced operational lifetimes, MXene-based materials are increasingly positioned as cost-effective and high-performance candidates for the industrial CO₂RR.

Conflicts of interest

There are no conflicts to declare.

Data availability

The data will be available upon request to the authors.

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