

Review

Perspectives on the status and future of sustainable CO₂ conversion processes and their implementation

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ABSTRACT

The rapid rise in atmospheric carbon dioxide (CO₂) concentrations continues to threaten global climate stability, underscoring the urgent need for scalable, economically viable, and sustainable CO₂ mitigation strategies. Among emerging solutions, CO₂ conversion technologies offer a transformative pathway by enabling the utilization of CO₂ as a renewable carbon feedstock for the production of fuels, chemicals, and materials, thereby promoting a circular carbon economy. The review begins by exploring foundational CO₂ capture and pre-treatment methods, emphasizing advanced materials, as well as integration strategies that directly couple capture with conversion processes as a gateway to improved CO₂ conversion. Recent advancements in CO₂ conversion technologies, spanning thermochemical, electrochemical, photochemical, and biological domains are then covered. The integration of CO₂ conversion systems with renewable energy and industrial infrastructures is explored through case studies and commercialization efforts, highlighting opportunities for sector-wide decarbonization. Furthermore, the increasing role of artificial intelligence (AI) and machine learning (ML) in predictive modeling, catalyst design, and process optimization, as well as the techno-economic analyses that frame the practical deployment of these technologies is also presented. Persistent challenges including energy efficiency, long-term stability, product selectivity, and regulatory constraints are critically analyzed, and emerging solutions are proposed. The review concludes by outlining future research directions, including the development of next-generation technologies and strategies to promote interdisciplinary collaboration and public-private partnerships. By synthesizing cutting-edge advancements and identifying key barriers and opportunities, this work provides a roadmap for accelerating the global deployment of CO₂ conversion technologies toward a sustainable and decarbonized future.

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1. Introduction

The relentless rise in atmospheric carbon dioxide (CO₂) concentrations due to combustion of fossil fuels, largely driven by industrial expansion and global urbanization, has triggered the most pressing environmental challenges of the 21st century: climate change, ocean acidification, ecosystem destabilization and wide-reaching socio-economic disruptions (Ramesh, 2025). According to the Intergovernmental Panel on Climate Change (IPCC), limiting global warming to below 1.5 °C above pre-industrial levels requires an ambitious 45 % reduction in CO₂ emissions by 2030 and the achievement of net-zero emissions by 2050 (Summary for Policymakers, 2022; Huang and Zhai, 2021). Failing to meet these targets risks crossing irreversible climate thresholds, with cascading consequences on global health, food security, water availability, and biodiversity. Carbon capture, utilization, and storage (CCUS) technologies have emerged as indispensable tools in global mitigation portfolios. Beyond mere sequestration, the utilization of captured CO₂ as a feedstock for the synthesis of fuels, chemicals, and functional materials presents a transformative opportunity to shift from a linear to a circular carbon economy. Converting greenhouse gases into value-added products simultaneously drives decarbonization and economic development, and aligns climate goals with industrial sustainability.

Recent decades have witnessed rapid progress across various CO₂ conversion processes. These include thermochemical processes such as catalytic hydrogenation and reforming; electrochemical CO₂ reduction (ECR) into carbon-rich fuels and chemicals; photochemical and photoelectrochemical strategies that harness solar energy; and biological pathways that leverage microbial or enzymatic systems for carbon fixation (Vega et al., 2024; Ashraf et al., 2024). Each of these approaches offers unique advantages in terms of selectivity, scalability, energy integration, and compatibility with existing infrastructure. The growing sophistication of these technologies is paralleled by improvements in catalyst design, reactor engineering, and process integration, leading to enhanced efficiencies and reduced energy demands. Multiple scholarly reviews have extensively covered individual CO₂ conversion modalities. For example, recent thermochemical reviews focus on the design of bimetallic and nanostructured catalysts for CO₂ hydrogenation and dry reforming (Ye et al.; Chaudhari et al., 2025). Electrochemical reviews emphasize the development of advanced electrode materials, mechanistic understanding of product pathways, and strategies for enhancing selectivity and stability. Biological reviews have documented breakthroughs in synthetic biology, metabolic pathway engineering, and the development of autotrophic organisms for CO₂ valorization (Onyeaka and Ekwebelem, 2023; Della Valle et al., 2024). Current studies also underscore the transformative role of artificial intelligence (AI) and machine learning (ML) in optimizing catalyst design, reaction conditions, and system-level efficiencies (Jamali et al., 2025; Wang et al., 2025). Techno-economic analyses have demonstrated promising the commercial and environmental footprint of these technologies (Zhang et al., 2025).

Despite this momentum, significant challenges persist that hinder the practical deployment of CO₂ conversion technologies at scale (Abdallah and Farrauto, 2023; Akbari et al., 2025; Zentou et al., 2025). Many existing reviews tend to be narrowly focused, offering deep dives into specific conversion pathways or catalyst types while neglecting broader integration issues such as energy sourcing, life cycle sustainability, regulatory barriers, and industrial compatibility (Beniwal et al., 2025; Chipangamate and Nwaila, 2024). Furthermore, the field is yet to comprehensively incorporate the rapid advancements in AI-driven materials discovery, which hold great promise for accelerating innovation (Bai and Zhang; Rashid and Kausik, 2024).

This review seeks to address these gaps by presenting a holistic interdisciplinary overview of the current state and future potential of CO₂ capture and conversion technologies. Organized into thematic sections, the review begins with foundational advances in CO₂ capture

materials and pre-treatment methods, emphasizing the importance of feedstock purity and capture efficiency. Subsequent sections explore cutting-edge developments across thermochemical, electrochemical, photochemical/photoelectrochemical, and biological conversion platforms, highlighting breakthroughs in catalyst design, system integration, and performance metrics. Special attention is given to the integration of CO₂ conversion with renewable energy systems and industrial processes, demonstrating the feasibility of embedding these technologies into real-world settings. An additional focus of the review is the transformative role of AI and ML in accelerating research and deployment. We examine how data-driven approaches are revolutionizing catalyst discovery, reaction optimization, and process scaling. Complementing this, is a detailed techno-economic analysis that highlights the cost structures, investment requirements, and policy frameworks necessary to foster widespread adoption. The final sections discuss persistent challenges such as selectivity, catalyst stability, and energy efficiency, and offer actionable recommendations for future research directions, industrial collaboration, and policy reform.

By weaving together advances in materials science, chemistry, engineering, biology, data science and policy, this review aspires to provide a unified roadmap for researchers, industry stakeholders, and policymakers. The goal is to catalyze coordinated efforts that will translate laboratory breakthroughs into commercial solutions, ultimately contributing to the global imperative of building a carbon-neutral and sustainable future.

2. CO₂ capture and pre-treatment: the foundation for effective conversion

2.1. Advances in capture materials

In advancing sustainable CO₂ conversion technologies, the development of high-performance capture materials is essential to achieving greater selectivity, durability, and energy efficiency. Recently, several next-generation sorbents like metal organic frameworks (MOFs), covalent organic frameworks (COFs), porous organic polymers (POPs), amine-based sorbents, carbon-based adsorbents have attracted considerable attention due to their exceptional surface areas, tunable porosity, and strong CO₂ adsorption capabilities. Collectively, these materials represent a versatile and evolving platform for efficient CO₂ capture, forming a critical foundation for downstream conversion processes.

Metal organic frameworks (MOFs)

MOFs offer modular design through the combination of metal nodes and organic linkers, enabling tailored binding sites for CO₂ capture and facilitating high storage capacity (Fan et al., 2025). Recent innovations have improved the thermal and chemical stability of MOFs, with variants such as ZIFs and UiO-66 demonstrating enhanced selectivity and lower regeneration energy requirements, key attributes for industrial deployment (Arya et al., 2025).

Covalent organic frameworks (COFs)

COFs, by contrast, provide rigid, crystalline architectures with high chemical resistance, making them suitable for use in harsh operating environments (Essalhi et al., 2025). Complementing these frameworks, nanoporous carbons also play a vital role, offering large accessible surface areas and high CO₂ uptake. Surface functionalization and pore structure tuning have further refined their selectivity and performance under real-world conditions (Altaf et al., 1234).

Porous organic polymers (POPs)

POPs have emerged as highly efficient materials for CO₂ capture and conversion due to their tunable porosity, high surface areas, and chemical stability (Wang et al., 2022). For example, hyper-crosslinked polymers (HCPs), conjugated microporous polymers (CMPs), ionic porous organic polymers, and porous aromatic frameworks (PAFs) have demonstrated exceptional CO₂ uptake (e.g., PAF-1 with ~1100 m²/g surface area and CMP-1 with ~1000 m²/g) and selectivity (Tian and Zhu, 2020; Lee and Cooper, 2020; Liu and Han, 2019; Tan and Tan,

2017). Particularly, when functionalized with amine groups like Epoxide-functionalized tetraethylenepentamine POP, under the premise of ensuring good cycle stability, demonstrated good working adsorption capacity of $1.9 \text{ mmol} \cdot \text{g}^{-1}$, a low adsorption heat of $48.5 \text{ kJ} \cdot \text{mol}^{-1}$, low desorption temperature of 393 K, and high hydrophobicity, so that the energy penalty for sorbent regeneration has been reduced to $2.3 \text{ MJ} \cdot \text{kg}^{-1}$ (CO_2) (Yang et al., 2020). Their robust frameworks enable recyclability and stability under humid conditions. For CO_2 conversion, POPs integrated with catalytic sites, such as metalloporphyrin-based POPs, have been used as a promising heterogeneous catalyst for CO_2 conversion with high turnover number (Guo et al., 2021), while ionic POPs have been used for cyclic carbonate synthesis—enhancing reaction efficiency by providing confined active sites and facilitating reactant diffusion (Mao et al., 2025).

Amine based adsorbents

Amine-based solid sorbents are among the most widely studied materials for CO_2 capture due to their high selectivity and capacity, particularly in post-combustion flue gas and direct air capture (DAC) applications (Duan et al., 2023). These sorbents typically consist of amines (e.g., polyethylenimine (PEI), tetraethylenepentamine (TEPA), or aminopropylsilanes) immobilized on porous supports like mesoporous silica (SBA-15, MCM-41), alumina, or carbon nanotubes, where the amine groups chemically react with CO_2 to form carbamates or bicarbonates, enabling efficient capture even at low CO_2 concentrations (Shen et al., 2017; Kumar et al., 2022). For instance, PEI-impregnated mesoporous multilamellar silica exhibits high adsorption capacity up to 4.73 mmol/g in pure and dry CO_2 flow at 90°C (Zhang et al., 2016), while TEPA-grafted mesoporous silica enhances moisture tolerance and cyclic performance (Wang et al., 2015). Recent advances include amine-MOF hybrids, which combine the high surface area of MOFs with amine reactivity, and alkylamine-functionalized cellulose aerogels, offering sustainable, low-cost alternatives (Daud and Najib, 2025; Dong et al., 2023). Amine-rich sorbents can be integrated with catalytic systems, such as $\text{Cu/ZnO/Al}_2\text{O}_3$ -based catalysts, to directly hydrogenate captured CO_2 into methanol (Suhail et al., 2024).

Carbon based adsorbents

Carbon-based adsorbents, such as N-doped activated carbons, amine-grafted biochars, and KOH-modified porous carbons, offer high CO_2 uptake due to their tunable porosity and surface chemistry (Li et al., 2022; Spessato et al., 2022). For example, functionalized graphene oxides and carbon nanotubes enhance selectivity through π -complexation, and recent advances integrate these materials with catalytic moieties (e.g., Cu-Zn on carbon nanofibers) for simultaneous CO_2 capture and conversion to methanol, leveraging their conductivity and stability in modular systems, though challenges remain in balancing adsorption kinetics with regeneration energy efficiency for scalable deployment (Ahmad et al., 2025).

2.2. Pre-treatment techniques

The success of CO_2 capture is often contingent on effective pre-treatment techniques (Makepa and Chihobo, 2024). Pre-treatment techniques enhance CO_2 capture and conversion efficiency by modifying feed gases or sorbents to remove impurities, improve reactivity, or reduce energy demands. Pre-treatment processes such as pressure and temperature regulation, along with impurity removal, are crucial in maximizing CO_2 purity and concentration, thus enhancing the efficiency of the conversion step. Pressure swing adsorption (PSA) and temperature swing adsorption (TSA) are commonly used to increase the CO_2 concentration in the feed stream, ensuring that the capture material operates within its optimal adsorption range (Shah et al., 2021; Fouladi et al., 2020; Zerobin and Pröll, 2020; Lian et al., 2019). Additionally, the removal of impurities such as water, nitrogen, and oxygen can prevent the clogging of porous materials and minimize their degradation over time (Siegelman et al., 2021; Khabazipour and Anbia, 2019). The integration of pre-treatment with CO_2 capture systems has led to more

energy-efficient cycles, as these processes allow for the tailoring of operating conditions to match the specific material properties and conversion goals.

For flue gas treatment, scrubbing with amine-based solvents (e.g., monoethanolamine, MEA) removes SO_x and NO_x , thereby preventing sorbent degradation in MOFs or ionic liquids (Luis, 2016). In contrast, alkali pre-treatment (e.g., KOH activation) of biochar or activated carbon increases porosity and enhances CO_2 adsorption capacity (Heidarinejad et al., 2020). Membrane pre-separation enriches CO_2 concentration before capture, improving process economics. For direct air capture (DAC), moisture removal via silica gel or alumina prevents competitive adsorption in MOFs, while electrochemical pre-treatment of ionic liquids (e.g., [Emim][BF₄]) reduces viscosity, enhancing CO_2 diffusivity (Surkatti et al., 2025; Li et al., 2021). In biomass-derived CO_2 conversion, steam reforming pre-treatment (e.g., using Ni-based catalyst) produces syngas for subsequent catalytic hydrogenation to methanol (Farooqi et al., 2021). Meanwhile, plasma activation (non-thermal plasma jets) breaks CO_2 bonds, facilitating electrochemical reduction to ethylene (Cu-based gas diffusion electrodes) (Tandava et al., 2025). For mineral carbonation, mechanochemical pre-treatment (such as ball milling serpentine or olivine) increases the surface area, thereby accelerating CO_2 mineralization (Cau et al., 2024). These methods optimize downstream processes, though trade-offs exist between energy input, cost, and scalability, necessitating tailored approaches for industrial deployment.

2.3. Recent integration of capture with conversion technologies

The latest advancements in CO_2 conversion technologies emphasize the integration of capture and conversion in a seamless process, optimizing both energy efficiency and material usage. One of the most promising approaches is the combination of direct air capture (DAC) with electrochemical reduction (Gutierrez-Sanchez et al., 2022). This method captures CO_2 directly from the atmosphere and converts it into valuable products like fuels or chemicals through electrochemical processes (Kim et al., 2023). Such integrated systems reduce the need for separate CO_2 capture and conversion steps, which lower operational costs and improve energy efficiency (Debergh et al., 2023). The electrocatalytic system captures CO_2 electrochemically and transforms it into CO, formate, or ethylene using metal-organic framework (MOF)-enhanced electrodes or ionic liquid (IL)-based electrolytes (Fortunati et al., 2023). Another emerging strategy combines amine scrubbing with catalytic hydrogenation, where captured CO_2 in monoethanolamine (MEA) at moderate temperatures, bypassing energy-intensive CO_2 release steps (Rochelle, 2009). Electrocatalytic CO_2 reduction (CO_2R) can convert captured CO_2 into valuable products using renewable electricity, enabling a carbon-neutral cycle. However, DAC itself is energy-intensive, and integrating electrocatalysis requires further optimization (Zhang et al., 2025).

Current electrocatalysts (e.g., copper-based materials) selectively convert CO_2 , but their efficiency and durability under real-world DAC conditions need improvement. High overpotentials and competing reactions (like hydrogen evolution) reduce effectiveness. Additionally, the dilute CO_2 concentration in air ($\sim 400 \text{ ppm}$) demands efficient capture and concentration before conversion, increasing energy costs (Ozkan et al., 2024). While electrocatalysis alone may not fully offset global emissions, it can complement other carbon removal strategies, provided costs decrease and improved performance. To address emissions from power plants during DAC and electrocatalysis, renewable energy must power the processes to ensure net-negative CO_2 removal (Ozkan et al., 2024). While carbon capture and storage (CCS) can trap residual emissions from fossil-based plants, advanced electrocatalysts (e.g., oxide-derived copper or single-atom catalysts) should minimize energy waste, and system integration—such as pairing DAC with flue gas capture or using waste heat can improve efficiency (Lau et al., 2021). Circular approaches like converting byproducts (e.g., O_2 from electrolysis)

for industrial use can further reduce the carbon footprint, ultimately requiring policy incentives and scaled infrastructure to make the combined system economically viable.

A more detailed look at the key components of recent CO₂ capture and conversion integration, highlighting the significant advancements, challenges, and opportunities in these combined technologies is presented in Table 1. Recent research has focused on enhancing the efficiency of these catalysts while minimizing energy consumption, a challenge that has been addressed through the optimization of electrolyzer designs and improved electrode materials. Integrating DAC with electrochemical reduction not only captures CO₂ but also closes the loop by converting it into useful byproducts, making this a sustainable solution for mitigating climate change. Furthermore, catalytic systems that integrate CO₂-adsorbing materials can be used for CO₂ conversion and separation. A notable example is TEA-treated Mg-MOF-74 crystals possessing Lewis acid sites (open metal sites) were reported with remarkable CO₂ (350 mg.g⁻¹) and water vapor (593 mL.g⁻¹) sorption capacities at 298 K. Further investigations reveal an extreme reduction in the isosteric adsorption heat from 42 to 22 kJ.mol⁻¹ as the CO₂ loading increased. Realistically, the separation of CO₂ from N₂ was achieved with about 179 mg g⁻¹ saturation capacity (Yang et al., 2012). Meanwhile, biocatalytic approaches employ carbonic anhydrase-mimicking MOFs or engineered bacteria (e.g., Cupriavidus necator) to convert captured CO₂ into bioplastics (PHB) or biofuels (Wright et al., 2018). For industrial scalability, biphasic solvent systems containing N, N-dimethylpropylamine, DMPA, and 50 wt% physical solvent (polyethyleneglycol dimethyl ether, NHD) are being examined to decrease the energy barrier of carbamate generation from zwitterions (DMPA⁺ COO⁻) to enhance chemical absorption (Chen et al., 2022). These integrated systems represent a paradigm shift toward circular carbon economies, though challenges remain in long-term stability, cost, and large-scale deployment.

Additionally, thermal capture of CO₂ typically involves chemisorption at high temperatures using solid sorbents like calcium oxide (CaO) or magnesium oxide (MgO), which react with CO₂ to form carbonates (e.g., CaCO₃) and can be regenerated via calcination (~900 °C)—a process used in calcium looping (CaL) for post-combustion capture (Dunstan et al., 2021). Alternatively, hydrotalcite-based materials (e.g., Mg-Al layered double hydroxides, LDHs) adsorb CO₂ at 200–400 °C, making them suitable for pre-combustion capture in syngas streams. Once captured, thermal catalysis converts CO₂ into value-added products through endothermic reactions, often requiring high temperatures (200–600 °C) and metal-based catalysts (Bernard et al., 2022). Recent advances focus on lowering energy demands via redox-active oxides (e.g., CeO₂-ZrO₂) or chemical looping systems, where oxygen carriers (e.g., Fe₂O₃) split CO₂ into CO while regenerating in a second reactor (Kim et al., 2022).

3. Thermochemical CO₂ conversion technologies

Thermochemical conversion of carbon dioxide (CO₂) is a technical procedure that uses CO₂ to create high-value products, such as fuels, chemicals, building materials, and polymers. Among the various routes, hydrogenation is the most prominent technology (Roy et al., 2018). In principle, a CO₂ and H₂ reactant mixture contains the necessary elements (C, H, and O) to yield a diverse spectrum of products. However, in practice, the outcome is strongly dictated by conversion efficiency, product selectivity, operating conditions, and kinetic limitations (Karakaya and Parks, 2023). Importantly, while the reactions involved are thermodynamically exothermic (Equations 1 and 2), practical feasibility hinges less on exo/endothermicity and more on the specific reaction conditions. Parameters such as temperature, pressure, and catalyst environment critically influence equilibrium, reaction pathways, and achievable yields.

For instance, in CO₂ methanation (Sabatier reaction), the reaction is highly exothermic, and efficient CH₄ production typically occurs at

250–400 °C under pressures of 1–30 bar, where lower temperatures improve equilibrium conversion but slow down kinetics, while higher temperatures enhance rates but risk side reactions (Tommasi et al., 2024). Conversely, methanol synthesis from CO₂ requires moderate temperatures (200–300 °C) and elevated pressures (50–100 bar) to balance kinetic constraints with favorable equilibrium conditions (Pham et al., 2024). Similarly, higher hydrocarbons or long-chain products (via Fischer–Tropsch-type processes) demand even more stringent tuning of operating windows, often involving bifunctional catalysts and elevated pressures (Amin et al., 2024). These examples highlight that product distribution and overall efficiency are not determined solely by whether a reaction is exothermic or endothermic, but by the careful optimization of thermodynamics and kinetics through temperature–pressure–catalyst interplay



Precious metals including Pt catalysts are widely used in RWGS reactions especially when supported on reducible metal support (Kim et al., 2012; Chen et al., 2016). Wang et al. (2023) reported the thermochemical hydrogenation of CO₂ to CO using a reverse water gas shift reaction. In their study, they prepared a platinum single-atom catalyst on ceria and titania referred to as Pt-nanoceria-CeO₂ (PCC) and Pt-nanoceria-TiO₂ (PCT), respectively. The effect of temperature and catalyst support was investigated, and the result is presented in Fig. 1.

As illustrated in Fig. 1, both catalysts demonstrate high efficiency in the thermochemical reduction of CO₂ to CO, with catalytic performance improving as temperature increases. Between 200 °C and 300 °C, PCT exhibits superior activity compared to PCC; however, beyond 320 °C up to 400 °C, PCC outperforms PCT. This contrasting behavior is likely due to the synergistic interactions between the active components and their respective supports. While precious metals are frequently employed in thermochemical CO₂ conversion processes, their high cost poses significant challenges for large-scale commercialization. Consequently, research efforts have increasingly focused on developing cost-effective alternatives based on non-precious metals (Peng et al., 2023). In a recent study, Pascual-Colino et al. (2023) employed supramolecularly synthesized porous MOF-based heterometallic catalysts (CuCo@F, CuNi@F and CuZn@F) for the thermochemical conversion of CO₂ to CO. The reaction was conducted at 550 °C using a CO₂/H₂ gas mixture as the feedstock. Remarkably, the catalysts achieved CO₂ conversions exceeding 70 %, with a CO selectivity of 100 %.

Similarly, Porosoff and Chen (2013) designed a Pt/Co bimetallic heterogeneous catalysts system using cerium oxide and alumina as support material. They reported a very good selectivity for the conversion of CO₂ to Co. They also compared the results of the monometallic Pt catalyst with the Pt-Co catalyst, they observed a higher conversion rate with the bimetallic catalyst. In addition, the selectivity of Pt/Co-CeO₂ was higher than Pt/Co-γ-Al₂O₃ for CO production. This suggests that the support material for the catalyst also plays a critical role in CO₂ reduction

3.1. Conventional thermochemical CO₂ conversion catalysts

Catalysts accelerate chemical reactions by lowering the activation energy required for conversion, thereby reducing operational costs and enhancing product selectivity (García-Serna et al., 2022). Due to the inherent thermodynamic stability and chemical inertness of CO₂, its activation remains a significant challenge, often resulting in low conversion efficiencies. As such, catalysts are indispensable across all CO₂ reduction pathways including thermochemical, electrochemical, photochemical, and biological routes. As illustrated in Fig. 1g, various CO₂ conversion technologies rely heavily on catalytic processes, which are essential to overcoming the kinetic barriers that limit reaction rates and selectivity (Su et al., 2023). The catalytic transformation of CO₂

Table 1

Summary of the recent integration of CO₂ capture and conversion technologies, specifically focusing on the combination of Direct Air Capture (DAC) with electrochemical reduction.

Aspect	Details	Research Focus	Technological Developments	Challenges	Potential Benefits	Ref.
CO ₂ Capture Methods	DAC: A technology to capture CO ₂ directly from the atmosphere.	Capture efficiency, scalability, and energy requirements for DAC systems.	- Development of large-scale DAC plants using amine-based sorbents.- Solid sorbent and liquid solvent systems.	- High energy consumption.- Cost of capturing CO ₂ from ambient air is still relatively high.- Regeneration of sorbents can be energy-intensive.	- Ability to capture CO ₂ directly from ambient air.- Potential for deployment in various locations.	(Li and Yao, 2024; McQueen et al., 2021; Chowdhury et al., 2023; Zhu et al., 2022; Al Yafiee et al., 2024; Mostafa et al., 2022)
Conversion Technologies	Electrochemical Reduction: Converts captured CO ₂ into valuable products (fuels, chemicals).	Catalysts development, energy efficiency of electrochemical cells, and product selectivity.	- Development of novel catalysts, including transition metals and metal alloys.- Optimization of electrolyzers and electrode materials.	- High energy demand for electrochemical processes.- Catalyst degradation and long-term stability.- Scaling issues related to electrochemical reactors.	- Direct conversion of CO ₂ into valuable products (e.g., methane, ethylene).- Reduction of dependency on fossil fuels.	(Zheng et al., 2018; Overa et al., 2022; Lin et al., 2020; Li et al., 2020; Ashraf et al., 2024)
Catalysts for CO ₂ Reduction	Transition metals or metal alloys used to catalyze the electrochemical conversion of CO ₂ .	Development of efficient, durable, and low-cost catalysts.	- Enhanced catalysts like Cu-based alloys (for hydrocarbons) and Sn-based catalysts (for CO production).- Electrocatalysts with higher selectivity for desired products.	- Catalyst deactivation over time.- Lack of understanding regarding catalyst mechanisms.- Expensive or scarce materials (e.g., platinum group metals).	- Enhanced efficiency in converting CO ₂ to hydrocarbons.- Possibility of using sustainable or abundant materials for catalysts.	(Zhang et al., 2018; Yousaf et al., 2024; Senthilkumar et al., 2024; Pourebrahimi et al., 2023; Ejeromedoghene et al., 2024)
Integration of DAC and Conversion	Integration of DAC with electrochemical reduction for a seamless CO ₂ capture-to-conversion process.	Enhancing integration between capture and conversion processes for energy savings and efficiency.	- Development of hybrid systems that integrate CO ₂ capture and electrochemical reduction in a single process.- Optimization of energy use across both capture and conversion steps.	- Coordination between capture and conversion technologies requires complex system design.- Potential for energy loss in integration.- Infrastructure challenges for seamless coupling.	- Reduced operational costs due to integrated processes.- Higher energy efficiency and sustainability.- Closing the CO ₂ loop, converting it to valuable byproducts.	(Mostafa et al., 2022; García-Bordejé and González-Olmos, 2024; Drechsler and Agar, 2021)
Electrolyzer and Reactor Design	Optimizing electrolyzers for CO ₂ conversion efficiency and reducing energy requirements.	Design of more efficient electrochemical reactors and electrolyzers for higher CO ₂ reduction rates.	- Improvements in membrane design for electrolyzers.- Development of multi-phase flow reactors for CO ₂ conversion.- Enhanced reactor configurations for higher throughput.	- Balancing efficiency with cost in large-scale systems.- Material degradation in long-term use.- High voltage or temperature requirements for efficient conversion.	- More efficient CO ₂ reduction processes.- Potential for scalable reactors suited to industrial applications.	(Jalili et al., 2023; He et al., 2023; Moore et al., 2023; Wang et al., 2018; Yang et al., 2020)
Energy Considerations	Ensuring that both CO ₂ capture and conversion processes are energy-efficient.	Minimizing energy consumption in DAC and electrochemical reduction systems.	- Development of low-energy capture systems (e.g., using renewable energy sources for DAC).- Electrochemical reduction using renewable electricity (e.g., solar, wind).	- Maintaining low energy requirements while achieving high conversion efficiency.- Dependency on the availability of renewable energy for both capture and conversion.	- Reduction of greenhouse gas emissions through low-energy CO ₂ conversion.- Alignment with renewable energy goals.	(Rahimi et al., 2022; Sharifian et al., 2021; Wang et al., 2023; Aleta et al., 2023)
Sustainability and Byproducts	Converting captured CO ₂ into useful byproducts that benefit the economy.	Sustainability and market readiness of CO ₂ -derived products.	- Developing markets for CO ₂ -based chemicals and fuels.- Design of processes for the sustainable use of byproducts.	- Market acceptance and demand for CO ₂ -derived products.- Competition with traditional production methods (e.g., from fossil fuels).	- Creation of valuable products from CO ₂ , contributing to a circular carbon economy.- Reduction of overall CO ₂ emissions in industrial processes.	(Ramirez-Corredores, 2024; Lehtonen et al., 2019; ; Alii et al., n. d.; Shah et al., 2023)
Cost and Scalability	Integration of DAC and electrochemical processes should ideally lead to lower operational costs.	Cost reduction strategies for scaling DAC and electrochemical conversion technologies.	- Development of low-cost materials for DAC and electrochemical systems.- Process optimization for cost-effective scaling.	- High initial capital costs for integrated systems.- Need for significant advances in process efficiency and scalability for commercial viability.	- More affordable solutions for large-scale CO ₂ mitigation.- Potential for cost-effective deployment in industries like energy and chemicals.	(Li and Yao, 2024; McQueen et al., 2021; Al Yafiee et al., 2024; Erans et al., 2022; Küng et al., 2023; Chauvy and Dubois, 2022; DiMartino, 2023)

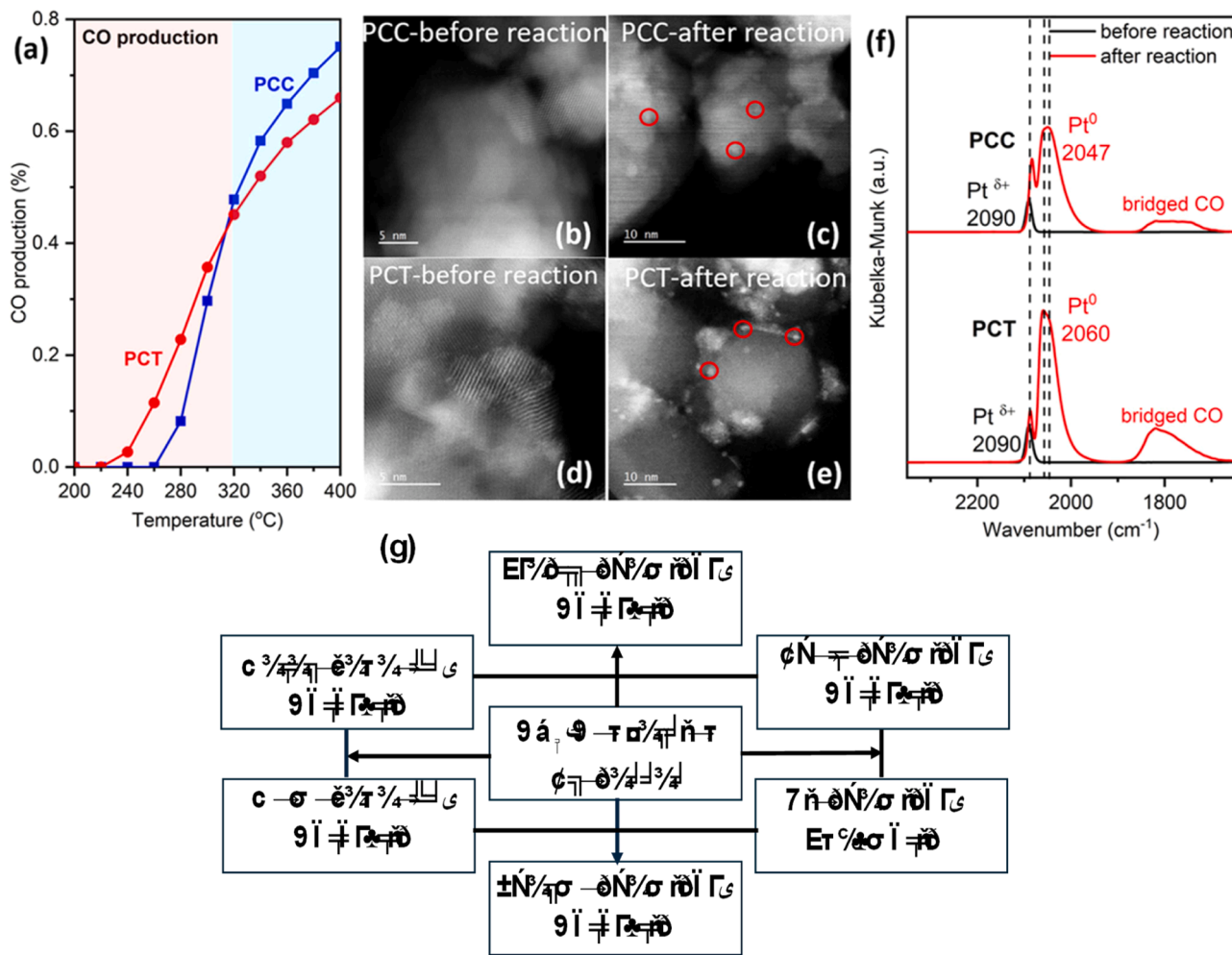


Fig. 1. (a) Comparison of CO production efficiency for PCC and PCT catalysts across different temperature ranges. (b) TEM image of PCC before the reaction. (c) TEM image of PCC after the reaction. (d) TEM image of PCT before the reaction. (e) TEM image of PCT after the reaction. (f) CO-probed DRIFTS spectra showing CO desorption profiles for PCC and PCT before and after the reaction. Adapted with permission from reference (Wang et al., 2023). Copyright © 2023, Springer Nature. (g) Overview of various strategies employed in CO₂ conversion processes.

began in the early 20th century, pioneered at the Dalian Institute of Chemical Physics (DICP) through studies in thermal catalysis (Shang et al., 2024). Since then, the field has expanded to encompass electrocatalysis and photocatalysis, significantly broadening the scope of CO₂ utilization technologies (Cheng et al., 2025). Numerous catalytic systems have since been engineered to enhance CO₂ conversion rates and improve selectivity toward targeted products. Among these, heterogeneous catalysis is particularly favored for its operational stability and ease of separation from reaction products, offering practical advantages over homogeneous systems (Anekwe et al., 2025).

The first reported heterogeneous catalytic hydrogenation of CO₂ to formate was documented in 1914 by Bredig and Carter, employing palladium black as the catalyst (Lvarez et al., 2017). Although the initial outcomes were limited by large metal particle sizes and aggregation, this work laid the foundation for further advances in the field. The advent of nanocatalysts has since driven significant progress, with their high surface-to-volume ratios and unique electronic properties contributing to improved activity and selectivity (Chaturvedi et al., 2012). A selection of recent studies on catalyst-mediated CO₂ reduction including reaction conditions and performance outcomes is summarized in Table 2.

Apart from the catalysts listed in Table 2, Cu-based catalysts are becoming increasingly popular for methanol synthesis (Li et al., 2019). This is because of its relatively low price and unique catalytic activity. Also, it is commonly believed that Cu provides an active site for

Entry	Catalyst	H ₂ / CO ₂ (bar)	Temp. (°C)	Additive	TON	Ref
1	CPC-Ru-1	50/30	120	–	179	(Bankar et al., 2023)
2	Ru ₃ (CO) ₁₂	40/30	70	BMMI. OAc.	17,000	(Weilhard et al., 2018)
3	Au/TiO ₂	20/20	70	NEt ₃	111	(Filonenko et al., 2016)
4	Pd@Ag/ TiO ₂	10/10	100	NaHCO ₃	14,839	(Mori et al., 2018)
5	MOF1/Pd	22.5/ 7.5	170	KOH	1500	(Makuve et al., 2022)
6	Ru-Co ₃ O ₄	20.7/ 41.4	120	NEt ₃	219	(Wang et al., 2023)
7	Au/Al ₂ O ₃	20/20	70	NEt ₃	215	(Maru et al., 2018)
8	Au/SiO ₂ -NH	50/30	90	NEt ₃	1026	(Liu et al., 2017)
9	Au36 (TBBT)24	22.5/ 7.5	120	–	935	(Yang et al., 2020)
10	Pd/AC	50/30	40	–	594	(Wu et al., 2019)

hydrogen gas dissociation in the CO₂ conversion process (Wang et al., 2020). Several reports have been published for methanol synthesis from CO₂ reduction, and the results are summarized in Table 3 entries 1–6.

Nickel-based catalysts play a pivotal role in the catalytic conversion of CO₂, particularly in the dry reforming of methane (DRM). Owing to their high hydrogen adsorption capacity, elevated CO₂ conversion rates, and excellent selectivity toward methane, Ni-based systems are among the most extensively studied non-precious metal catalysts (Zafarnak and Rahimpour, 2025; Pizzolitto et al., 2019). However, a key limitation is their susceptibility to deactivation under harsh DRM conditions, primarily due to the aggregation and sintering of Ni particles (Lai et al., 2024).

CO₂ methanation converts CO₂ and H₂ into CH₄ (methane) using nickel (Ni)-, ruthenium (Ru)-, or cobalt (Co)-based catalysts supported on Al₂O₃, CeO₂, or ZrO₂, with Ni/Al₂O₃ being the most common due to its cost-effectiveness and moderate activity (Beniwal et al., 2025). In a notable study, Sepehri et al. (Sepehri, 2015) investigated CO₂ methanation using a supported Ni catalyst (Ni/Al₂O₃) under reaction conditions of H₂/CO₂ molar ratio of 3.5, GHSV of 9000 mL/g.cat-h, and a temperature range of 200–500 °C. The catalyst achieved a remarkable 70 % CO₂ conversion and 100 % selectivity to methane, demonstrating performance comparable to that of precious metal catalysts, but with significantly lower cost. Recent advances include bimetallic catalysts. For instance, Tan et al. (2019) employed a Ni-MgO/ZrO₂ catalyst for CO₂ methanation using a CO₂/H₂/N₂ mixture (molar ratio: 8/32/10) at a total flow rate of 50 mL/min and temperatures ranging from 200–500 °C. They reported an outstanding 95 % CO₂ conversion at 300 °C with complete selectivity to methane (100 %). Several other studies have also demonstrated the effectiveness of Ni-based catalysts in DRM, with key findings summarized in Table 3 (entries 6–10). Although challenges in H₂ sourcing costs, catalyst deactivation from sintering/coking, and energy-intensive compression have been identified, emerging solutions involving MOF-derived catalysts (e.g., Ni/ZIF-8) and electrocatalytic routes (e.g., Cu-ZnO/Al₂O₃ membranes) are being explored to improve selectivity and durability (Hoang et al., 2021; Xiang et al., 2024; Liu et al., 2023).

Furthermore, converting CO₂ to aromatics is another promising approach that typically involves cascade reactions: first, CO₂ hydrogenation to methanol occurs via Cu/ZnO/Al₂O₃, then methanol-to-aromatics (MTA) follows suit via zeolite catalysts (e.g., ZSM-5, Ga-modified HZSM-5). Alternatively, direct CO₂-to-aromatics routes employ multifunctional catalysts (e.g., Co-Fe/K-Al₂O₃) or oxide-zeolite (OXZEO) systems (e.g., Cr₂O₃/H-SAPO-34). A breakthrough by Carbon Recycling International uses biocatalytic pathways (engineered microbes) to produce styrene from CO₂. Key hurdles are low single-pass

yields, catalyst coking, and high H₂ demand, with research focusing on non-thermal plasma activation and single-atom catalysts (e.g., Pt₁/ZnO-ZrO₂) to boost efficiency.

3.2. Improved thermochemical catalysts

Recent advancements in thermochemical catalysis have significantly enhanced CO₂ reduction processes, particularly through the development of bimetallic and nanostructured catalysts. Bimetallic systems, comprising two distinct metals, have emerged as promising platforms due to their ability to synergistically combine the advantageous properties of each component, thereby improving catalytic activity and selectivity (Deshmukh et al., 2025). For instance, copper-based catalysts alloyed with noble metals such as gold or palladium demonstrate superior performance copper facilitates CO₂ activation, while gold or palladium enhances intermediate stabilization and electron transfer, collectively reducing catalyst deactivation (Zhong et al., 2025). (Chen et al) exemplified this approach by developing atomically dispersed Fe–Co bimetallic catalysts embedded in Co-zeolitic imidazolate frameworks (C–Co–ZIF), which were pyrolyzed to form a highly active electrocatalyst for electrochemical CO₂ reduction reactions (ECO₂RR) (Fig. 2a). The incorporation of Fe introduced synergistic interactions that increased the number of active sites and induced favorable distortions in the local coordination environment, leading to enhanced CO selectivity. The optimized C–Fe–Co–ZIF catalyst achieved a CO Faradaic efficiency (FE) of 51.9 %, with a tunable H₂/CO ratio ranging from 0.8 to 4.2 across a broad potential window (–0.35 to –0.8 V vs. RHE), and maintained a high total FE of 93 % (CO + H₂) over 10 hours, highlighting its stability and performance.

Oxide-based catalysts have also attracted attention, particularly those incorporating ceria (CeO₂), zirconia (ZrO₂), and alumina (Al₂O₃), owing to their robustness and multifunctional roles in CO₂ activation. Ceria is especially notable for its redox flexibility between Ce³⁺ and Ce⁴⁺ states, which facilitates oxygen storage and release, key to lowering CO₂ activation energy (Fig. 2b). The addition of zirconia and alumina improves mechanical strength and catalytic efficiency, making these oxides effective in reactions such as CO₂ hydrogenation and the reverse water-gas shift (RWGS) (Wang et al., 2025). Moreover, the oxygen vacancies and mobility in ceria-based systems contribute to improved thermodynamic performance (Zhang et al., 2025).

Nanostructured catalysts including metal nanoparticles (e.g., Cu, Ag, Au) and carbon nanotubes represent another innovative frontier. Their high surface area and dense distribution of active sites enhance CO₂ adsorption and conversion, allowing for increased reaction rates and selectivity. Furthermore, their ability to operate at lower temperatures and pressures makes them more energy-efficient and cost-effective than traditional catalysts (Yu et al., 2023).

Wang et al. (No Title, 2024) demonstrated the power of nanostructured design by constructing a photoelectrochemical (PEC) system using crystal phase-engineered silver (Ag) nanocrystals deposited on a silicon heterojunction photocathode (Fig. 2c). The Ag nanocrystals, featuring unconventional hexagonal close-packed phases, significantly improved charge transfer and CO₂-to-CO conversion. By decoupling light absorption from the catalytic layer, this system minimized parasitic absorption and achieved a CO Faradaic efficiency exceeding 90 % across a wide potential range, peaking at 97.4 % at –0.2 V vs. RHE. At the CO₂/CO equilibrium potential, the photocurrent density reached –2.7 mA cm^{–2} with a CO FE of 96.5 %, outperforming traditional Au-based benchmarks. These developments underscore the transformative potential of advanced catalyst design in CO₂ conversion. The integration of bimetallic, oxide-based, and nanoscale catalysts offers a pathway to scalable, energy-efficient, and sustainable CO₂ reduction technologies critical for mitigating greenhouse gas emissions across industrial sectors.

Table 3

The catalytic performance of Ni and Cu catalysts for CO₂ conversion.

Entry	Catalyst	Temp. (K)	Conversion %	Selectivity %	Ref
1	Cu/AlCeO	473–553	<22.5	<94	(Li et al., 2019)
2	Cu/ZnO/ZrO ₂	503–543	<23	<66.8	(Dong et al., 2016)
3	Cu/SiO ₂	533	15–20	<98	(Prieto et al., 2013)
4	Cu/ZrO ₂	493–553	<13	<76.4	(Witoon et al., 2016)
5	O/H-Cu/ZnO	523	27.54	76.86	(Li et al., 2018)
6	O/I-Cu/ZnO	523	29.22	83.56	(Li et al., 2018)
7	25 %Ni/Al ₂ O ₃	623	74	99.0	(Darouhegi et al., 2017)
8	6 %Ni/ZrO ₂	523	90	100	(Tan et al., 2019)
9	6 %Ni-MgO/ZrO ₂	573	84 %	100	(Tan et al., 2019)
10	Ni/ZrO ₂	612	71.9	100	(Jia et al., 2019)

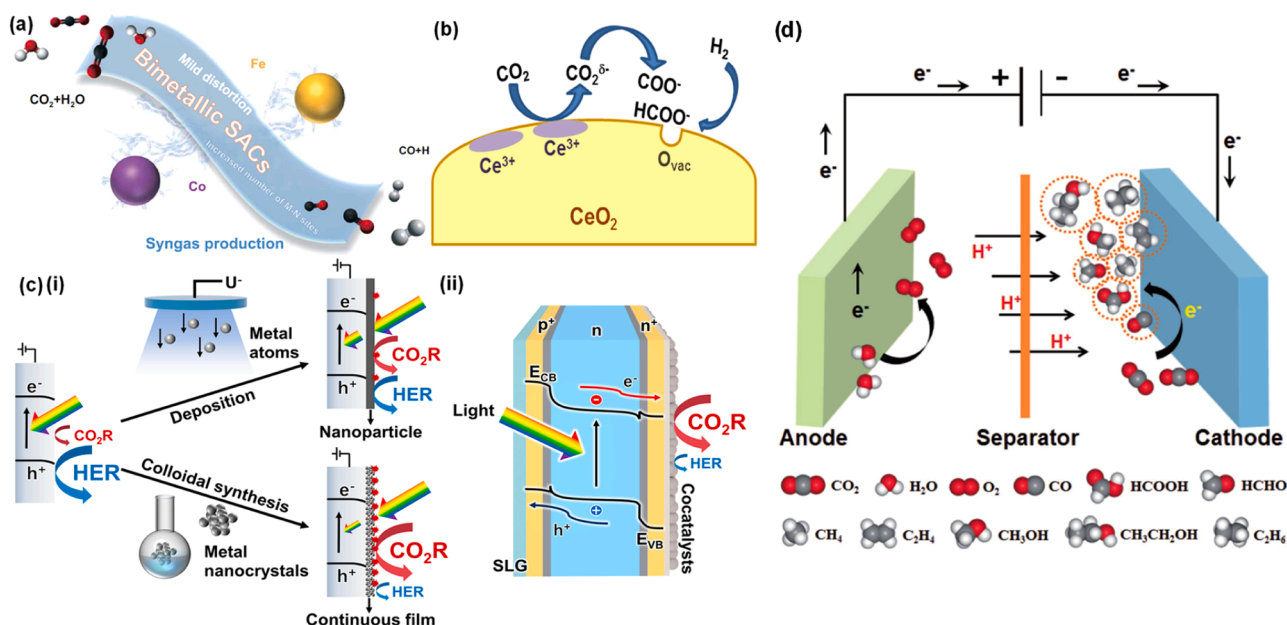


Fig. 2. (a) Schematic depicting the reaction mechanism of bimetallic catalysts during electrochemical CO₂ reduction (ECO₂RR) (Peng et al., 2023). (b) Illustration of the CO₂ activation process on a ceria surface. (c) Design strategies for photocathodes in CO₂ reduction (CO₂R), including: (i) schematic representations of various cocatalyst synthesis methods applied to front-side illuminated photocathodes, and (ii) a schematic of heterojunction silicon (HJ-Si) photocathodes with illumination and reaction decoupling to minimize parasitic light absorption. HER: hydrogen evolution reaction (Lvarez et al., 2017). (d) Schematic overview of CO₂ electrochemical reduction (CO₂ECR) occurring within an electrolytic cell. Adapted with permission from reference (Chaturvedi et al., 2012). © 2022 MDPI.

4. Electrochemical CO₂ reduction (ECR) technologies

Electrochemical CO₂ reduction (CO₂ECR) was first pioneered by Y. Hori in the 1980s and has since attracted significant interest due to its operation under relatively mild conditions compared to other CO₂ conversion methods (Kas et al., 2020; Wiranarongkorn et al., 2023). CO₂ECR involves the electrochemical conversion of carbon dioxide into valuable chemicals and fuels within an electrolytic cell (Jin et al., 2022). A typical electrolytic cell comprises two electrodes (a cathode and an anode) immersed in a chamber filled with a CO₂-saturated liquid electrolyte (Sajna et al., 2023). These electrodes are often separated by an ion-conductive membrane to prevent electrical short circuits and avoid product crossover. During operation, oxygen evolution occurs at the anode, while CO₂ reduction takes place at the cathode. As illustrated in Fig. 2d, CO₂ molecules diffuse to the electrode surface where the electrochemical reduction reactions occur. Consequently, the development of stable, selective, and efficient electrode materials is critical to optimizing the CO₂ECR process.

4.1. Innovations in electrode materials

Electrode design, including its structure and morphology, plays a pivotal role in the efficiency of the ECR process by ensuring optimal contact and interaction among CO₂ molecules, protons, and electrons (Chen et al., 2025). Typically, the electrocatalyst is either directly deposited onto the electrode surface or integrated within the electrode itself. Recent research has focused intensively on the development of advanced electrode architectures, with nanostructured electrodes emerging as a particularly promising class. These electrodes are fabricated by nanostructuring metallic catalysts, significantly increasing their electrochemically active surface area (ECSA), which is a critical factor influencing catalytic performance.

It is widely accepted that the catalytic activity of heterogeneous catalysts correlates strongly with their accessible surface area; thus, maximizing ECSA forms the fundamental strategy behind nanostructured electrode design. Various metals have been employed in crafting these nanostructured electrodes, including silver (Ag), gold

(Au), copper (Cu), palladium (Pd), tin (Sn), and cobalt (Co) (Li et al., 2022; Ewis et al., 2023; Tsubonouchi et al., 2021; Yousaf et al., 2024). Among these, copper-based catalysts stand out as particularly effective for CO₂ electroreduction, owing to their relatively low cost, excellent electrical conductivity, and high surface area. Moreover, copper electrodes uniquely stabilize chemisorbed CO intermediates, which are crucial for facilitating selective and efficient CO₂ conversion pathways.

In addition to metallic nanostructures, MOFs represent an exciting class of porous hybrid materials composed of metal ions or clusters coordinated to organic ligands (Shahzad et al., 2023). MOFs are distinguished by their exceptional surface areas, tunable structural frameworks, facile functionalization, and high porosity (Zhang et al., 2022; Adegoke and Maxakato, 2021). These properties make MOFs highly advantageous for electrochemical CO₂ capture and conversion. Specifically, MOFs offer: (i) diverse and customizable frameworks that enable targeted functionalization; (ii) large porosity facilitating efficient mass transport of reactants and products; and (iii) expansive surface areas that enhance catalytic reactivity. Consequently, MOFs have been extensively studied for their potential in electrochemical CO₂ reduction applications, with key findings summarized in Table 4.

Although Cu-mediated catalysts in nanostructure and MOF-designed electrodes are efficient for CO₂ conversion using the ECR process. However, they still suffer some challenges such as irreversible HER, sluggish kinetics, and low FE (Ma et al., 2017). Carbon-based materials have gained attention in recent years. The advantages include high surface area, resistance to acids and bases, high thermal and chemical stability, and availability in large quantities which are beneficial to ECR. Examples of carbon materials used in electrocatalysis include g-C₃N₄, graphene oxide, 2-dimensional 2D graphene, carbon nanofibers, carbon nanotubes etc. (Ma et al., 2017). Yuan et al. (2018) reported a metal-free pyridoxine functionalized graphene oxide electrode GO-VB6 for electrochemical CO₂ conversion to ethanol. They reported a very good FE coupled with remarkable selectivity to the targeted product. Similarly, Jia et al. (2020) fabricated an electrode using reduced graphene oxide (rGO) for ECR CO₂ reduction to CO. They reported an excellent FE of 94.5 % with very good product selectivity (94 %).

Nowadays, research into additive manufacturing of functional

Table 4
MOFs and electrocatalyst used for ECR CO₂ conversion processes.

Entry	Pristine MOF	Electrocatalyst	Major product	FE %	Ref
1	HKUST-1	PTFE/CuxOyCz	C2+ products	54	(Sikdar et al., 2021)
2	Cu-ASP	Porous Cu ₂ O	C2 products	70	(Yang et al., 2020)
3	HKUST-1	Cu/Ag	C2+ products	21	(Sikdar et al., 2022)
4	Cu-TCNQ	Cu@NxC	C2 products	80	(Li et al., 2021)
5	Cu-Co-MOF-74	M-Cu-Co/C	C2 products	10.1	(He et al., 2022)
6	HKUST-1	Cu-Cu ₂ O	C2+ products	58	(Han et al., 2021)
7	BEN-Cu-BTC	Cu@N-doped C	C2 products	11.2	(Cheng et al., 2019)
8	HKUST-1	Cu Clusters	Ethene	45	(Nam et al., 2018)
9	Cu-doped ZIF-8	Cu-SA/NPC	Acetone	36.7	(Zhao et al., 2020)
10	Co-doped	CoCu single atom	Ethene	15.6	(Kim et al., 2023)

devices to fabricate functional electrodes for electrochemical CO₂ reduction is getting attention. For example, Vaněčková et al. (2021), demonstrated the design and fabrication of functional electrodes with

controlled architecture via 3D printing, similarly Foo et al. (2018) also achieved 3Dprinting of electrochemically active materials to functioning electrodes, they reported that the additively manufactured electrodes demonstrated similar activity compared to conventional electrodes. Another advantage of 3D-printed electrodes is their flexibility and on-demand production.

4.2. ECR in tandem with renewable energy sources

We previously discussed the tandem strategy in catalysis, and its application is now gaining momentum in electrochemical CO₂ reduction (ECR) processes. Integrating tandem ECR systems with renewable energy sources, such as wind and solar power, has emerged as a promising route for achieving sustainable CO₂ conversion. Niu et al. (2021) developed a Cu₂O–Ag tandem catalyst for the electrochemical reduction of CO₂ to C₂ products, reporting an impressive Faradaic efficiency (FE) of 72.85 %. The enhanced performance was attributed to the synergistic interaction between Ag nanoparticles and cuprous oxide (Cu₂O) nanocubes. Similarly, Zhang et al. (2020) demonstrated the use of Cu/ZnO tandem electrodes for CO₂ electroreduction to ethylene, achieving higher FE than pristine Cu electrodes. A schematic representation of the tandem electrocatalyst system is shown in Fig. 3a.

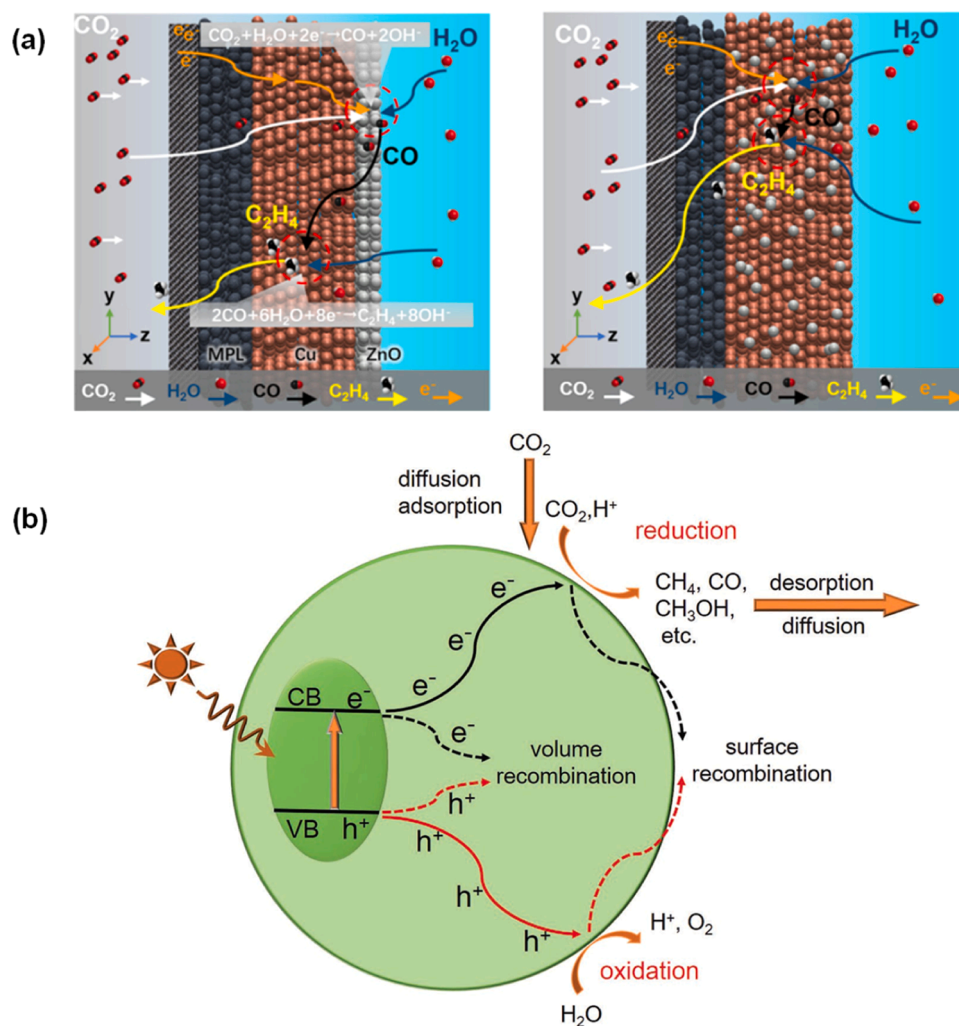


Fig. 3. (a) Schematic representation of the Cu/ZnO tandem electrode as reported by Zhang et al. Reproduced with permission from Ref. (Zhang et al., 2020), © 2020 Elsevier. (b) Fundamental mechanism of the photocatalytic process. Reproduced with permission from Ref. (Du et al., 2020), © 2020 Elsevier.

5. Photochemical and photoelectrochemical CO₂ reduction technologies

There are several methods to convert CO₂ using renewable solar energy, broadly classified into two main categories: photochemical (PC) and photoelectrochemical (PEC) conversion (Kalamaras et al., 2018). Photochemical conversion involves the direct reduction of CO₂ into value-added products using sunlight as the primary energy source. In contrast, photoelectrochemical conversion combines solar energy with electrochemical energy to transform CO₂ into clean fuels or chemicals (Zhang et al., 2020). In PEC systems, the photocatalyst functions as an electrode, generating photogenerated electrons that migrate to the electrode surface under an external electric field. This process enhances CO₂ conversion efficiency and helps overcome some limitations associated with purely photochemical methods (Gozzi et al., 2024). While PEC shares similarities with electrocatalysis, the integration of solar energy significantly reduces overall energy consumption (Lin et al., 2024; Minh et al., 2022). This field is gaining increasing attention due to its innovative potential for addressing climate change and advancing sustainable development. Fundamentally, both PC and PEC processes rely on semiconductor light absorption, which induces the separation of electron-hole pairs. The excited electrons then drive the reduction of CO₂ into useful products.

5.1. Advances in photocatalysts

Inspired by natural photosynthesis, light-driven catalytic reactions have attracted significant attention as environmentally friendly chemical processes. Among these, photochemical CO₂ reduction stands out as a promising approach, harnessing abundant solar energy and converting CO₂ into valuable chemicals without relying on fossil fuels. The pioneering work of Fujishima et al. in 1967 demonstrated the first photocatalytic reduction using a semiconductor-based catalyst sparking decades of research in this field (Chakravorty and Roy, 2024; Ashu Abey et al., 2025). The photocatalytic mechanism, depicted in Fig. 3b, initiates with the photoexcitation of electrons from the valence band (VB) to the conduction band (CB), resulting in the generation of electron-hole (e^-h^+) pairs in equal proportions. Upon formation, these charge carriers undergo separation and directional migration toward the semiconductor surface. At the reactive sites, the photogenerated electrons, possessing sufficient reducing potential, participate in CO₂ reduction pathways to yield C₁ products, while the photogenerated holes simultaneously oxidize water molecules, generating oxygen or reactive oxygen intermediates. The overall photocatalytic efficiency strongly depends on the semiconductor's ability to achieve rapid charge separation and suppress recombination, as this process governs the effective utilization of the electron-hole pairs in driving the surface redox reactions (Zhu et al., 2022; Chakravorty and Roy, 2024).

Early photocatalytic studies focused on semiconductor materials such as TiO₂, ZnO, CdS, and Cu₂O, primarily for pollutant degradation. Although these materials are inexpensive and stable, their drawbacks include corrosion susceptibility, limited visible-light absorption, rapid electron-hole recombination, and wide band gaps (Ashu Abey et al., 2025). Consequently, recent efforts have aimed to develop advanced photocatalysts such as MOFs, perovskites, and organic semiconductors (Al-Saedi, 2023; Khan et al., 2024). Moreover, applications of photocatalysis have expanded to converting CO₂ into methane, methanol, formic acid, and other valuable chemicals. Among these, formic acid is particularly notable for its potential as a hydrogen storage medium (Dong et al., 2024).

To overcome limitations of traditional photocatalysts, designing efficient, stable, and scalable materials with tailored surface properties and architectures has become a research priority. Current photocatalysts are predominantly semiconductor-based, including transition metal oxides (e.g., TiO₂, Co₃O₄), metal chalcogenides (CdS, MoS₂, SnS₂), nitrides, bismuth halide oxides, MOFs, and metal halide perovskites (Alli

et al., 2023c, 2023b). While these catalysts possess suitable band gaps for CO₂ reduction, their primary response to ultraviolet (UV) light constrains their overall efficiency (Lu et al., 2024). Thus, enhancing their catalytic activity through material modifications is a major focus. Photocatalysts can be broadly classified into single-component, two-component, and multicomponent systems.

One of the most effective strategies to boost photocatalytic performance involves forming heterojunctions by combining conductors with differing properties. This approach broadens the visible light absorption range and reduces electron-hole recombination rates (Alli et al., 2023; Wang et al., 2024). For example, Tan et al. (2018) synthesized Pd/Ag nanoalloys supported on N-doped TiO₂ nanosheets (AgxPd_y/TiO₂) for CO₂-to-methane conversion. Compared to single-metal TiO₂ catalysts (Ag/TiO₂ and Pd/TiO₂), the Ag₂Pd₁/TiO₂ heterojunction catalyst achieved a significantly higher methane production rate of 79.0 $\mu\text{mol g}^{-1} \text{h}^{-1}$, attributed to improved charge separation via heterojunction formation. Heterojunctions are generally categorized into three types based on their charge separation mechanisms (Fig. 4a).

Type I heterojunctions occur when semiconductor A has a smaller bandgap than semiconductor B, resulting in closely aligned conduction and valence bands with a straddling configuration. This alignment typically leads to low charge separation efficiency, as both electrons and holes accumulate in the same material (Liu et al., 2022). Despite this, appropriate material combinations can yield significant photocatalytic enhancements. For instance, Zhang et al. (2025) reported a type I heterojunction composite of BiOCl and etched SiC (BOC/eSiC) for CO₂-to-CO conversion, exhibiting an 11.9-fold increase in activity compared to individual components. In contrast, type II heterojunctions exhibit staggered band alignment that promotes more efficient spatial separation of charge carriers, enhancing photocatalytic performance. Due to this advantage, type II systems have garnered considerable research interest (Sudrajat et al., 2025; Sambyal et al., 2025). (Li et al.) developed a UiO-66/Bi₄O₅Br₂ composite photocatalyst, which demonstrated CO₂ conversion rates 1.64 and 2.15 times higher than pure Bi₄O₅Br₂ and UiO-66, respectively. Type III heterojunctions share a similar band alignment to type II but with non-overlapping bands, creating a "broken gap" that requires a stronger driving force for charge transfer (Sudrajat et al., 2025). Consequently, type III heterojunctions show poor charge separation and are rarely reported in literature (Alli et al., 2023).

Among these, type II heterojunctions generally exhibit the best photocatalytic activity, inspiring ongoing efforts to develop advanced photocatalysts based on this configuration. Recent innovations have introduced novel type II heterojunction photocatalysts utilizing charge transfer mechanisms known as S-scheme and Z-scheme systems (Fig. 4b and c).

The Z-scheme photocatalytic concept was first introduced by Bard in 1979 to overcome the limitations of redox potential in type-II heterojunction materials (Balapure et al., 2024). This system offers several advantages, including enhanced light absorption, strong redox capability, and improved catalytic performance. As illustrated in Fig. 4b, the name "Z-scheme" derives from the zigzag (Z-shaped) transfer pathway of charge carriers within the heterojunction structure. Z-scheme photocatalysts are categorized into two types: direct Z-scheme (involving intimate contact between semiconductors without a mediator) and indirect Z-scheme (involving an electron mediator). Among the commonly used materials, graphitic carbon nitride (g-C₃N₄) stands out due to its appropriate band gap, as well as its excellent thermal and chemical stability (Bairamis and Rapti, 2023; Lai and Lee, 2021).

Numerous studies have demonstrated the successful application of Z-scheme photocatalysts in CO₂ conversion to valuable products such as carbon monoxide, methane, methanol, and formic acid (Kumaravel et al., 2020; Yazdanpour and Sharifnia, 2013; Yuan et al., 2024; Wang et al., 2020). Despite their promise, Z-scheme systems still face challenges such as undesired electron-hole recombination, poor selectivity in multi-step reactions, and thermodynamic limitations (Alli et al.,

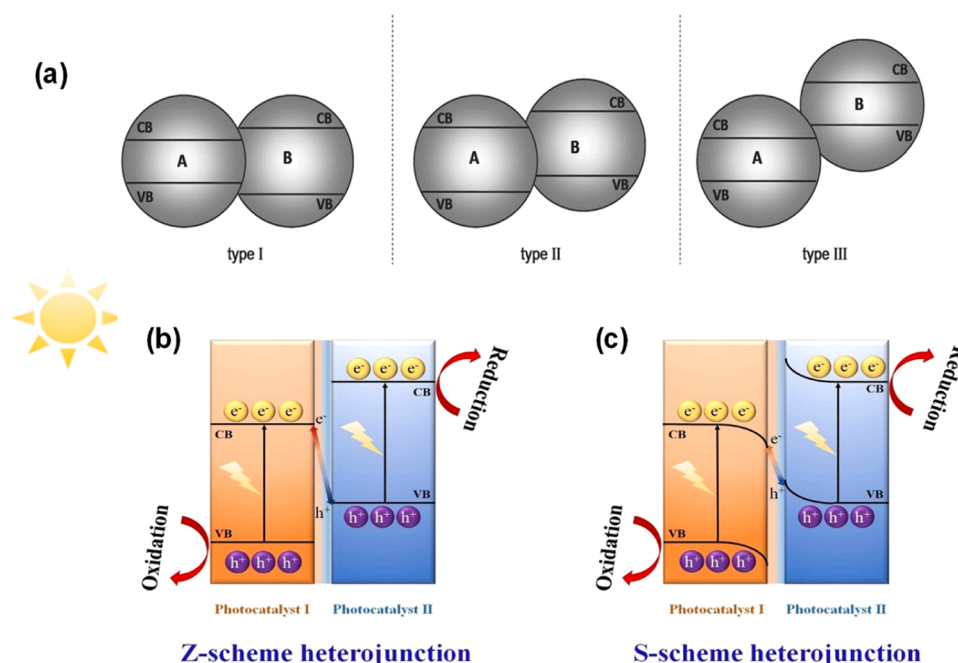


Fig. 4. (a) Various types of semiconductor heterojunctions. Adapted with permission from Ref. (Schumacher and Marschall, 2022), © 2022 Springer Nature. (b) Schematic illustration of charge transfer and separation in Z-scheme heterojunctions. (c) S-scheme heterojunctions. Adapted with permission from Ref. (Zhang et al., 2024), © 2024 Wiley.

2023). To address these issues, Yul and colleagues proposed the S-scheme photocatalytic system in 2019 (Qahtan et al., 2024). In an S-scheme heterojunction, an oxidation photocatalyst (OP) is paired with a reduction photocatalyst (RP), typically comprising two n-type semiconductors, unlike the n/p-type configuration common in Z-schemes. The term "S-scheme" is derived from its staggered band alignment, which visually resembles the letter 'N' at the microscopic level (Wang et al., 2024). Several comprehensive reviews on S-scheme photocatalysts have been published, including our recent contribution (Alli et al., 2023, 2024). The S-scheme design has gained increasing attention in CO₂ photoreduction due to its superior charge separation and retention of high redox potentials. For instance, Tao et al. (2023) developed a BiOBr/g-C₃N₄ S-scheme photocatalyst, which exhibited a CO production rate 8.1 times higher than that of bulk g-C₃N₄. This enhancement was attributed to improved charge carrier dynamics and preserved redox activity. More recently, an S-scheme WO₃/BiOBr photocatalyst was fabricated for efficient CO₂ reduction to CO (Li et al., 2024), further confirming the growing potential of this strategy in carbon capture and utilization.

5.2. Improved CO₂ reduction through improved photoelectrochemical cell designs

We have previously described the PEC process. In practice, the PEC reduction takes place in a PEC reactor or electrolytic cell. A PEC cell is a device that employs semiconductor solar cells to convert chemical energy into value added chemicals (Zhang et al., 2020). It was discovered in 1972 for water splitting using TiO₂ photocatalyst (Yu and Jang, 2023). Since then, its application has extended fuel production, CO₂RR and degradation of organic pollutants (Wu et al., 2020).

A typical PEC electrolytic cell is usually constructed based on 3 phase electrode configuration viz working electrode, reference electrode and a counter electrode (Jiang et al., 2020). The functional units of a PEC cell are electrodes, electrolyte and voltage. The electrodes play critical roles as they help to convert photons into electron hole pairs; therefore, it is important to select and appropriate photocatalytic material for the photoelectrodes. The semiconductor material must be stable, durable,

selective and possess the appropriate bandgap. For PEC CO₂ reduction systems, there different types of design, these include photoanode, photocathode, photoanode/cathode, and PV-assisted tandem (Abarca et al., 2023).

As shown in Fig. 5, the photoanode architecture is illustrated in Fig. 5a, in this system, the anode is exposed to the light source, and it is the simplest type of PEC design. In the photocathode system, the cathode is exposed to the light source, in the third design (Photoanode/photocathode system), both the anode and the cathode are illuminated at the same time. The PV-assisted tandem is the combination of PV and PEC technologies for direct conversion of solar energy and CO₂ into sustainable fuels (Fig. 5d).

It is worth mentioning that most literature reports on PEC for CO₂RR process are conducted in a batch reactor system. The continuous flow PEC (CFPER) reactor is also getting tremendous attention as it offers multiple benefits compared to its batch counterpart. The advantages include improved mixing, faster reaction (Endrödi et al., 2017), and scale up benefits for commercial applications. The design of CFPEC reported by Jung et al. (2024) is illustrated in Fig. 5e. They reported an impressive 30 folds increase in CO FE, and 16 folds increase in CO production rate when compared to traditional PEC cell. Similar design has been employed by (Endrödi et al., 2017; Jung et al., 2023) for CO₂ reduction and they reported excellent conversion and great CO selectivity.

6. Biological CO₂ conversion technologies

Harnessing biological systems to convert CO₂ into valuable organic compounds represents a promising pathway toward carbon neutrality and the development of sustainable societies. Organisms such as microorganisms, plants, and algae naturally assimilate CO₂ through specialized metabolic pathways and utilize reducing power to drive this transformation. This section delves into key microbial CO₂ fixation routes including the Calvin-Benson-Bassham (CBB) cycle, the reductive tricarboxylic acid (rTCA) cycle, and the acetyl-CoA pathway and highlights the essential enzymes that facilitate these processes (Fig. 6). It also discusses the energy and electron sources necessary for regenerating

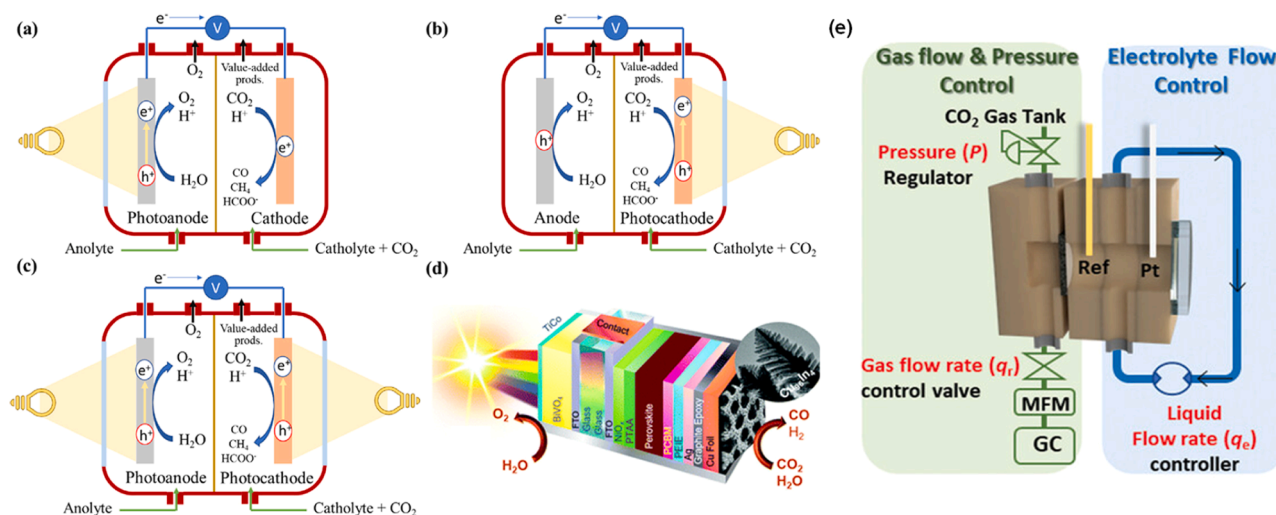


Fig. 5. Schematic architectures of photoelectrochemical (PEC) systems for CO₂ reduction: (a) photoanode-based system, (b) photocathode-based system, (c) integrated photoanode/photocathode system, and (d) photovoltaic (PV)-assisted tandem configuration. Panels (a–d) adapted with permission from reference (Antonio Abarca et al., 2023), © 2023 Elsevier. (e) Continuous-flow PEC reactor for CO₂ conversion, adapted with permission from reference (Jung et al., 2024), © 2024 Wiley.

reducing power, which is critical to improving CO₂ fixation efficiency. Recent advancements in genetic engineering and synthetic biology are explored, illustrating how both native and engineered microbial platforms are being leveraged to convert CO₂ into food sources and high-value bioproducts. Collectively, these innovations underscore the transformative potential of biological CO₂ conversion technologies in mitigating greenhouse gas emissions and supporting a sustainable future.

6.1. Microbial CO₂ reduction pathways

Recent studies have significantly advanced our understanding of microbial CO₂ reduction, highlighting the potential of autotrophic microorganisms to convert CO₂ into useful organic compounds. Autotrophic microorganisms, such as certain species of bacteria, algae, and archaea, possess natural CO₂-fixing pathways, including the Calvin-Benson-Bassham (CBB) cycle, the reductive tricarboxylic acid (rTCA) cycle, and the acetyl-CoA pathway (Fig. 3) (Lee et al., 2025; Claassens et al., 2016; Liang et al., 2020). These pathways allow microbes to capture CO₂ directly from the atmosphere or from industrial emissions and convert it into biomass or valuable metabolites like ethanol and methane (Srisawat et al., 2022). Recent studies have also explored the optimization of these natural CO₂-fixing pathways through metabolic engineering, improving the efficiency and yield of microbial CO₂ conversion (Choi et al., 2022). Enzyme-based conversion within these organisms is being engineered to increase CO₂ reduction rates, with some promising results in enhancing carbon fixation through directed evolution and gene editing (Long et al., 2017). Additionally, the integration of synthetic biology approaches has opened up new avenues for creating hybrid pathways that combine the best features of natural and engineered systems to maximize CO₂ conversion efficiency.

6.2. Enzyme-based CO₂ conversion

Enzyme-based CO₂ conversion has gained significant attention due to the specificity and efficiency of biological catalysts. Carbonic anhydrases (CAs), for instance, are enzymes that play a pivotal role in CO₂ fixation, facilitating the reversible hydration of CO₂ to bicarbonate (Sharma et al., 2020). The catalytic activity of carbonic anhydrases is critical for processes such as photosynthesis, and recent advances have focused on optimizing these enzymes for industrial CO₂ conversion applications (Russo et al., 2022). Other enzymes, such as carbon monoxide dehydrogenase and other CO₂-reductase enzymes, are also being studied

for their role in reducing CO₂ into valuable products (Bährle et al., 2023). These enzymes exhibit high specificity for CO₂, making them ideal candidates for use in bioreactors or other conversion systems (Bierbaumer et al., 2023). Advances in enzyme engineering, including site-directed mutagenesis and protein stabilization techniques, are helping to enhance the catalytic efficiency and stability of these enzymes, allowing for their application in more demanding industrial processes (Liu et al., 2019). The development of artificial enzyme systems and enzyme cascades, combining multiple enzymes for stepwise CO₂ conversion, is also a promising area of research to improve overall conversion rates and product selectivity (Qiao et al., 2023).

6.3. Strategies in genetic engineering and synthetic biology

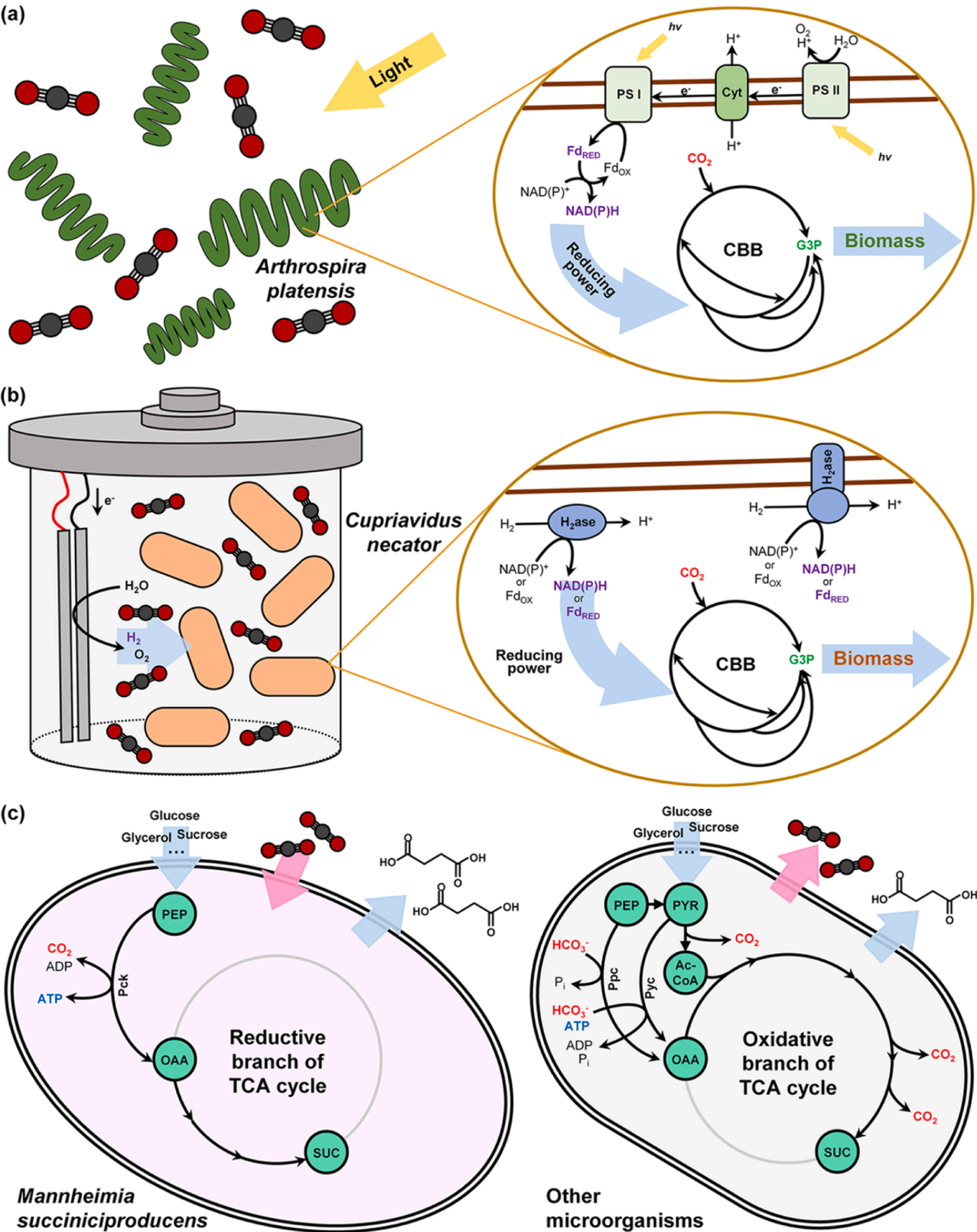
Genetic engineering and synthetic biology are transforming the potential of biological CO₂ conversion by enabling the creation of custom-designed organisms and pathways for enhanced CO₂ fixation (Gurawalia et al., 2024; Almomani et al., 2023; Tan and Nielsen, 2022). One of the most exciting innovations in this field is the use of CRISPR-Cas9 gene editing to modify microorganisms for more efficient CO₂ assimilation (Garg et al., 2023). By precisely editing the genomes of microbes, researchers can enhance their natural CO₂ fixation abilities (Priyadharsini et al., 2022) or introduce entirely new pathways, such as the incorporation of non-native carbon fixation pathways like the 3-hydroxypropionate cycle (Zahed et al., 2021; Barati et al., 2021; Hendriks, 2023). In addition to CRISPR, synthetic biology tools like pathway optimization and gene synthesis allow for the construction of entirely synthetic microbial systems that can efficiently convert CO₂ into desired products (Chen et al., 2018; Correa et al., 2023; Salehizadeh et al., 2020; Ko et al., 2020). Advances in genome-wide engineering, along with the development of modular genetic parts, are making it possible to engineer more robust microbial platforms that can operate in diverse and challenging environmental conditions (Wang et al., 2024). These synthetic biology approaches are key to realizing the commercial potential of CO₂ bioconversion, as they can improve both the rate and efficiency of CO₂ fixation, while also enabling the production of high-value bioproducts from CO₂.

7. Integration of CO₂ conversion with industrial and renewable systems

The unprecedented rise in carbon dioxide emissions poses an urgent environmental challenge that demands innovative strategies to mitigate

its harmful effects. Both human activities and natural processes contribute to CO₂ emissions, with fossil fuel combustion accounting for the largest share globally. Power plants, which burn fuels such as natural gas, oil, and coal, are among the primary sources of CO₂ emissions.

Additionally, industrial processes including cement manufacturing, steel production, and chemical synthesis release significant amounts of CO₂, as do various other production methods (Dang et al., 2024). Other notable contributors include energy generation, transportation, and



(caption on next page)

Fig. 6. Biological Conversion of CO₂ into Valuable Organic Compounds via CO₂-Utilizing Bacteria and Their Native Metabolic Pathways. (a) Spirulina Production: *Arthrospira platensis*, a photosynthetic cyanobacterium, converts CO₂ into nutrient-rich biomass (spirulina) through the Calvin-Benson-Bassham (CBB) cycle. Light-harvesting photosystems (PS I and PS II) generate high-energy electrons from water (H₂O), providing the reducing power necessary for CO₂ fixation. (b) Microbial Protein Production: The chemolithotrophic bacterium *Cupriavidus necator* synthesizes proteins using CO₂ during fermentation. Renewable energy sources (e.g., solar, wind, or tidal) drive in situ water electrolysis to produce H₂ and O₂. These gases are consumed by the bacterium, where hydrogenases (H₂ases) facilitate electron transfer, generating reducing equivalents and ATP. These energy carriers enable CO₂ conversion into protein and biomass via the CBB cycle. (c) Succinic Acid Production: *Mannheimia succiniciproducens*, a heterotrophic bacterium, assimilates CO₂ and renewable carbon substrates to produce succinic acid. Unlike most microbes that emit CO₂ during the oxidative tricarboxylic acid (TCA) cycle, *M. succiniciproducens* uses a reductive TCA cycle, fixing two CO₂ molecules to generate two succinic acid molecules from one six-carbon sugar (e.g., glucose) or two three-carbon compounds (e.g., glycerol). In the figure, CO₂ and HCO₃⁻ are marked in red, pathway products in green, reducing agents in purple, and ATP in blue. Native metabolic pathways are shown with black arrows, while unused or alternative routes are indicated in grey for comparison. Key Metabolites: Ac-CoA (acetyl-CoA), FdOX (oxidized ferredoxin), FdRED (reduced ferredoxin), G3P (glyceraldehyde 3-phosphate), PEP (phosphoenolpyruvate), PYR (pyruvate), OAA (oxaloacetate), SUC (succinate). Key Enzymes: Cyt (cytochrome), H₂ase (hydrogenase), Pck (phosphoenolpyruvate carboxykinase), Ppc (phosphoenolpyruvate carboxylase), PS I/II (photosystems I/II), Pyc (pyruvate carboxylase) (Jung et al., 2023).

diverse industrial operations. Integrating CO₂ conversion technologies, as illustrated in Fig. 7, with industrial and renewable energy systems offers a promising pathway to transform greenhouse gases into valuable, market-ready products while advancing sustainable energy solutions (Zhao, 2024). This strategy could help industries achieve up to half of their carbon neutrality goals and reduce global CO₂ emissions by 4 to 10 gigatons annually by 2050.

Many researchers show intense interest in building and deploying massive-scale systems that capture and transform CO₂ emissions. CO₂ utilization technologies have recently achieved promising results through current technological developments. These technologies offer the opportunity to transform CO₂ into useful liquid fuels and chemicals through complex capture systems including solvent-based, solid sorbent-based and membrane-based systems that work together with multiple conversion pathways such as thermochemical electrochemical photochemical and biochemical processes (Jiang et al., 2024). The combination of electrochemical methods with photocatalytic and photosynthetic technologies has shown successful production of chemical fuels and building materials (Karishma et al., 2024; Dang et al., 2024). The environmental impact of CO₂ decreases alongside large-scale implementation potential when renewable energy sources are employed to run CO₂ conversion operations. Several advantageous points emerge from this integrated approach. Industry participation

leads to reduced non-renewable resource usage while advancing the adoption of circular economy principles by using carbon dioxide-derived materials instead of fossil fuel-based initial materials. As such, CO₂ utilization has increased because it represents an alternative to geologic storage systems and creates valuable products while improving economic viability.

Furthermore, the transformation of CO₂ into fuels along with plastics, fertilizers and building materials represents an advanced technology being actively developed today (Zhao, 2024; Kuang et al., 2025; Al Harthi et al., 2024; Alok et al., 2022). The widespread implementation of these technologies depends on solving fundamental problems regarding their power consumption and the scale of necessary infrastructure deployment. Researchers currently focus on three main objectives, developing methods to overcome current obstacles while building affordable conversion technologies and finding solutions to existing commercial and regulatory barriers for wide-scale implementation.

7.1. Coupling CO₂ conversion with renewable energy systems

Carbon dioxide conversion technologies represent a promising research direction for converting powerful greenhouse gases into useful products (Jiang, 2025; Shen et al., 2025). These adopt the use of

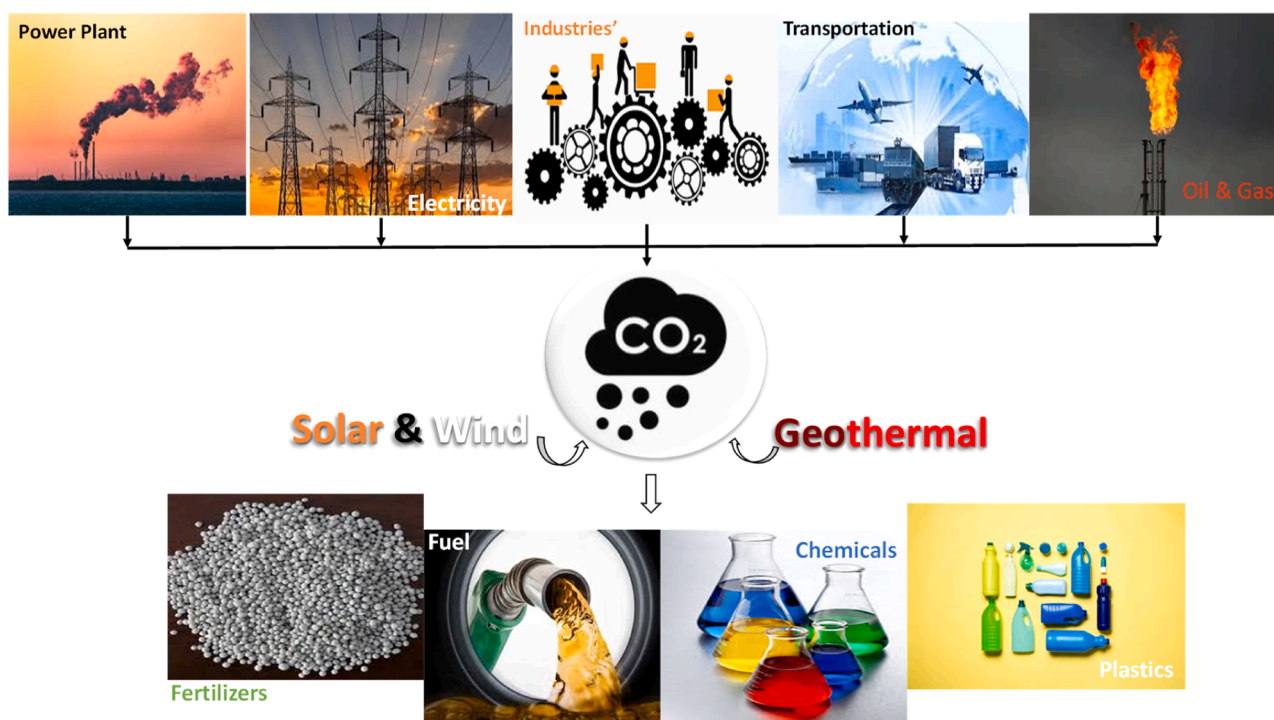


Fig. 7. Conversion of Carbon dioxide into Value-added products.

renewable energy systems which include, wind, solar and geothermal-driven CO₂ conversion systems.

Wind Energy

Wind energy has emerged as a leading enabler of CO₂ conversion technologies, offering a renewable and low-carbon alternative to fossil fuels for powering energy-intensive processes. By integrating wind power into CO₂ conversion systems, particularly for fuel production, it becomes possible to significantly reduce greenhouse gas emissions while advancing the global transition to sustainable energy (Assareh *et al.*, 2024; Gabbar and Ramadan, 2025). Wind energy's intermittent yet abundant nature makes it ideal for scalable CO₂-to-fuel applications such as methanol synthesis, hydrogen generation, and methanation. Recent advances focus on power-to-liquid (PtL) strategies, combining wind electricity with electrochemical CO₂ reduction. For example, Fogel *et al.*, (Schreiber *et al.*, 2024) conducted a life-cycle assessment of methanol and dimethyl ether production using wind-powered electrolyzers, demonstrating substantial emission reductions compared to conventional methods.

In their study, Fogel *et al.* described the synthesis of methanol via the catalytic hydrogenation of CO₂ and H₂ at 80 bar and 250 °C using a CuO/ZnO/Al₂O₃ catalyst. The process involves compressing feed gases, pre-heating via heat exchange with the product stream, and incorporating two recycled streams obtained through sequential flash separation. The final output, a 50:50 molar mixture of methanol and water, is separated via distillation to yield methanol with >99.85 wt.% purity.

Expanding on this, Stefan Fogel *et al.* (2024) emphasized the role of proton-conducting solid oxide electrolysis (SOE) cells coupled with wind energy in power-to-methanol pathways. Their study highlighted the cost-effectiveness and reduced carbon footprint of this integration, positioning it as a critical solution for sustainable fuel production. Moreover, Yunxia Long *et al.* (2023) assessed the global impact of installed wind capacity in curbing CO₂ emissions. In 2021, 837 GW of wind energy across 31 countries generated approximately 2186 TWh of electricity, reducing emissions by around 1311 Mt. Projections suggest wind could supply over 30 % of global electricity by mid-century, potentially cutting CO₂ emissions by 14,871 Mt by 2050 and 32,864 Mt by 2100. Importantly, the geographic shift of wind energy potential toward southern regions enhances deployment prospects in low-latitude countries such as Brazil, Vietnam, and those in Central Africa. Overall, coupling wind energy with CO₂ conversion technologies not only mitigates climate change but also enhances the resilience and sustainability of global energy systems.

Solar-powered CO₂ conversion system

Solar-powered CO₂ conversion systems offer a sustainable path to reducing carbon emissions while producing valuable fuels and chemicals. Advancements in photocatalysis and material engineering continue to enhance efficiency and scalability. With further innovation, these systems can play a crucial role in achieving carbon neutrality and a cleaner energy future.

The conversion of CO₂ into value-added products requires substantial energy input, with solar energy emerging as a sustainable alternative to conventional power sources. Solar-powered CO₂ conversion represents a key technological advancement, enabling direct use of renewable energy and reducing reliance on fossil fuels (Al Harthi *et al.*, 2024; Nguyen and Zondervan, 2019; Kim *et al.*, 2025; Fu *et al.*, 2024). These technologies typically employ photochemical, photocatalytic, and photo-electrochemical methods to convert CO₂ into useful compounds through photonic energy input (Song *et al.*, 2025; Li *et al.*, 2021).

For example, H. Yamaguchi *et al.* (Orege *et al.*, 2023) developed a solar-powered Rankine cycle system utilizing supercritical CO₂ for both electricity and heat generation. The system, driven by evacuated solar collectors, heats CO₂ to supercritical temperatures, which then powers a turbine to generate mechanical energy. The resulting energy supports various applications, including refrigeration, air conditioning, and hot water supply. The system demonstrated stable operation in the trans-critical region, with estimated power generation and heat recovery

efficiencies of 0.25 and 0.65, respectively.

In another development, Hunter Shirley *et al.* (Zhao *et al.*, 2023) reported a durable photocatalytic system that uses a nickel-based redox-active bipyridyl-N-heterocyclic carbene macrocyclic ligand to convert CO₂ or CO into CH₄. This solar-driven system achieved up to 19,000 turnovers for CH₄ production from CO₂ and an exceptional 570,000 turnovers from CO hydrogenation using light, highlighting its potential for producing high-energy solar fuels.

The integration of CO₂ conversion with renewable energy platforms provides a promising route for greenhouse gas mitigation and sustainable chemical production. Notably, solar energy serves as a clean, abundant power source for driving electrochemical CO₂ reduction systems. Chen *et al.* (Jiang *et al.*, 2025), for instance, developed a biohybrid photosynthetic system that efficiently converts CO₂ into long-chain chemicals using solar energy. Similarly, a liquid-based direct air capture (L-DAC) system, incorporating hydrogen-fluidized solar calcination, was proposed to convert captured CO₂ into sustainable aviation fuels (Yin *et al.*, 2025).

Sue-Faye Ng *et al.* (Zheng *et al.*, 2025) advanced the field by designing low-dimensional carbon nitride-based nanostructures for selective CO₂ conversion into C₁–C₂ products. Graphitic carbon nitride (g-C₃N₄) and its allotropes, known for their high stability, surface-area-to-volume ratio, and tunable properties, offer metal-free photocatalytic alternatives. These materials have demonstrated strong potential for energy-rich chemical production and raise important considerations for scalable catalyst design and economic feasibility.

Further innovation was achieved by Dong-Eun Lee *et al.* (Shen *et al.*, 2025), who created a ternary hybrid photocatalyst—NiAl-LDH@TiO₂/Ti₃C₂—with an S-scheme heterointerface via in situ growth. This hybrid system, responsive to ultraviolet, visible, and near-infrared light, achieved 99 % CO selectivity over H₂ and an apparent quantum yield of 0.81 at 365 nm, while maintaining strong stability across multiple CO₂ reduction cycles. Their work presents a strategic approach to constructing efficient photocatalysts for solar-powered CO₂ reduction. Additionally, Rehana Shahin *et al.* (Sun *et al.*, 2025) introduced a solvent-free sulfur-bridge eosin-Y (SBE-Y) polymeric framework photocatalyst synthesized via in situ thermal polymerization. The integration of elemental sulfur enhanced the light absorption capabilities of eosin-Y. The resulting photocatalyst, when used in an enzyme-assisted artificial photosynthesis system, achieved a high NADH regeneration efficiency of 86.81 % and enabled formic acid production (210.01 μmol) along with fine chemical synthesis at 99.9 % yield. This work underscores the potential of solar-driven photocatalytic systems for environmental purification and advanced chemical synthesis.

Overall, solar-powered CO₂ conversion technologies present a sustainable and scalable path for reducing carbon emissions while generating valuable chemicals and fuels. Continued advancements in photocatalyst design, material engineering, and integration strategies will be critical to realizing the full potential of these systems in the global pursuit of carbon neutrality.

Geothermal-powered CO₂ conversion system

The growing interest in geothermal systems as a means to address climate change has been amplified by the global shift toward renewable energy sources. Geothermal energy presents a compelling opportunity for CO₂ conversion by leveraging the Earth's natural heat. Utilizing CO₂ as a working fluid in geothermal power generation offers multiple advantages, including carbon sequestration, enhanced heat extraction efficiency, and reduced environmental impact during power generation. Its unique thermophysical properties make CO₂ an effective medium for subsurface heat extraction, thus expanding the feasibility of land-based geothermal systems.

Integrating CO₂ conversion with geothermal systems offers a promising route for sustainable energy and carbon management. These integrated systems not only enable long-term CO₂ storage but also facilitate its conversion into valuable chemicals or fuels. For instance,

Justin Ezekiel et al. (Lamichhane et al., 2024) investigated the use of supercritical CO₂ as a working fluid in deep natural gas reservoirs to serve dual functions: enhanced gas recovery (EGR) and CO₂-Plume Geothermal (CPG) energy extraction. Their study proposed a Carbon Capture, Utilization, and Underground Storage (CCUUS) system that leverages a shared subsurface infrastructure and a common working fluid. Simulations demonstrated that the injection of CO₂ for EGR could seamlessly transition into the CPG phase, where a CO₂ mass flow rate of 110 kg/s yielded a net power output of 2 MWe in a pilot-scale setup—highlighting the scalability and efficiency of this approach.

Similarly, Jimmy B. Randolph et al. (Ghazi et al., 2024) emphasized the potential of using CO₂ not as a waste product but as a viable working fluid for geothermal energy capture. Due to its superior thermodynamic and fluid dynamic properties compared to water, CO₂ can transfer geothermal heat more efficiently. This not only improves energy recovery but also enhances the economic viability of CO₂ sequestration. Furthermore, it opens up possibilities for utilizing lower-temperature geological formations that are typically considered uneconomical for conventional geothermal systems.

In another notable study, Mark R. Fleming et al. (Ewis et al., 2023) introduced the Flexible CO₂-Plume Geothermal (CPG-F) system, which employs geologically stored CO₂ to provide on-demand power, energy storage, or both simultaneously. Their findings showed that while a CPG-F system could deliver 7.2 MWe for 8 hours—a 190 % increase over standard CPG power output—its total daily energy production dropped by 61 % (from 60 MWe-h to 23 MWe-h). Despite a 70 % higher initial cost than traditional CPG systems, the CPG-F design offers flexible operational modes and generates 90 % to 310 % more power, depending on the configuration. The cost difference between a CPG-F facility with dual-mode capability and one dedicated solely to energy storage was marginal, at just 3 %.

Additional studies have further explored innovative integrations of CO₂ utilization with geothermal systems. One such study (Yang et al., 2025) examined the combination of geological CO₂ sequestration with Aquifer Thermal Energy Storage (ATES), demonstrating the feasibility of simultaneously storing CO₂ and harvesting thermal energy for electricity generation and district heating. Luo (2024) reported on coupling CO₂ electrochemical conversion with geothermal systems, wherein renewable electricity drives CO₂ reduction—achieving high efficiency and carbon neutrality.

Enhanced Geothermal Systems (EGS) that employ supercritical CO₂ are particularly promising. These systems enhance geothermal energy recovery while directly utilizing CO₂ as the heat transfer medium, thus contributing to emission reductions (Liu et al., 2025). Furthermore, hybrid models integrating solar, wind, and geothermal energy have been proposed for CO₂ conversion and mitigation, enhancing both sustainability and economic viability (Cho et al., 2024; Ali et al., 2024).

Collectively, these advancements underscore the transformative potential of integrating CO₂ conversion with geothermal technologies. By combining carbon sequestration, energy generation, and resource recovery, such systems pave the way toward carbon neutrality and a resilient, renewable energy future.

7.2. Industrial applications of converted CO₂ products

Addressing climate change demands the urgent adoption of sustainable solutions to reduce greenhouse gas emissions. One promising approach is the conversion of carbon dioxide into valuable products such as methanol, ethylene, and formic acid, as illustrated in Fig. 8. Among these, the utilization of CO₂ for methanol production has attracted considerable attention, offering an efficient pathway to transform a major greenhouse gas into commercially useful chemicals

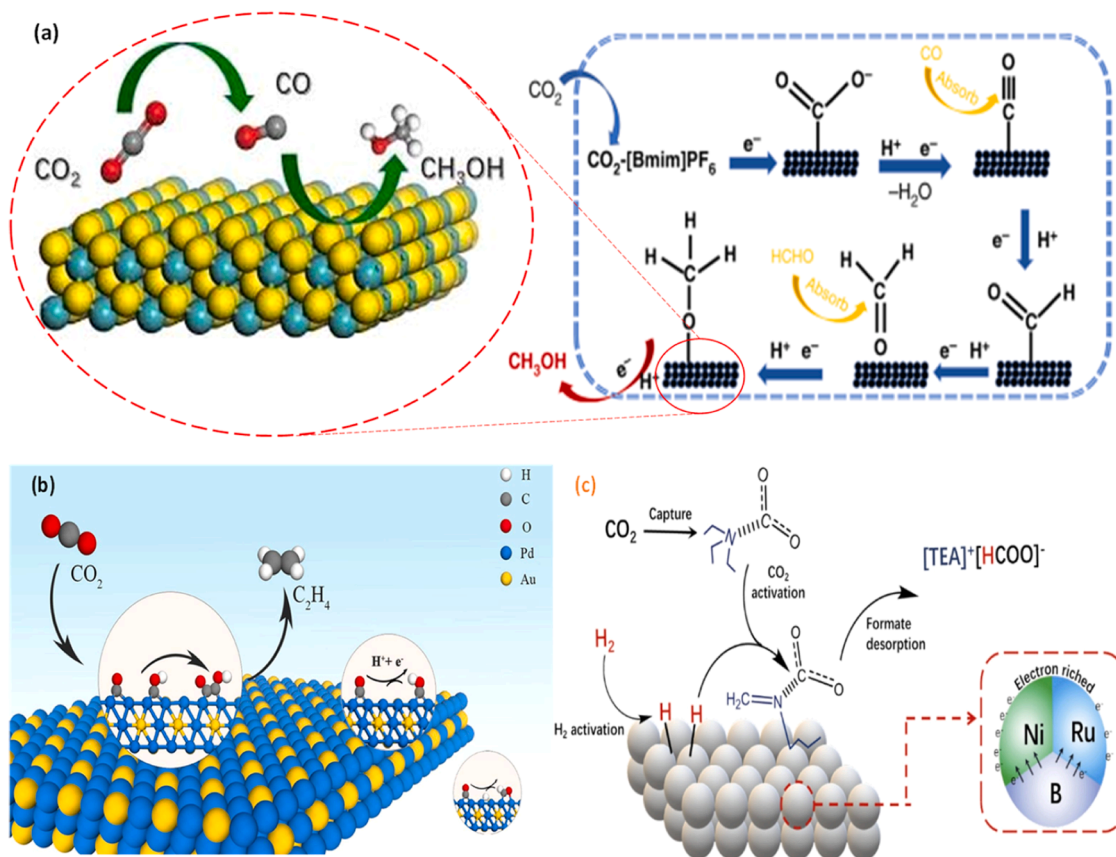


Fig. 8. Conversion of CO₂ into (a): Methanol. Printed with permission from (Yang et al., 2019). Copyright 2019, Springer Nature (b): Ethylene. Adapted with permission from (Zheng et al., 2022). Copyright 2022, Elsevier and (c) Formic acid. Adapted with permission from (He et al., 2021). Copyright, 2021, Elsevier.

and fuels.

The conversion of CO₂ into methanol presents a promising avenue for sustainable manufacturing, offering a dual benefit: reducing carbon emissions and generating valuable synthetic methanol. As global concerns over climate change intensify, CO₂-derived products have gained significant industrial relevance. Researchers have demonstrated several efficient chemical pathways for methanol synthesis from CO₂, including direct hydrogenation and syngas production via bi-reforming (Marques da Cunha et al., 2025; Nguyen and Zondervan, 2019).

Methanol is a versatile platform chemical widely used in fuels, plastics, and pharmaceuticals, making its production from captured CO₂ a compelling strategy for sustainable industry. For instance, Sachin Kumar Sharma et al. (Kim et al., 2025) developed a highly stable MgO-enhanced Cu/ZnO catalyst that achieved over 99 % selectivity for methanol via CO₂ hydrogenation. The inclusion of Mg atoms in ZnO created defect sites enhancing CO₂ adsorption, while the Cu-ZnO interface facilitated activation of CO₂ molecules. A catalyst containing 20 wt % MgO proved most effective for selective hydrogenation. In a complementary study, Jinfeng Fu et al. (2024) conducted a process simulation to evaluate methanol production via CO₂ hydrogenation in a packed bed reactor. Their findings revealed that the reactor temperature initially increased due to exothermic reactions, followed by a slight decline near the top section. CO₂ conversion improved with higher reaction temperatures and pressures rising from 18.18 % at 475 K to 23 % at 498–555 K, and increasing with inlet pressures from 35 bar to 55 bar, reaching a peak conversion of 22.96 %.

Further advancement in catalyst design was demonstrated by Lixin Song et al. (2025), who investigated cation rearrangement in Cu/ZnAl₂O₄ spinel catalysts. Their study revealed that disordered structures (e.g., AlO₄ and ZnO₆) promoted the formation of oxygen vacancies and surface hydroxyl groups, which facilitated the dispersion of small Cu species. This enhanced metal-support interaction (MSI) and hydrogen spillover, ultimately boosting CO₂ conversion and methanol space-time yield (STY). These findings offer new insight into optimizing spinel catalysts for CO₂ hydrogenation. In addition, recent research has emphasized integrating renewable energy sources into CO₂-to-methanol processes. The combination of reverse water-gas shift reactions and green hydrogen (via electrolysis) enables industrial-scale methanol production while utilizing waste CO₂ streams (Li et al., 2021; Orege et al., 2023). Improvements in Cu-based catalysts have further increased reaction rates and selectivity, supporting the feasibility of large-scale deployment. Collectively, these innovations position CO₂-to-methanol conversion as a pivotal element in the transition to a circular carbon economy—addressing emissions while supplying key industrial chemicals.

Moreover, the transformation of CO₂ into high-value products such as ethylene represents another major advancement in sustainable industrial chemistry. Ethylene, a vital precursor for plastics, adhesives, and solvents, has seen increasing interest in production from CO₂ through electrochemical, catalytic, and plasma-assisted processes. Among these, electrochemical reduction has emerged as a leading approach, with recent studies demonstrating high selectivity and efficiency. Notably, innovations like bilayer ionomer coatings have enabled ampere-level current densities and significant Faradaic efficiencies (Zhao et al., 2023; Jiang et al., 2025; Yin et al., 2025). These developments are paving the way for scalable CO₂ electrolysis systems aimed at ethylene and ethanol production.

Electrochemical CO₂ reduction has emerged as a promising strategy to mitigate environmental challenges while generating value-added chemicals and fuels. According to Zheng et al. (2025), converting CO₂ into ethylene (C₂H₄) via electrochemical methods offers an effective route to address energy and environmental concerns. Functionalizing copper-based metal-organic frameworks (MOFs) with crown ether (CE) significantly enhances C₂H₄ selectivity, improving the faradaic efficiency (FE) of CuBTC, CuBDC, and CuBDC-NH₂ by factors of 3.1, 1.7, and 2.4, respectively. Among these, CuBTC demonstrated the highest FE for

ethylene, reaching approximately 52 % at 120 mA cm⁻². Shen and co-workers (Shen et al., 2025) reported nitrogen-doped Cu₂O catalysts with tunable Cu⁰/Cu⁺ ratios for selective CO₂-to-ethylene conversion. Through NH₃/Ar plasma treatment, the Cu⁰/Cu⁺ ratio was varied from 0.16 to 15.19, with an optimal value of 0.43 yielding enhanced C₂ product formation. This strategy provides a rational pathway for designing high-performance electrocatalysts. Similarly, Sun and co-authors (Sun et al., 2025) developed an Ag-modified CuO catalyst (CuO/Ag@C) derived from MOFs, where the porous carbon framework controlled nanoparticle size and exposure of active sites. The catalyst achieved a FE of 48.6 % for ethylene at -0.7 V vs. RHE, exhibiting strong stability and catalytic performance. Plasma-assisted CO₂ conversion has also demonstrated potential for C₂H₄ generation, leveraging plasma discharges to form reactive intermediates that interact with CO₂ to produce hydrocarbons like ethylene and polyethylene precursors (Lamichhane et al., 2024). These approaches, due to their scalability and compatibility with renewable energy, reinforce the commercial viability of CO₂-derived ethylene for use in packaging, polymers, and fuels.

Formic acid is another key CO₂-derived product gaining industrial relevance due to its diverse applications and role as a hydrogen carrier. Electrochemical reduction of CO₂ to formic acid has shown high faradaic efficiencies, making it commercially attractive (Ghazi et al., 2024; Ewis et al., 2023). With its high hydrogen density, non-toxicity, and liquid-phase stability, formic acid is an ideal medium for hydrogen storage and transport (Ghazi et al., 2024). Photocatalytic and photo-electrochemical routes have further enhanced CO₂ conversion efficiency. Yang et al. (2025) introduced a nickel-perylene-carbon nitride nanosheet (Nickel-Perylene-C₃N₄) for selective solar-driven CO₂ reduction to formic acid. The complexation at nitrogen sites and band structure optimization resulted in 60 % selectivity toward formic acid. Ya Liu et al. (2025) explored a Cu₂O-based multilayer photoelectrode (Cu₂O/Ga₂O₃/TiO₂/In) for CO₂ photoelectroreduction, achieving a photocurrent density of 2.21 mA/cm² at -0.9 V (vs. Ag/AgCl) and a 62.1 % FE for formic acid, maintaining operational stability for up to 180 min. Jinwon Cho et al. (2024) developed 2D metal/graphene and metal/graphene/metal hybrid systems, where metal monolayers were deposited on graphene to create highly active electrocatalysts. Strong covalent bonding and sp-d orbital hybridization enabled excellent CO₂-to-HCOOH conversion, particularly with Pd/G, Pt/G/Ag, and Pt/G/Au catalysts. Sajjad Ali et al. (2024) investigated aza-doped graphene-analogous 2D materials as bifunctional catalysts for CO₂ hydrogenation and electroreduction to formic acid. Their reaction pathway showed a low energy barrier (0.78 eV) for thermal conversion and an electroreduction overpotential of just 0.46 V, indicating high catalytic efficiency. In industrial applications, formic acid serves multiple roles: as a feed preservative and silage additive in agriculture, a reducing agent and intermediate in pharmaceuticals, and as a key chemical in hydrogen energy systems. Recent advances in tin- and indium-based electrocatalysts have significantly improved the efficiency and selectivity of formic acid production from CO₂, supporting its scalability for industrial use (Ghazi et al., 2024; Zhang et al., 2023; Theußl et al., 2024; Yang et al., 2025). Integrating such processes into broader hydrogenation strategies and reducing dependence on fossil fuels is pivotal for sustainable development across sectors like construction and energy.

8. Artificial intelligence (AI) in CO₂ conversion technologies

AI is crucial to the success and swift maturity of CO₂ utilization technologies and achieving a carbon neutral future (Chen et al., 2023). AI is crucial for accelerated transition towards carbon-neutrality and several attempts are already being made to use it to identify research gaps, improve and discover new catalysts covering aspects such as the active materials, performance and lifecycle; optimize CO₂ conversion reaction pathways, reactors and processes to obtain specific products, and identify new/replacement value added fuel or chemical products that use high amounts of CO₂; and carry out techno-economic and life

cycle assessments to predict performance ranges of conversion technologies to inform decision making (Jerng et al., 2024; Hussin et al., 2023; Guo et al., 2021; U. States Department of Energy, 2024). Several artificial intelligence aspects have already been applied in CO₂ utilization aspects, with machine learning coupled with computational methods such as density functional theory (DFT) and the relative force-field (ReaxFF) occupying most reports in literature (Jerng et al., 2024). Hussin et al. applied bibliometric analysis and noted a drastic increase in publications containing keywords to do with CO₂ utilization and the use of AI and machine learning in the recent years indicating the reception of these subjects (Hussin et al., 2023). AI tools have been applied to predict the thermodynamic and electronic properties of materials and reveal catalytic mechanisms, helping with the discovery, optimization and acquisition of high-performance (activity and selectivity) CO₂ conversion catalysts, as well as optimize reaction conditions (Zhong et al., 2020; Jerng et al., 2024). Several successful comprehensive machine learning models have already been used to discover novel catalysts, reveal complex reaction mechanisms and attain high predictive performance (Jerng et al., 2024; Guo et al., 2021). Table 5 summarizes various analyses of AI algorithms in providing solutions for CO₂ utilization strategies, as well as typical works where the tools have provided guidance in the works. A typical AI generated maps that can be useful in making informed decisions during development of catalysts for CO₂ utilization is also presented in Fig. 10 (Zhong et al., 2020).

Accelerated catalyst design and discovery can mainly be attributed to AI tools being computationally efficient surrogates which carry out less expensive/resource intensive quantum chemical calculations (Jerng et al., 2024; Zhang et al., 2022). The biggest advantage of artificial intelligence lies in the ability of algorithms to effectively analyze large data sets and understand relationships or patterns that cannot be easily or immediately picked up by humans using descriptors that are designed to reflect prior human knowledge. As such, faster, efficient and cheaper screening of innovative and superior CO₂ conversion catalysts and better reaction pathways can be accomplished (Jerng et al., 2024). Complex compositions and hierarchical structures which cannot be solved independently or cannot be easily solved using traditional methods can also be addressed through artificial intelligence.

Given the growing interest in applying AI to CO₂, there is a pressing need to establish standardized benchmarks and methodologies to guide its implementation and accelerate progress. Advanced machine learning (ML) models are essential to fully exploit the vast and growing databases of molecules and materials, as well as to explore untapped regions of chemical space. However, significant gaps remain in the application of cutting-edge techniques such as self-supervised learning, deep generative models, and large language models, which have yet to be fully harnessed. Furthermore, the development of comprehensive databases and detailed, step-by-step protocols for implementing ML algorithms in CCSU processes is urgently needed (Zhu et al., 2025).

Jerng et al. conducted a comprehensive comparative study of ML algorithms applied to CO₂-to-methanol conversion, evaluating their performance across various case studies. They emphasized key research priorities, including addressing data scarcity, improving model interpretability, standardizing evaluation metrics, integrating domain knowledge, and minimizing overfitting (Vanjari et al., 2023). Experimental data, in particular, is critical for the success of ML applications, and its limited availability in certain areas remains a major barrier. Notably, there is a discernible bias in the literature toward the use of AI/ML in carbon capture and storage, compared to utilization. This can largely be attributed to the more mature industrial development and data availability in the former fields (Li et al., 2023; Alimi et al., 2020; Onisuru et al., 2021).

Despite the promise of AI, its heavy reliance on descriptor-performance relationships poses limitations, especially when extrapolating to novel systems with new variables (Alimi et al., 2020). To overcome these challenges, hybrid approaches are emerging such as combining conditional generative models with ML simulations or

integrating ML with experimental validation to create more effective and adaptive frameworks (Alimi et al., 2019). Improving model interpretability is also crucial, particularly in revealing reaction mechanisms and informing catalyst design.

A more holistic adoption of AI across the research pipeline is advocated, as demonstrated by Nia et al., who used ML to predict CO₂ conversion efficiency, methanol and CO selectivity, while enabling process optimization, techno-economic analysis, and life-cycle assessment (Alimi et al., 2020). Numerous other studies have also begun to showcase the growing integration of AI in CO₂ utilization research (Alimi and Meijboom, 2021; Potgieter and Meijboom, 2021; Guzmán et al., 2021). Importantly, AI is not a replacement for rigorous theoretical and experimental work; rather, it serves to enhance and accelerate discovery by narrowing search spaces and directing resources toward high-potential systems (Alimi et al., 2020). The future of AI in advancing CO₂ utilization technologies is promising. As summarized in Table 5, there is a prevailing preference for Gradient Boosted Regression Trees (GBRT) and Artificial Neural Networks (ANNs), with the latter often demonstrating superior accuracy and desirability for predicting catalyst performance (Arya et al., 2025; Centi et al., 2020; Lee et al., 2023; Hepburn et al., 2019; Schmidt et al., 2018; Martins et al., 2023).

In thermochemical conversion, the widespread adoption of AI and new technologies has influenced catalyst design, characterization and rapid evaluation of catalysts in the future. For instance, new catalysts and reactors have been developed by additive manufacturing techniques (Alimi et al., 2020; Onisuru et al., 2021; Alimi et al., 2020, 2019, 2020, Alimi and Meijboom, 2021), rapid screening of catalysts using high throughput systems (Potgieter and Meijboom, 2021), new reaction technologies; flow chemistry, lab on a chip and microreaction technology will promote faster reaction. In addition, the introduction of synthesis robots in the laboratory will promote safety, reduce human error, eliminate repetitive tasks and improve precision and accuracy.

9. Techno-economic analysis on CO₂ conversion technologies

While there are several CO₂ conversion technologies ranging from electrochemical, photochemical, biochemical to thermocatalytic, technoeconomic analyses have mainly been applied to electrochemical and thermocatalytic processes, or their combination, since the former is regarded as due to the use of renewable electricity and the latter being the most efficient in yielding profitable products (Guzmán et al., 2021).

Considering the hype towards utilization of CO₂ and its importance as a tool for reducing atmospheric CO₂ there is no doubt about the importance of carrying out techno-economic and life-cycle assessments of the various proposed approaches to weigh their feasibility for industrial implementation and their overall benefits on climate mitigation (Centi et al.). Lee et al. indicate that the choice of CO₂ source is more than an issue of raw input feedstock cost since the quality (concentration and purity) have a crucial impact on the carbon intensity of the final products (Lee et al., 2023). Scaling up the cheapest CO₂ utilization pathways will facilitate market penetration, and several techno-economic assessments have been carried out in that regard (Hepburn et al., 2019). However, several challenges are cited to impede the success of most of these pathways, including cost competitiveness, technology limitations and energy sources (Hepburn et al., 2019). Lack of complete demonstration of these pathways and lack of agreement on generally acceptable techno-economic assessment methods have been cited as considerable challenges (Centi et al., 2020; Schmidt et al., 2018; Martins et al., 2023). Proper guidance during data analysis and contextualization of the results is needed to effectively draw conclusions from reports (Centi et al.). Verma et al also identify lack of information on durability and cell potentials as a challenge for assessment of commercial viability systems (Verma et al., 2016). Most reports apply technical parameters representative of current technological states in their baseline cases and draw input data and assumptions from literature (Grim et al., 2022). On the outlook, it is important to consider a future

Table 5Literature demonstrating application of AI models in CO₂ utilization strategies as well as contrasting the capabilities of the algorithms used.

Aspect	AI approach	Investigation	Findings	Ref
Electrochemical CO ₂ reduction catalysts	DFT studies were conducted using the VASP within the Atomic Simulation Environment. Intermetallic crystal structures obtained from the Materials Project were analyzed using pymatgen to enumerate symmetrically distinct surface facets with Miller indices ranging from -2 to 2	To establish a fully automated framework for the continuous generation and storage of DFT data using a screening approach that integrates machine learning and optimization algorithms to guide density functional theory calculations for predicting electrocatalyst performance	Identified candidate surfaces across intermetallics with a potentially high CO ₂ reduction activity and Hydrogen evolution, most of which have already been validated by literature experiments	(Tran and Ulissi, 2018)
Electrochemical conversion catalysts	Artificial neural network	Determining CO adsorption energies on multi-metallic alloy catalyst surfaces.	100 high-performance terminated Cu complex potential catalysts were identified.	(Ma et al., 2015)
Electrochemical catalysts	DFT studies using VASP	To elucidate the complete C ₁ and C ₂ reaction pathways for CO reduction on Cu(111), with a particular focus on the role of surface-bound H ₂ O in the electrochemical dehydration reduction process	Surface water on Cu important in the selectivity for hydrocarbon products over the oxygen-containing alcohol products by promoting dehydration and a strong proton donor for electrochemical dehydration reductions. Routes for major products are pH dependent.	(Xiao et al., 2017)
Electrochemical conversion catalysts	An iterative machine learning model refinement framework coupled with DFT	To investigate the nature and location of active sites in Ni/Ga intermetallic systems	Ni atoms surrounded by Ga atoms demonstrated to be optimal for CO ₂ conversion.	(Ulissi et al., 2017)
Electrocatalyst	Machine learning protocols developed	To determine ways of improving the energy efficiency and productivity (current density) of copper (the predominant electrocatalyst) for production of more valuable multi-carbon products such as ethylene at cost-competitive prices.	Density functional theory calculations coupled with active machine learning Identified Cu-Al as more efficient for reducing CO ₂ to ethylene with the highest Faradaic efficiency reported so far. Cu-Al was found to provide multiple sites and surface orientations with near-optimal CO binding for both efficient and selective CO ₂ reduction.	(Zhong et al., 2020)
Electrochemical CO ₂ reduction catalyst.	New artificial learning framework using the d-band width from muffin-tin orbital theory and the electronegativity as descriptors.	To develop a model for predicting chemisorption energies.	Highly accurate model in predicting the energies of CO adsorption onto alloy systems was developed. Cu ₃ Y@Cu* was identified as a promising electrochemical CO ₂ reduction catalyst with a lower overpotential than Au.	(Noh et al., 2018)
Electrochemical CO ₂ reduction catalyst.	AL framework	To develop protocols for the discovery of effective CO ₂ reduction electrocatalysts through theoretical screening to guide DFT calculations for reduction and H ₂ evolution.	131 candidate surfaces across various alloys of 31 different elements were determined to be potentially high-performance electrochemical catalysts.	(Tran and Ulissi, 2018)
Electrocatalysts	Machine learning-genetic algorithm (ML-GA)	To improve the CO ₂ RR capabilities of NPC regarding C ₂ products in a flow cell setup by altering process parameters during electrode preparation.	ML algorithm developed as a predictive mechanism to complement the genetic algorithm. Extreme gradient boosting regression (XGBR) algorithm has highest prediction. Experimental validation only 2.34 % off predicted result.	(Lok et al., 2023)
Single-atom alloy electrochemical reduction catalysts	XGBoost, gradient boosting regression (GBR), and ExtraTrees models using descriptors related to reaction pathways, metals, charge transfer, hydrogen-bond interactions, and geometry.	To predict CO ₂ RR reaction intermediates and products using zeolite-supported single-atom catalysts.	ZnCu, AgCu, GaCu, GeCu, and PCu single-atom alloy catalysts were identified as promising CO ₂ RR catalysts.	(Zhu et al., 2022)
Electrochemical CO ₂ and CO reduction	Probabilistic and unbiased approach by combining DFT and supervised machine learning using the Gaussian process regression model.	To predict CO and H ₂ adsorption energies on surfaces of disordered CoCu-, GaNiZn and AgAuCuPdPt alloys for enhanced selectivity for CO reduction and H ₂ suppression.	Model predicted GaNi as an optimal catalyst candidate for CO ₂ and CO reduction, even without prior knowledge of its catalytic properties. Model validated by an independent experiment.	(Pedersen et al., 2020)
Single-atom catalysts (SACs) in zeolites electrochemical reduction catalysts	DFT and machine learning models using XGBoost, GBR, and ExtraTrees algorithms.	To develop easily accessible descriptors for predicting reaction intermediates and products in CO ₂ RR using SACs in zeolites.	Adsorption free energies were highly correlated with catalytic activity. XGBoost and ExtraTrees algorithms successfully predicted free energy for all possible intermediates and product probabilities of CO ₂ reduction to methanol, methane and formaldehyde.	(Zhu et al., 2025)
Data-driven design of dual-metal-site electrochemical reduction catalysts	gradient boosting regression (GBR) model.	To determine the reaction activity and selectivity of 1218 dual-metal-site catalysts.	Mn-Ru, Mn-Os, Zn-Ru, and Co-Au-N6-Gra-model 3 were identified as promising catalysts.	(Feng et al., 2022)
(Photo)electrochemical cells	Kernel density estimation	To construct a product-performance map that shows relationships between performance figures and different classes of materials and optimization strategies for electrochemical CO ₂ reduction by analyzing	Developed experimental in situ techniques and model systems that complement theoretical efforts on unveiling performance descriptors for rational design of catalysts. Formate was	(Gastón et al., 2017)

(continued on next page)

Table 5 (continued)

Aspect	AI approach	Investigation	Findings	Ref
Photocatalysis	ML algorithms of regression, kernel and neural network-based models (ANN). The K- fold cross-validation method was employed to fine-tune the hyperparameters of the ML models.	and screening various literature approaches for designing electrocatalysts. To develop an approach for predicting the gas-phase CO ₂ photoconversion rate using various machine learning (ML) technique algorithms.	identified to potentially become the first commercially successful potentially product. ANN model showed an outstanding rating of performance evaluation metrics compared to the other ML models. Consistency of performance indicator values also observed. Good agreement of predicted CO ₂ conversion at predicted (71.32 %) vs experimental (70.60 %).	(Hossen et al., 2025)
Thermocatalysts	Generalized regression neural network (GRNN), Cascade forward neural network (CFNN), Multilayer perceptron neural network (MLP), and Radial basis function (RBF) neural network.	To predict the CO selectivity, CO ₂ conversion, and olefin selectivity	Absolute error values of 1.56 %, 6.70 %, and 3.35 % for CO selectivity, CO ₂ conversion, and olefin selectivity, respectively. CFNN and GRNN models exhibited the highest accuracy with R ² values of 0.997 for CO selectivity, 0.979 for CO ₂ conversion, and 0.975 for olefin selectivity.	(Sedighi et al., 2025)
Thermocatalysts	Artificial neural network (ANN) models based on Bayesian-Regularisation (BR) and Levenberg-Marquardt (LM) backpropagation learning algorithms. Linear, tree-based, and kernel-based ML models used to evaluate the performance of the developed ANN models.	Prediction of catalyst CO ₂ conversion activity and selectivity for lower olefins.	ANN-BR can predict CO ₂ conversion & LO selectivity with less deviation from experimental data (R = 0.90 & 0.8). Two- to three-fold increases in yields with optimized catalyst composition, operating conditions, and novel combination of catalysts compared to reported experimental results predicted.	(Chandana et al., 2023)
Thermocatalysts	Simple descriptive statistics for pre-analysis of the database. random forest (RF) model for prediction and Boruta analysis for identification of significant variables.	Predicting CO ₂ conversion through analysis of 100 catalytic CO ₂ methanation publications.	The random forest model was found to be effective at predicting CO ₂ conversion with the training and testing root mean square error (RMSE) of 6.4 and 12.7 respectively; R ² was 0.97 for training while it was 0.85 for testing. The model was validated by computing CO ₂ conversion profiles for individual experiments in test data and comparing them with literature outputs.	(Yilmaz et al., 2023)
Thermocatalysts	Data mining tools on a comprehensive dataset compiled from published literature with over 1400 experimental datapoints (including catalyst composition, synthesis methods, and reaction conditions)	Assess the performance of Cu-, Pd-, In ₂ O ₃ -, and ZnO-ZrO ₂ -based catalysts on the thermocatalytic hydrogenation of CO ₂ to methanol through a data driven framework.	Established a generic and interpretable ML framework with robust prediction abilities of methanol space time yields of various types of catalysts by coupling models with experimental assessments.	(Suvama et al., 2022)
Thermocatalysts	Artificial neural network, support vector machine regression, and gaussian process regression. Principal Component Analysis (PCA) for training and preliminary evaluation of the algorithms with guidance from a 10-fold cross-validation method.	Develop a machine learning model for predicting methanol outputs with CO ₂ conversion, methanol selectivity, CO selectivity, and methanol space-time yield.	Predictive model developed and validated experimentally using different catalysts at varying conditions of temperature, pressure, and space velocity was found to predict typical heterogeneous catalytic reaction outputs with R ² > 0.9 for all variables.	(Bhardwaj et al., 2023)
Thermocatalysts	Various ML models: Multi Linear Regression, Least Absolute Shrinkage Selection Operator, Ridge Regression, Support Vector Regression, Gaussian Process Regression (GPR), Random Forest Regression, Gradient Boost Random Forest Regression (GBRT) and Artificial Neural Network (ANN).	Development of methanol production catalyst performance prediction models based on published experimental data focusing on CO ₂ conversion and selectivity for methanol.	Best models were GBRT and ANN with R ² 0.95 and 0.94 for CO ₂ conversion and with R ² 0.95 and 0.95 for methanol selectivity, respectively.	(Vanjari et al., 2023)
Ionic liquid catalysts for CO ₂ cyclization	Random forest (RF), support vector regression (SVR) and multilayer perceptron (MLP). The shapely additive explanation (SHAP) method was used to interpret the ML models.	To develop a yield prediction model for the CO ₂ cycloaddition reaction.	The random forest (RF) model showed the best prediction accuracy with an R ² of 0.80 for the test data.	(Li et al., 2023)

where the energy system would have significantly decarbonized such that direct air capture of CO₂ becomes the main source of CO₂ (Gonzalez-Garay et al., 2022).

The Fischer-Tropsch method is at the centre of most literature reports as it is considered crucial for converting syngas into hydrocarbon products in the overview of Power-to-X, or at least generation of methanol which can then be converted into hydrocarbon fuels, especially jet fuel (Schmidt et al., 2018). This is especially because aviation is considered one of the difficult industries to decarbonize warranting for research towards finding sustainable aviation fuels (SAF) (Grim et al.,

2022). Obtaining SAF from CO₂ rather than fossil fuels is predicted to reduce carbon intensity of aviation fuels by 50–94 % (Grim et al., 2022). Also well covered in literature is electroreduction of CO₂ into several gas to liquid products ranging from CO to liquid products (Schmidt et al., 2018). The Fischer-Tropsch-to-jet using biomass as feedstock emits more CO₂ compared to pyrolysis-to-jet (Wang et al., 2022). It is therefore important to note that the process is only viable when coupled with captured CO₂ processes.

Throughout literature, there are strong recommendations around the need for better understanding around improved catalysts and synthesis

processes, scaling and industrial integration aspects, the use of renewable energy and sourcing of cheaper hydrogen, and policies around penalties and incentivization for emission or utilization of CO₂ (Zhou et al., 2025). Technological or process improvements are notably the key enablers and major drivers for the successful scalability Power-to-X and CO₂ conversion strategies with the use of cheap renewable energy and reduced cost of hydrogen also produced from electrolysis of water using renewable energy (Zhou et al., 2025; Li et al., 2016). Lowering hydrogen prices to below \$900/t is critical to making CO₂ conversion processes economically viable (Zhou et al., 2025). Electricity storage or at least integration of multiple renewable electricity sources is important for effective and continuous operation of electrolyzers to increase capacity factors and lower capital costs (Kulkarni et al., 2021). While storage of renewable energy in batteries can be efficient, their high cost and limited storage capacity for the CAPEX will not make economic sense. The use of electrolyzers such as PEM or SOEC that are can easily operate intermittently is also proposed although their CAPEX still remains too high compared to conventional systems. Combining renewable energy and natural gas has also been proposed to optimize operation and increase plant output and improve the techno-economic performance (Kulkarni et al., 2021). The contribution of CO₂ recycling has also been a subject for debate to its impact on the overall success of these technologies and Zhou et al. and Kulkarni et al. provide contrasting insights in that regard (Zhou et al., 2025; Kulkarni et al., 2021).

The importance of installing effective broad policy and regulatory frameworks that enable economic competitiveness and large-scale uptake of CO₂ products is relayed by several authors. Hepburn *et al.* suggest penalization of CO₂ emission and incentivization of verifiable reductions of CO₂ emissions with climate change in mind (Hepburn et al., 2019). The use of artificial intelligence and machine learning in techno-economic analyses and lifecycle assessments as an effective tool to process larger data sets and obtain more representative results as discussed in Section 8 cannot be ignored (Hussin et al., 2023). Overall, it is important to pay attention to various CO₂ utilization opportunities against other proposed technique such as biomass gasification and pyrolysis for carbon offsetting. Of greater importance are the social and environmental benefits more than economic benefits of CO₂ removal and reducing emissions. The technologies are modelled to reduce life cycle emissions by 25 % at present and 75 % by 2050 with technological advancements (Gonzalez-Garay et al., 2022). Table 6 below gives an overview of techno-economic analyses that have been carried out on various proposed integrated systems

10. Challenges and emerging solutions in CO₂ conversion technologies

CO₂ capture and utilization are at the forefront of industrial innovation, providing a solution to reduce climate change while improving process efficiency. Opportunities abound for converting waste carbon dioxide into useful products like fuels and chemicals, possibly changing the energy and manufacturing industries. However, obstacles remain in expanding technologies, lowering costs, improving efficiency and attaining industrial integration, while considering the environmental repercussions (Beniwal et al., 2025). Navigating technological, economic, and legal contexts is essential for unleashing the full potential of CO₂ capture and usage, opening the path for sustainable industrial growth. While some challenges are specific to different technologies, others are common across all CO₂ conversion processes.

This section gives brief information on the regulatory challenges, incentives for the adoption of CO₂ conversion technologies and its economic feasibility as shown in Fig. 9.

10.1. Technology considerations

Thermochemical conversion of CO₂

Although there have been significant research efforts to accelerate

the catalytic conversion of CO₂ into valuable chemicals and fuels, commercialization and process scale-up have been difficult. Other challenges include lower conversion, selectivity and stability of the catalyst due to sintering, coking, and oxidation in thermochemical catalysts (Yadav et al., 2024). For example, in the DRM process, the Ni-based catalyst usually suffers from instability at high temperatures while the Cu-based catalyst suffers a low conversion rate in the methanol production process from CO₂ (Table 3 lines 1–5). Another problem is catalyst selectivity to oxygenated compounds such as formic acid and methanol (Galadima and Muraza, 2019). Despite these challenges, the future of catalysts in CO₂ conversion is promising, with ongoing research efforts focusing on developing new and inexpensive catalysts at lower energy conditions (lower temperature and pressure). In the future, efforts may be dedicated to the development of new analytical and computational techniques to enhance understanding of reaction mechanisms. There is also a need for improving collaboration between engineers and chemists to develop new reactors to enhance catalyst efficiency, product formation and commercialization.

Future research efforts should prioritize enhancing the scalability of thermochemical CO₂ conversion technologies by designing catalysts that exhibit greater robustness and prolonged operational lifetimes. Additionally, the development of hybrid systems that synergistically integrate catalytic processes with complementary CO₂ reduction methods holds significant promise for improving overall conversion efficiencies. Innovations in process intensification and reactor engineering will be critical to lowering the energy consumption per unit of CO₂ converted, thereby improving the economic viability of these technologies. Moreover, leveraging advanced computational tools such as machine learning algorithms and high-throughput screening techniques can substantially accelerate the identification of novel catalysts and the optimization of reaction parameters. Achieving these objectives will require sustained interdisciplinary collaboration among materials scientists, chemists, and chemical engineers to overcome existing technical barriers and advance thermochemical CO₂ conversion toward commercial deployment.

Electrochemical CO₂ Reduction (ECR) Technologies

The transition of ECR technologies from laboratory-scale experiments to industrial-scale commercialization remains in its nascent stages. A primary bottleneck is the limited availability of catalysts that are not only cost-effective but also exhibit high selectivity, activity, and long-term stability. To date, the majority of research efforts have centered on small-scale catalyst development, often driven by computational modeling and theoretical predictions (Belsa et al., 2025). While these studies have provided valuable mechanistic insights, there is an urgent need to extend catalyst innovation toward scalable, industrially relevant systems. This includes greater emphasis on the design and engineering of robust electrolyzers, improved mass transport systems, and reactor configurations tailored for continuous operation.

Moreover, the inherently low solubility of CO₂ in aqueous electrolytes and its uneven distribution at the electrode-electrolyte interface significantly hinder the overall efficiency of the ECR process. These limitations often result in suboptimal CO₂ conversion rates and reduced Faradaic efficiency (FE), thereby constraining the viability of ECR for large-scale applications. Addressing these challenges will require a holistic approach that integrates advanced catalyst design with innovations in system architecture, gas-liquid interface engineering, and process optimization.

Photochemical and Photoelectrochemical CO₂ Reduction

Currently, most research effort focuses on the development of new photoelectrodes, however, to date, no commercially available photocathode have been developed (Lu and Wang, 2024). Another challenge is that the overall efficiency, conversion and selectivity of PEC cells is still very low, falling below 10 % (Kistler et al., 2021). Another problem is the stability issues of the photocathodes in the aqueous system. At the moment, the reaction mechanism in the PEC conversion of CO₂ is not very clear and requires further studies. Despite these challenges, the future of PEC technologies for CO₂ conversion is promising for

Table 6

An overview of techno-economic analyses that have been carried out on various proposed integrated systems.

Conversion technology	Process(es)	Analysis model(s)	Major findings	Comments	Ref.
Direct electrochemical conversion	Captured CO ₂ reduction reaction (cCO ₂ RR) in a monoethanolamine (MEA)-based medium vs electrochemical conversion process via the CO ₂ reduction reaction (CO ₂ RR) in aqueous electrolyte media (key difference between the two processes is the existence of a stripper column).	The National Energy Technology Laboratory (NETL) cost estimation methodology was used for Techno-economic analysis while ReCiPe 2016 (H) v1.1. was used for the life cycle impact assessment	Low economic feasibility. Levelized cost of product CO (LCOC) of the cCO ₂ RR process, which reflects the current technology level is 3.5 times higher than that of the CO ₂ RR process. The cCO ₂ RR process has more positive environmental impact than CO ₂ RR when using renewable electricity, even at the current technological performance level.	The cCO ₂ RR technology has good economic potential. Its development to the same level as that of the CO ₂ RR, can result in the levelized cost of product CO being 6.1 % lower than that of the CO ₂ RR process.	(Lee et al., 2023)
Electrolysis, fermentation and thermocatalysis	Three-step CO ₂ -to-SAF: (i) electrolysis front-end to produce CO (ii) biological syngas fermentation to produce ethanol (iii) thermocatalytic ethanol upgrading to SAF product.	Fully integrated Aspen Plus model based on a modelled pathway for CO ₂ -to-SAF design. Well-to-Wake, Well-to-Pump and Pump-to-Wake systems boundaries employed for life cycle analysis	CO ₂ -to-SAF is more costly compared to petroleum jet fuel. Current SAF production costs as low as \$3.51 per Gallon of gasoline equivalent (GGE) are achievable using currently available technology while costs as low as \$2.25–2.53 per GGE obtainable with advancements to the underlying technologies and substantial reductions in the price of electricity down to \$0.01 per kW h.	The gap can be reduced, but not fully closed, by pursuing high-efficiency, high-yield technologies in locations with access to low-cost renewable electricity. Producing SAF from CO ₂ is expected to lower the CI of the fuel by 50–94 % relative to fossil jet fuel, similar to other SAF production methods.	(Grim et al., 2022)
Fischer–Tropsch (FT) and Methanol to fuels (MtF).	Production of jet fuel via Fischer–Tropsch and Methanol-to-Fuels.	Resource-technology network (RTN) Model based on solar radiation as an energy source in Spain.	FT and MtF products eight to ten times more expensive than the current oil-based scenario. Production costs in 2020 per kg _{fuel} in Spain varied from 3.90 € (MtF) to 4.95 € (FT) using solar energy and point source CO ₂ . CO ₂ life cycle emissions cut by 25 % compared to their fossil-based counterpart. Future reduced jet fuel production costs to 2.5–3.3 € per kg _{fuel} possible with technological improvements.	More favourable renewable energy sources and cost reduction in photovoltaic and electrolysis technologies can result in significant CO ₂ reductions and final product prices. For perspective, these product prices represent a minimum increase of 100–150 % at present and 40–80 % by 2050 in the cost of a flight ticket. Future minimum carbon taxes of 500 h per tCO ₂ would be required for SAFs to become competitive.	(Gonzalez-Garay et al., 2022)
Electrolysis and thermocatalysis	Co-electrolysis of CO ₂ and H ₂ O to syngas using solid oxide electrolysis cells (SOECs) and thermocatalytic conversion of syngas to liquid products.	CHEMCAD 7.1.1 computer aided process simulation program for a 500 barrels per day (BPD) plant.	The levelized cost of liquid product is 1.29\$ per liter or 0.15\$ per kW h. The highest contribution (at 50 %) in the cost is from electricity for electrolysis. Levelized cost of products for 1500bpd and 5000bpd plants are 1.06\$ per liter and 0.91\$ per liter, respectively. 82 % CO conversion, 79 % C5+ selectivity, 67 % overall energy efficiency and stable operation of 4000 h.	The price of electricity, including its location and source, has the largest impact on the levelized cost of liquid products. Economy of scale important on the prices of products with large scale plants mainly benefiting from better CAPEX and OPEX contributions, especially maintenance and labour. Since RE is intermittent, storing electric energy in batteries is an efficient option, but their high cost and low energy storage capacity do not justify the economics. A hybrid process combining natural gas with renewable electricity may optimize operation and increase plant output, improving the techno-economic performance.	(Vega et al., 2024)

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Table 6 (continued)

Conversion technology	Process(es)	Analysis model(s)	Major findings	Comments	Ref.
Electrochemical reduction and thermocatalysis	Electrochemical reduction of CO ₂ to CO + Fischer–Tropsch process	Engineering and economic model framework was developed for the investigation. The cost analysis module is based on a DCF analysis adapted from the H2A model.8,17	Under the business-as-usual scenario, the model estimates the levelized cost of synthetic fuel at \$9.20 per gallon. In the optimistic case, the cost of synthetic fuel remains approximately 36 % higher than the current wholesale price of diesel. Energy efficiency across scenarios ranges between 41 % and 65 %. In terms of CO ₂ emissions, outcomes vary widely from an increase of 180 % (nearly double) to a reduction of up to 75 % when compared to the business-as-usual scenario without carbon sequestration.	Optimistic case incorporated a reduced price of H ₂ and electricity combined with the improved FT yields. If achieved, the price of this synthetic fuel could be in a range similar (but modestly higher) than today's petroleum fuel prices.	(Kulkarni et al., 2021)
Electroreduction	CO ₂ to C ₁ –C ₂ chemicals such as carbon monoxide, formic acid, methanol, methane, ethanol, and ethylene.	Gross-margin model = difference between the revenue and the cost of goods sold divided by the revenue.	Gross-margin model was developed and can be applied to analysis of electroreduction of CO ₂ to various products under different scenarios such as different products combinations, selectivity ratios, and process designs.	CO ₂ reduction catalysts need to be improved so that they last for thousands of hours. Using CO instead of CO ₂ , direct utilization of flue gas, or a combination CO ₂ capture conversion processes will be required for the electroreduction of CO ₂ to contribute significantly to reduction of CO ₂ emissions.	(Verma et al., 2016)
Electrochemical reduction and thermocatalysis	CO ₂ to liquid products (1) CO and subsequent Fischer–Tropsch conversion of syngas to diesel fuel (CO ₂ –CO–FTL), (2) ethanol in one step (CO ₂ –C ₂ H ₅ OH), (3) CO and subsequent reduction to ethanol in two steps (CO ₂ –CO–C ₂ H ₅ OH), and (4) formic acid (CO ₂ –HCOOH).	Capital cost analysis and Net present value analysis	With conceivable improvements in an optimistic scenario, the i. diesel process was projected to have the best pathway to making cost-effective fuels, ii. ethanol would be prohibitively expensive without major improvements to the present electrosynthesis performance. iii. Formic acid, though projected to be expensive relative to its stored energy content, was projected to have perhaps the simplest pathway to production at costs competitive with its commercial bulk price. CO and formic acid were the only economically viable products with NPVs of \$13.5 million and \$39.4 million, respectively under the current techno-economic conditions. Higher-order alcohols, such as ethanol and n-propanol are promising under future conditions if reasonable electrocatalytic performance benchmarks are achieved (e. g., 300 mA/cm ² and 0.5 V overpotential at 70 % Faradaic efficiency).	None of the processes can compete with current fuel prices. High CAPEX for electrolyzers is the primary limiting factor. Levelized costs of the liquid products strongly influenced by parameters that affect the electrolyzer CAPEX (i.e., current density, faradaic efficiency, and cost per electrode area). Improvements on high faradaic efficiency, improved current densities, and reduced electrolyzer costs per electrode area needed for economic viability.	(Spurgeon and Kumar, 2018)
Electrochemical reduction	CO ₂ to CO, formate, methanol, methane, ethylene, ethanol, n-propanol	The Generalized techno-economic model was used for eCO ₂ R using CO ₂ reduction figures of merit. An economic analysis was also carried out to calculate the end-of-life net present value. CAPEX and OPEX for the CO ₂ electrolyzer were based on the DOE Current Central H2A base case for an alkaline electrolyzer.	CO and formic acid were the only economically viable products with NPVs of \$13.5 million and \$39.4 million, respectively under the current techno-economic conditions. Higher-order alcohols, such as ethanol and n-propanol are promising under future conditions if reasonable electrocatalytic performance benchmarks are achieved (e. g., 300 mA/cm ² and 0.5 V overpotential at 70 % Faradaic efficiency).	With technological improvements electrochemical CO ₂ reduction for fuels and chemicals production can become a profitable option as part of the growing renewable energy infrastructure. Low market potential and profitability of formic acid and gaseous products due to Difficulties associated with storage and transportation. For higher-order alcohols to become profitable, cheaper electricity costs and improved catalytic performance are needed. Improved electrocatalytic performance benchmarks for these alcohols also achievable with continued research.	(Jouny et al., 2018)

(continued on next page)

Table 6 (continued)

Conversion technology	Process(es)	Analysis model(s)	Major findings	Comments	Ref.
Electrochemical reduction, thermocatalysis, photocatalysis, hybrid approaches	CO ₂ conversion to jet fuel supply chain in the United States. CO ₂ -CO-FTS-Fuel and CO ₂ -Methanol-Fuel. Direct thermocatalytic conversion, direct electrocatalytic conversion, direct photocatalytic conversion and hybrid approaches.	The Gross-Margin model was developed to assess the techno-economic viability of various C ₁ -C ₂ products produced through the electroreduction of CO ₂ . A mixed-integer linear programming model was developed to select source plants and conversion pathways, locations of conversion refinery sites, and the amount of captured CO ₂ across the United States.	Reducing H ₂ prices to below \$900/t and lowering operating costs to 5 %–6 % of current levels are critical to making CO ₂ conversion processes economically viable. i. FTS is economically viable under current H ₂ prices and reduced operating costs. ii. hydrogen price and electricity costs are critical determinants of economic feasibility. iii. Higher CO ₂ recycle percentages and conversion rates significantly enhance the economic and environmental performance of CO ₂ conversion pathways. iv. leveraging policy mechanisms, and fostering international cooperation can enhance the scalability and broader applicability of the studied conversion technologies, contributing to global carbon reduction and sustainable energy goals.	Hydrogen price as the most significant component of total production cost. Electricity cost constitutes a large percentage of operating costs and is a major factor for locating conversion refineries. The CO ₂ recycle percentage of the FTS pathway influences the choice of applied pathways at refineries. Additionally, a higher conversion rate holds a substantial promise for reducing the total production cost and can make the MeOH pathway a viable choice.	(Zhou et al., 2025)

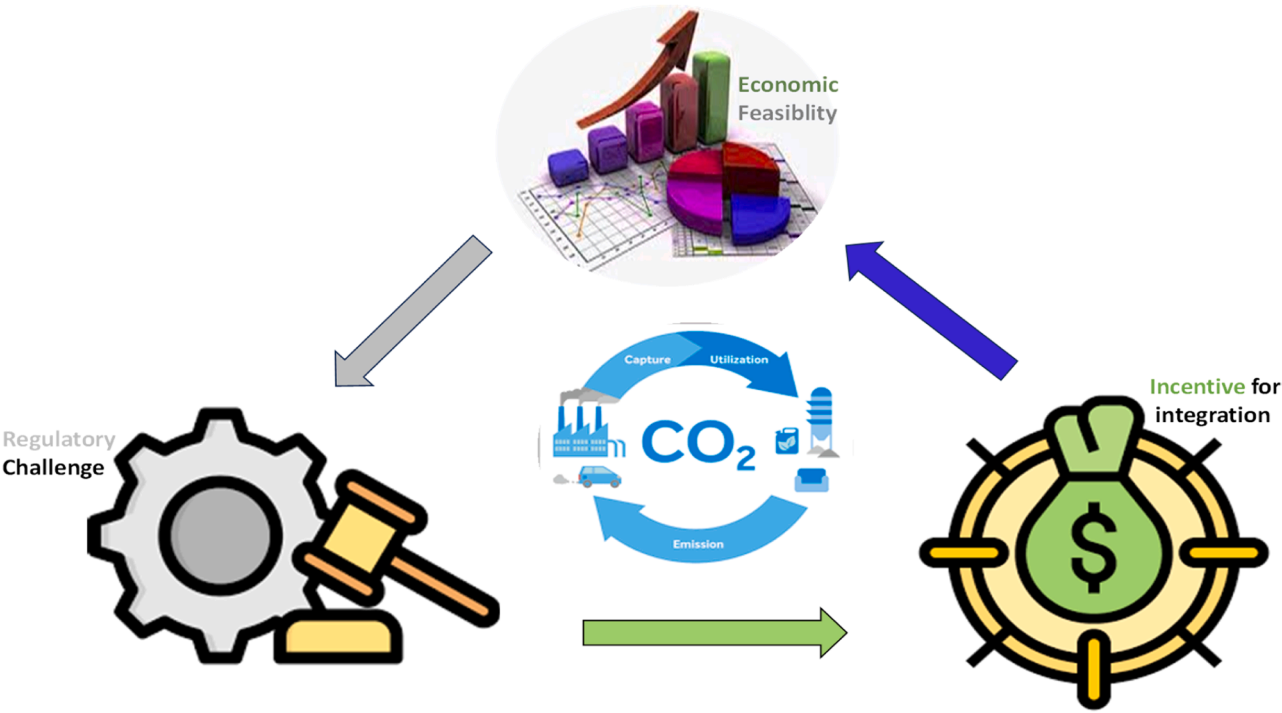


Fig. 9. Opportunities and Challenges in CO₂ Capture and Utilization.

mitigating climate change. The development of cost-effective, highly efficient, and stable catalysts must be considered. In addition, increasing efforts into reactor design and engineering is crucial to increasing PEC performance in the future. Further research into the regeneration of photocatalyst should be considered to make technology greener and environmentally friendly.

Bioconversion

While biological CO₂ conversion technologies offer significant

promise, several challenges remain in scaling these systems for industrial applications. One major limitation is scalability: biological systems, particularly those involving microbes, often struggle to operate efficiently at large scales, particularly in continuous flow reactors (Hassan et al., 2024). Maintaining high cell densities and ensuring optimal growth conditions for microbes in industrial settings can be difficult, particularly when dealing with large quantities of CO₂ (Bajracharya et al., 2017). Additionally, product selectivity remains a critical

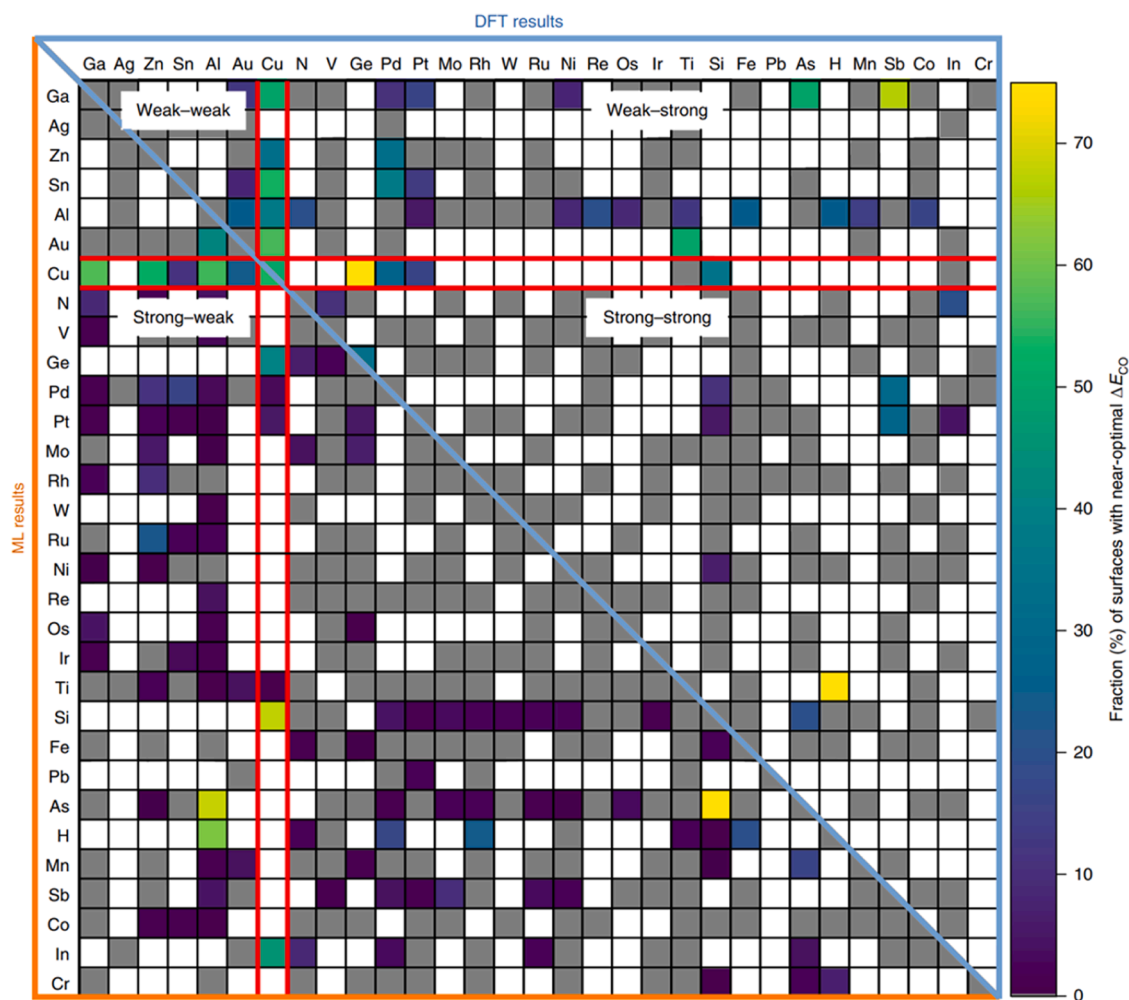


Fig. 10. A CO₂ reduction activity map for bimetallic systems to visualize two-component intermetallic surfaces with low-coverage CO adsorption energies (ΔE_{CO}) within the optimal range of -0.77 to -0.57 eV. In the map, white boxes indicate surfaces that were not evaluated, grey boxes represent surfaces with ΔE_{CO} values outside the desired range, and colored boxes highlight those with potential catalytic activity. The ΔE_{CO} values in the upper half of the map were obtained using DFT, while those in the lower half were predicted using a surrogate machine learning model. Copper-containing intermetallics are outlined in red, as copper's monometallic ΔE_{CO} is closest to the ideal adsorption energy of -0.67 eV. Adapted with permission from ref. (Zhong et al., 2020). Copyright 2020, Springer Nature.

challenge (Zhao et al., 2019). Many biological systems produce a range of products, but achieving high selectivity for desired compounds while minimizing unwanted byproducts is often difficult. Advances in synthetic biology and metabolic engineering are addressing this issue, but it remains a significant hurdle for commercial implementation. Stability is another challenge, as enzymes and microbial systems can degrade over time or under extreme industrial conditions, leading to reduced efficiency and the need for frequent replacements or regeneration. Developing more stable strains and enzyme formulations, as well as improving the longevity of bioconversion systems, is critical to their long-term viability. Finally, the economic feasibility of biological CO₂ conversion systems remain uncertain. While many of these technologies show great potential in laboratory-scale experiments, achieving cost-effective, large-scale CO₂ conversion requires ongoing research into optimizing productivity, reducing operational costs, and integrating these systems into existing industrial infrastructure.

10.2. General considerations

Efficiency and Cost-Effectiveness

Efficiency and cost-effectiveness are major challenges in CO₂ conversion regardless of the method of conversion. The low efficiency in CO₂ conversion is due to the thermodynamic stability of CO₂ which

requires large energy input for the conversion process thereby making it ineffective economically (Ezeji et al., 2007). To overcome this challenge, electrocatalysis and photocatalysis methods of CO₂ conversion have recently gained attention. This technology utilizes electricity and light energy to lower the activation energy and drive CO₂ conversions to form hydrocarbons and other valuable chemicals (Raganati and Ammendola, 2024). However, the metal oxides and earth abundant catalysts used in photocatalytic conversion (second and third row transition metals) face challenges in terms of light absorption efficiency, stability, and scalability (Li et al., 2023). Studies on heterojunctions (Kumar et al., 2022; Tahir et al., 2017) and ion doping (Mgolombane et al., 2021) are being explored to enhance catalyst performance, and improvements in CO₂ conversion have been observed.

There are several strategies that have shown promise. In bioconversion, *Chlorella vulgaris* and cyanobacteria have been used as microorganisms to absorb over 90 % of CO₂ and generate biomass at a rate greater than 0.45 g/L/day in a standard photobioreactor (Emmanuel and Rozina, 2025). It should however be noted that other factors contributed to the efficiency of CO₂ conversion. This includes the microorganism growth rate, tolerance of contamination and control of operating conditions (Gupta et al., 2024). Electrochemical volarization of CO₂ by eliminating the CO₂ stripping step and allowing for direct conversion of captured CO₂ (Hu et al., 2025). Studies show that

integrated systems can achieve nearly full conversion of CO₂ (Kim et al., 2018, 2024) with minimal energy input, and energy savings of up to 44 % compared to sequential processes (Li et al., 2021). Non-thermal plasma technology (NTP) technology has also shown a lot of promise although it involves optimizing several factors, including reactor design, catalyst use, and energy input. Studies done on improving the energy efficiency by optimizing the plasma discharge system showed that the microwave, radio frequency and the gliding arc discharge system are able to exceed a 60 % energy efficiency. However, the conversion efficiency is less than 40 % for the three discharge systems as seen in Fig. 11 (Snoeckx and Bogaerts, 2017).

To enhance conversion efficiency, integrating catalysts with non-thermal plasma (NTP) enables the development of a hybrid plasma-catalytic process, which offers significant potential for achieving plasma-catalytic synergy. This synergy can greatly improve CO₂ conversion, as well as the selectivity and yield of desired products (Xiong et al., 2024). However, current understanding of how to design cost-effective, highly active, and stable catalysts for plasma-assisted CO₂ conversion remains limited.

Long-Term Stability and Catalyst Deactivation

Another challenge affecting the scale-up of CO₂ conversion technology is massive coke deposition, sintering and particle growth on the surface of the catalyst and in some cases, structural and phase transformation which often leads to catalyst deactivation (Chen et al., 2023; Lai et al., 2023). This is mostly observed in the dry reforming of methane conversion process that is associated with methane decomposition and/or carbon monoxide degradation as seen in Eqs. (3)–(5).



Different solution pathways have been explored ranging from catalyst modification and reactor configuration have failed to provide long term solutions (Galadima and Muraza, 2019). Researchers have examined several noble metals such as Rh, Ru and Pd as a catalyst during the methanation reaction, however, their high cost makes scaling up the process a challenge (Vega et al., 2024). Also, the use of Nickel based support catalyst as Ni-Cu/MgO (Song et al., 2018) and Ni-Mn/Al₂O₃ (Vrijburg et al., 2020) have been explored, although they are prone to long term deactivation due to the Ni particle sintering and growth (Egawa, 2018). Studies have been done on the addition of Cobalt on the

Ni-based catalyst from as low as 3 % to up to 15 % catalyst which has shown to enhance CO₂ conversion, CH₄ selectivity, long-term stability, and coke resistance (Beniwal et al., 2025; Pastor-Pérez et al., 2018). The addition of Co suppresses Ni aggregation and improves stability (Wu et al., 2019). Similarly, the use of high-entropy alloys and structured supports such as CoNiCuPdRu/TiO₂ can enhance stability by preventing sintering and maintaining active sites (García-Moncada et al., 2021; Xiong et al., 2024).

Abate et al. (2016) developed a composite catalyst and assessed its methanation performance using a batch-type reactor under specific testing conditions: 0.6 g of catalyst, an H₂/CO₂ ratio of 4, temperatures ranging from 250 to 400 °C, and space velocities between 20,000 and 30,000 h⁻¹. The incorporation of oxides such as ZrO₂-TiO₂ and CeO₂ was found to significantly enhance the catalytic performance of the base Ni/Al₂O₃ catalyst. Among the tested composite systems, the Ni/Al₂O₃/ZrO₂/TiO₂ catalyst with 15 wt% CeO₂ achieved the highest CO₂ conversion rate of 82 %. Characterization studies revealed that, in addition to improving textural properties and nickel dispersion, increased CeO₂ loading enhanced the reducibility of NiO species, thereby boosting catalytic activity, particularly at lower reaction temperatures.

Selectivity and Product Control

CO₂ conversion often involves complex reaction pathways that can lead to side reactions and the formation of undesired byproducts. Additionally, the presence of multiple active sites on catalysts poses a challenge in controlling the selectivity toward the desired product. To address this, Cheng et al. [405] developed a relay catalyst system for CO/CO₂ hydrogenation, aimed at enhancing product selectivity. Relay catalysis entails constructing a single, well-orchestrated tandem reaction channel that directs the reaction pathway through selected intermediates and reaction steps. By employing optimally paired catalysts for each step, the system ensures controlled transformation toward the target product.

Li et al. [406] demonstrated the effectiveness of a nanostructured photocatalyst—atomically thin CuInS₂ layers for the selective reduction of CO₂ to methane. This system achieved nearly 100 % methane selectivity due to the formation of stable intermediates at specific catalytic sites. Selectivity in CO₂ electroreduction can also be tailored by exploiting the structural sensitivity of catalysts. For instance, modifying the shape, size, and composition of copper nanocatalysts has been shown to favor the formation of specific products [407, 408].

Beyond catalyst design, optimizing reaction conditions such as temperature, pressure, and catalyst supports can significantly influence both activity and selectivity. Mesoporous supports and the inclusion of metal promoters have been widely investigated for their ability to enhance catalytic performance. These systems improve not only product yield but also selectivity and overall reaction efficiency (Zhang et al., 2023). For example, Zhou et al. [409] employed a Ni/CeO₂ catalyst supported on a mesoporous structure in a fixed-bed reactor to assess CO₂ conversion and methane selectivity. Under optimal conditions (1 atm, 45,000 mL/g·h gas flow rate, varying temperatures, and 0.05 g catalyst loading), the system achieved 91 % CO₂ conversion and 100 % CH₄ selectivity, with stability maintained over a 12 hr reaction period.

Environmental and Regulatory Considerations

The environmental impact of CO₂ conversion is contingent on its life cycle assessment (LCA) which can be used to create a comprehensive regulatory framework. LCA studies on CO₂ conversion technology showed that the highest environmental impact contributions are from the energy use in the process; e.g. energy supply for water electrolysis (Rosental et al., 2020). This high energy input can negate environmental benefits if the energy is not sourced from renewables (Zhang et al., 2023). Additionally, material sourcing (catalysts, solvents, feedstocks), process efficiency, and waste generation pose risks, while concerns over water and land use further complicate large-scale deployment. Addressing these issues requires optimizing energy efficiency, integrating renewable energy sources, developing sustainable catalysts with

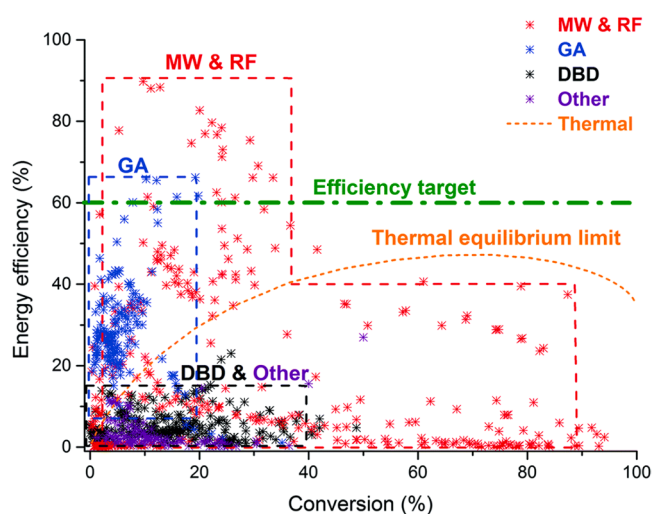


Fig. 11. Energy efficiency as a function of CO₂ conversion using different plasma systems (Reused with permission from (Snoeckx and Bogaerts, 2017)). Copyright 2016, Royal Society of Chemistry.

minimal environmental impact and closely regulating the distribution and usage of the resulting products (Emmanuel and Rozina, 2025). For example, the CO₂ electrochemical reaction for hydrogen production requires demineralized water and countries that face water shortages, such as those in the Mediterranean, may find water usage challenging. Studies on desalination have shown promise in mitigating this risk and providing fresh water for these technologies in areas with water supply issues, but this would further increase the demand for energy inputs and could potentially have environmental side effects (Cai et al., 2023).

On the regulatory side, the lack of standardized policies and clear carbon accounting frameworks makes commercialization difficult. Many CO₂-derived products require extensive regulatory approvals, and unclear carbon pricing mechanisms provide weak incentives for industry adoption. Governments can support the sector by establishing universal certification standards, streamlining approval processes, and implementing strong carbon pricing policies that reward CO₂ utilization (Chai et al., 2025). Public-private partnerships and targeted funding for research and infrastructure can also accelerate deployment. To overcome these barriers, industry stakeholders must work closely with policymakers to create supportive regulations and market incentives. Expanding carbon credit systems to include CO₂-derived products, providing tax benefits, and ensuring regulatory clarity can attract investment (Liu et al., 2023). Additionally, integrating CO₂ conversion technologies with existing industrial operations, such as power plants and refineries, can improve feasibility by leveraging existing infrastructure. Investment in innovative materials and process improvements will further enhance efficiency and reduce costs.

Considerations for industrial integration

The combination of CO₂ conversion technologies throughout industries shows great potential to transform greenhouse emissions into marketable products (Karishma et al., 2024; Yaashikaa et al., 2019). Research activities along with development efforts have produced encouraging results in CO₂ conversion technologies despite existing technical challenges. The conversion of CO₂ into fuels as well as chemicals and construction materials show promise through three emerging technologies: electrochemical processes, photocatalysis, and biological systems. Unique industrial applications from these advancements simultaneously reduce emissions while contributing to cleaner plant operations. However, integrating CO₂ conversion in industries faces numerous regulatory barriers, primarily due to the complexity and variability of policies across jurisdictions. Current frameworks often lack specific guidelines for CO₂ utilization, which impedes large-scale deployment. Additionally, stringent environmental regulations for industrial byproducts and storage safety can delay project approvals. A significant challenge lies in aligning CO₂ utilization regulations with carbon pricing mechanisms. Without harmonized global standards, industries may struggle to adopt conversion technologies cost-effectively. For example, the European Union's Emissions Trading System (ETS) incentivizes CO₂ reduction but lacks direct provisions for CO₂ conversion, creating a policy gap.

Most technologies exist at basic levels of development despite facing various commercial and regulatory barriers yet their capacity to decrease emission output and produce revenue solidifies their significance for more advanced investigation and funding. The economic viability of CO₂ conversion technologies is a critical determinant of their industrial adoption. High capital and operational costs for CO₂ capture, conversion, and infrastructure development remain major hurdles. Advanced catalysts and energy-efficient processes, while promising, are often expensive. A study in the steel industry revealed that integrating CO₂ conversion into production lines will help mitigate the emission of CO₂ (Li et al., 2024), but in turn, could increase production costs. Scaling these technologies to achieve economic parity with fossil-based processes requires significant investments and technological breakthroughs. However, economic feasibility improves when CO₂-derived products, such as methanol or polymers, capture niche markets with premium pricing.

Policy incentives are instrumental in driving the widespread adoption of CO₂ conversion technologies. Mechanisms such as carbon credits, subsidies for integrating renewable energy, and tax incentives for industries utilizing captured CO₂ serve as key enablers. For example, the U. S. Department of the Treasury has issued guidelines to assist businesses in accessing tax credits for the storage of eligible carbon oxides and for use in tertiary oil recovery. These credits provide up to \$50 per metric ton for permanent carbon storage and \$35 per metric ton for enhanced oil recovery (Lok et al., 2023), thereby encouraging investment in carbon capture and promoting environmentally responsible storage practices. In addition, public-private partnerships can help mitigate financial risks and stimulate technological innovation. Regulatory frameworks, including mandatory emission reduction targets set by international agreements like the Paris Accord, further compel industries to adopt CO₂ utilization strategies as part of their compliance and sustainability efforts.

11. Perspectives on the future of CO₂ conversion

The evolution of CO₂ conversion technologies promises to profoundly influence global energy and chemical sectors, providing pathways for sustainable production of fuels, chemicals, and materials while mitigating greenhouse gas emissions. Achieving this transformative potential requires the development of next-generation systems that combine high efficiency, selectivity, and scalability with environmental sustainability. Realizing such objectives demands a multidisciplinary approach, integrating expertise from materials science, chemical engineering, environmental science, and computational modeling to address the complex challenges associated with carbon capture, conversion, and utilization.

Central to this endeavor is the design and development of advanced catalysts that can operate efficiently under diverse conditions while maintaining high selectivity toward desired products. Multifunctional and adaptive catalysts, including SACs, have emerged as highly promising, offering exceptional activity due to maximized atomic utilization and tunable electronic environments (Anekwe et al., 2025). The incorporation of catalysts with electronically active supports further enhances activity and stability by modulating surface properties, enabling more precise control over reaction pathways. High-throughput screening platforms, combining density functional theory (DFT), molecular simulations, and machine learning, have accelerated the discovery and optimization of catalytic materials, allowing for predictive tailoring of performance prior to experimental validation (Wen et al., 2025; Gu et al., 2022; Nyangiwe, 2025).

Alongside catalyst development, process intensification remains critical for translating laboratory success into industrially relevant outcomes. Microreactor designs, continuous-flow systems, and modular reactor architectures enhance mass and heat transfer, improving overall conversion efficiency. Integrating CO₂ capture with conversion in unified platforms reduces energy consumption and operational costs, particularly in electrochemical and hydrogenation processes, and improves the economic viability of large-scale deployment (Vega et al., 2024). These integrated approaches also provide opportunities for adaptive operation, allowing processes to respond dynamically to fluctuations in feedstock composition or renewable energy availability.

The incorporation of renewable energy sources, such as solar, wind, and hydroelectric power, into CO₂ conversion systems is essential for minimizing reliance on fossil fuels and achieving truly sustainable processes. Coupling renewable electricity with electrochemical or photo-electrochemical CO₂ reduction has been shown to enhance energy efficiency and product selectivity, enabling decentralized and modular conversion systems that can flexibly meet varying energy and chemical demands (Nnabuife et al., 2025). These hybrid systems, which unify capture, conversion, and energy input, represent a promising avenue for scaling CO₂ valorization technologies sustainably.

Digitalization, AI, and ML are increasingly pivotal in optimizing CO₂

conversion processes. AI-driven predictive modeling, process control, and real-time optimization enable precise adjustment of operating parameters, maximizing conversion efficiency and minimizing energy waste. For example, ML-guided design of CO₂ capture solvents, including amines and ionic liquids, has led to significant improvements in absorption efficiency and selectivity (Chaudhari et al., 2025). The integration of digital twins into reactor systems can facilitate continuous process monitoring and predictive maintenance, bridging the gap between laboratory research and reliable industrial operation.

Scaling CO₂ conversion technologies from bench-scale to pilot and industrial scales poses further challenges, including reactor design, materials durability, and process integration. Modular and continuous-flow electrochemical reactors have demonstrated promising scalability, maintaining high performance across increased reaction areas, highlighting the potential for commercial viability (Onyeaka and Ekwebelem, 2023). Alongside technical development, policy and economic frameworks play an indispensable role in accelerating adoption. Regulatory incentives, carbon pricing mechanisms, and targeted investment strategies can foster a circular carbon economy by supporting both R&D and industrial deployment. National programs, such as those outlined by the U.S. Department of Energy, underscore the importance of integrating AI and renewable energy to achieve research, development, demonstration, and deployment objectives in CO₂ conversion (Della Valle et al., 2024).

Ultimately, the future of CO₂ conversion lies in the convergence of advanced catalysts, integrated and renewable-powered systems, digital optimization, scalable reactor design, and supportive policy landscapes. Addressing these interconnected challenges through sustained, collaborative research will enable the transformation of CO₂ from an environmental liability into a renewable carbon feedstock. Such progress will not only accelerate decarbonization and mitigate climate change but also establish sustainable industrial practices and a resilient circular carbon economy, reshaping global carbon management strategies.

12. Conclusions

The escalating atmospheric CO₂ concentrations present a formidable challenge to global climate stability, necessitating the development of scalable, economically viable, and sustainable mitigation strategies. CO₂ conversion technologies offer a transformative pathway by enabling the utilization of CO₂ as a renewable carbon feedstock for the production of fuels, chemicals, and materials, thereby promoting a circular carbon economy. This review has systematically explored advancements across various domains, including catalyst development, integration of CO₂ capture with conversion processes, and the incorporation of renewable energy sources. Recent innovations in catalyst design, particularly the development of multifunctional and adaptive catalysts, have significantly enhanced the efficiency and selectivity of CO₂ conversion processes. The integration of CO₂ capture with conversion technologies within unified systems has demonstrated potential in reducing energy requirements and operational expenditures, thereby improving economic feasibility. Furthermore, the coupling of CO₂ conversion processes with renewable energy sources, such as solar and wind, has been identified as crucial for achieving sustainability goals and reducing reliance on fossil fuels. The application of artificial intelligence and machine learning in CO₂ conversion technologies has shown promise in optimizing processes, accelerating development, and improving efficiency. These technologies facilitate predictive modeling, process control, and real-time optimization, thereby enhancing the overall performance of CO₂ conversion systems. However, challenges related to energy efficiency, long-term stability, product selectivity, and regulatory constraints persist, necessitating continued research and development efforts.

Looking ahead, the successful commercialization of CO₂ conversion technologies will require the development of modular, scalable reactor designs, validation of processes at pilot and industrial scales, and

alignment with supportive policy frameworks. Interdisciplinary collaboration and public-private partnerships will be pivotal in accelerating the adoption of these technologies. By addressing existing challenges and leveraging emerging opportunities, CO₂ conversion technologies can play a critical role in mitigating climate change and advancing sustainable industrial practices.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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