



Recent advances in semiconductor quantum dots for photocatalytic CO₂ reduction

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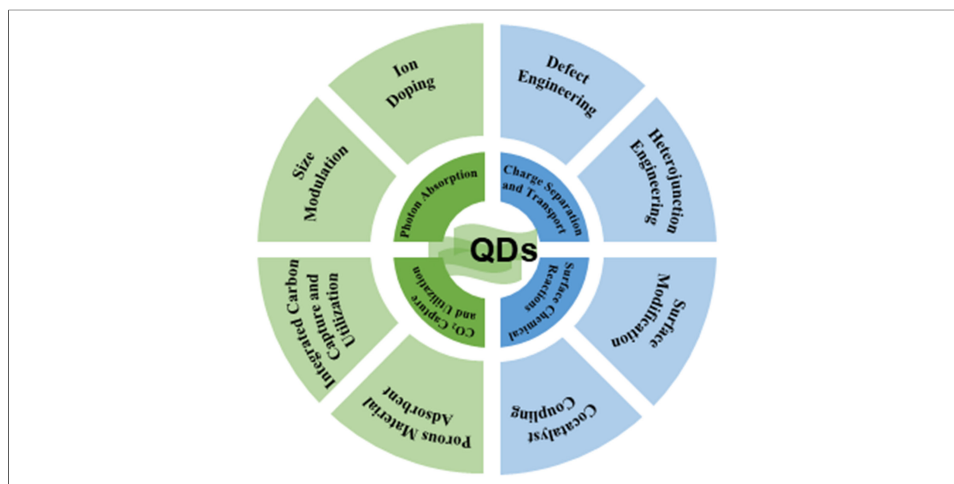
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Abstract

Developing efficient carbon capture, utilization and storage methods is essential to offset adverse global climate changes. Among those methods, photocatalytic CO₂ conversion is emerging as an effective and sustainable solution. Among the various photocatalysts, semiconductor quantum dots (QDs) are particularly promising for the CO₂ reduction reaction (CO₂RR) due to their unique features, such as quantum confinement effect, large absorption coefficient, and beneficial surface properties. This review provides a comprehensive and distinctive perspective by integrating three critical dimensions: advanced mechanistic understanding through cutting-edge characterization techniques, systematic stability analysis under realistic operating conditions, and direct CO₂ capture-utilization integration. We highlight recent strategies for improving the CO₂RR performance of QDs, including bandgap tuning, ion doping, defect and heterojunction engineering, ligand modification and cocatalyst loading. We also explore integrated approaches that couple CO₂ capture with photocatalytic conversion. Furthermore, we address the critical transition from laboratory demonstrations to real-world

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implementation by analyzing long-term stability, degradation mechanisms, and realistic cyclic operating conditions inadequately addressed in current research. Finally, we address prevailing challenges and future prospects, aiming to spark continuous innovation in applying QDs to CO₂ capture and conversion.

INTRODUCTION

The extensive consumption of fossil fuels over the past centuries has led to the release of substantial amounts of greenhouse gas, particularly CO₂, posing a serious threat to global ecosystems and human society^[1]. In response, significant efforts have been directed toward developing effective carbon capture, utilization and storage technologies to reduce atmospheric CO₂ levels^[2,3]. Nature provides an exemplary model in photosynthesis, which uses solar energy to convert atmospheric CO₂ into value-added products, thereby storing solar energy as chemical energy^[4,5]. However, natural photosynthesis is limited by low energy conversion efficiency, limited product selectivity, and its reliance on complex biological systems^[6]. These limitations have spurred the development of artificial photocatalytic systems designed to overcome such challenges.

Considerable progress has been made in developing various photocatalysts for the CO₂ reduction reaction (CO₂RR), including metal oxides, carbon-based materials, and composite structures, with some demonstrating promising conversion rates under laboratory conditions [Figure 1A]^[7-9]. Despite this progress, artificial photocatalysts still face significant challenges, such as insufficient visible-light absorption (as evidenced by the wide bandgaps (> 3.0 eV) of many benchmark photocatalysts that only absorb ultraviolet (UV) light), rapid charge recombination (carrier lifetimes often shorter than nanoseconds) and low solar-to-fuel conversion efficiency ($< 1\%$). Furthermore, the inherent stability of the CO₂ molecule, with a high dissociation energy of $750 \text{ kJ}\cdot\text{mol}^{-1}$ for the C=O bond, demands substantial energy input for its activation^[10].

The past decades have witnessed remarkable advances in both materials design and mechanistic understanding of photocatalytic CO₂ reduction^[11]. Among the diverse range of photocatalysts, semiconductor quantum dots (QDs) have emerged as particularly promising candidates. Defined by their nanoscale dimensions (typically 1-10 nm, smaller than the Bohr exciton radius), QDs exhibit unique optoelectronic properties that distinguish them from their bulk counterparts and molecular catalysts^[12-14]. These advantageous characteristics include: (1) High Absorption Coefficients: QDs typically possess high molar extinction coefficients, enabling highly efficient harvesting of photon energy. For example, the molar extinction coefficient of CsPbX₃ (where X is a halogen ion) is approximately 10^5 - $10^7 \text{ L}\cdot\text{mol}^{-1}\cdot\text{cm}^{-1}$ ^[15]; (2) Tunable Bandgaps: the quantum confinement effect allows for precise tuning of their band structures simply by varying their sizes^[16], facilitating optimization of the thermodynamic driving force and product selectivity for specific CO₂RR pathways; (3) Efficient Charge Separation: QDs often exhibit lower exciton binding energies (E_b), promoting the dissociation of excitons into free electrons and holes that can migrate to surface active sites; (4) Multiple Exciton Generation: Under high-energy photon excitation ($\geq 2E_g$), QDs can generate multiple electron-hole pairs from single photons through Auger processes, potentially achieving internal quantum efficiencies exceeding 100%. This enhanced efficiency results from their discrete energy levels that suppress non-radiative relaxation, unlike bulk semiconductors; (5) Abundant Surface Sites: The high surface-to-volume ratio of QDs provides abundant surface sites, including coordinatively unsaturated atoms, vacancies, or defects, which can be tailored for CO₂ adsorption and activation; (6) Favorable Band Positions: The conductive band (CB) of most QDs is situated at sufficiently negative potentials to thermodynamically drive various CO₂ reduction pathways^[17]. In summary, these unique properties establish QDs as highly promising photocatalysts for CO₂RR, which is also evidenced by the exponential growth in related publications, as evidenced by keyword trends in the Web of Science database [Figure 1B and C].

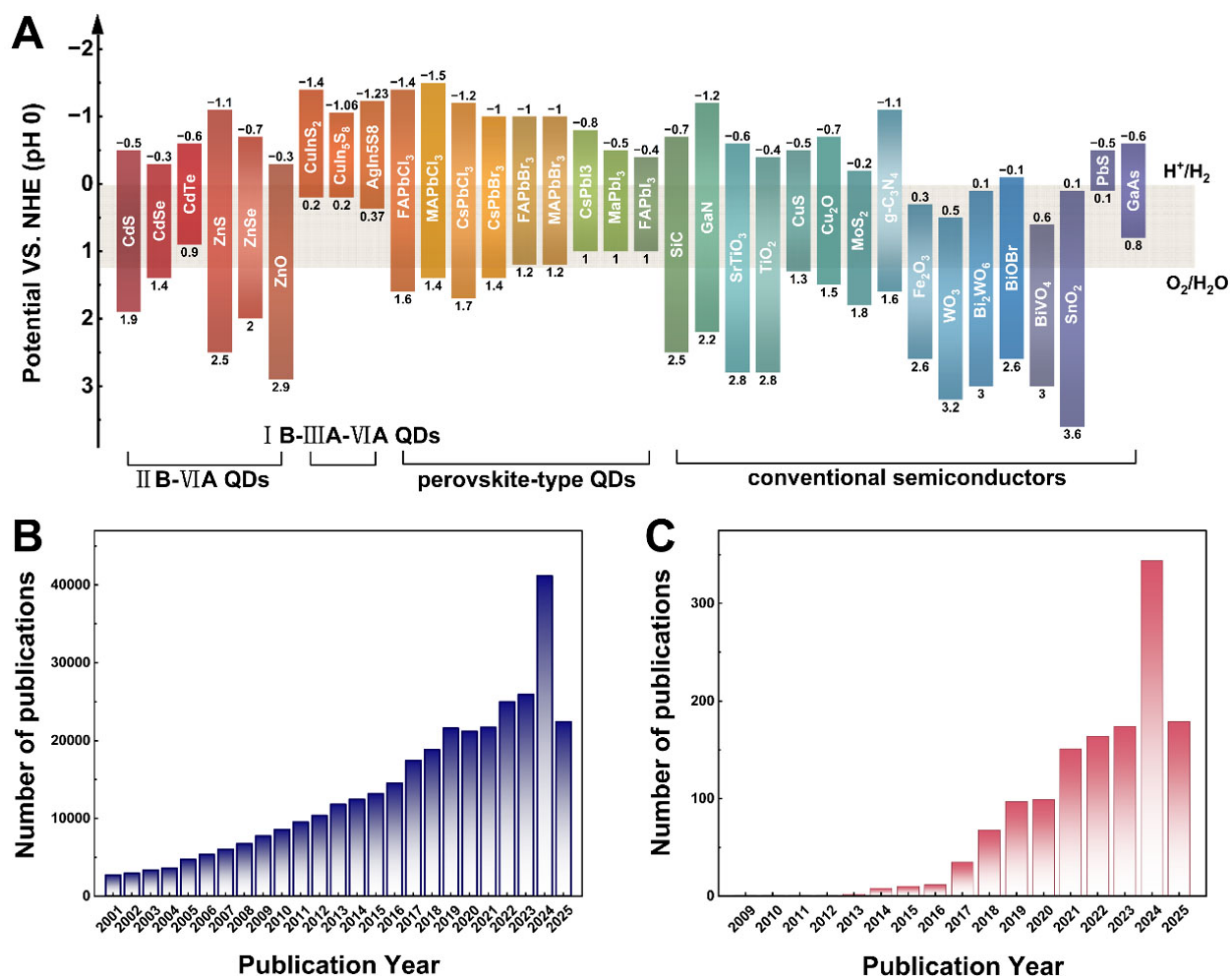


Figure 1. (A) Band energy diagrams of representative semiconductors for CO₂ photoreduction (NHE: Normal Hydrogen Electrode). Number of published manuscripts categorized by the keywords of (B) Annual publication counts for "quantum dots" from 2001-2025. (C) Annual publication counts for "quantum dots" combined with "photocatalytic CO₂ reduction" from 2009-2025. Data sourced from the Web of Science database.

Common QD families include binary compounds from groups II-VI (e.g., CdS, CdSe, ZnO)^[18-20], ternary I-III-VI compounds (e.g., CuInS₂, CuAlS₂)^[21-23], and a new generation of perovskite-type QDs (e.g., CsPbBr₃, CH₃NH₃PbBr₃, Cs₂AgBiBr₆) renowned for their exceptional optoelectronic properties^[24-26]. In this review, we focus on the application of semiconductor QDs in photocatalytic CO₂RR and the direct coupling of CO₂ capture with its utilization. We begin by summarizing the fundamental thermodynamics and kinetics of photocatalytic CO₂ reduction. Subsequently, we discuss key strategies for enhancing the performance of QD photocatalysts, including bandgap engineering, heterostructure design, and surface modification to improve light absorption, charge separation, and surface reaction kinetics. Distinctively, we provide an in-depth examination of cutting-edge characterization techniques that enable real-time monitoring of reaction intermediates, active site evolution and photocatalyst stability, addressing a critical knowledge gap in mechanistic understanding. We also present comprehensive analysis of integrated CO₂ capture and utilization (CCU) approaches using QD-metal-organic framework (MOF) and QD-covalent organic framework (COF) composites, evaluating both technical feasibility and realistic energy balance considerations. We also examine integrated approaches for direct CO₂ CCU, addressing associated challenges and potential solutions. Finally, we present a perspective on the remaining challenges and future directions in this vibrant field, particularly emphasizing the transition from laboratory demonstrations to practical implementation through realistic stability testing and energy-efficient system design, aiming to provide a roadmap for developing high-performance QD-based systems for sustainable carbon management.

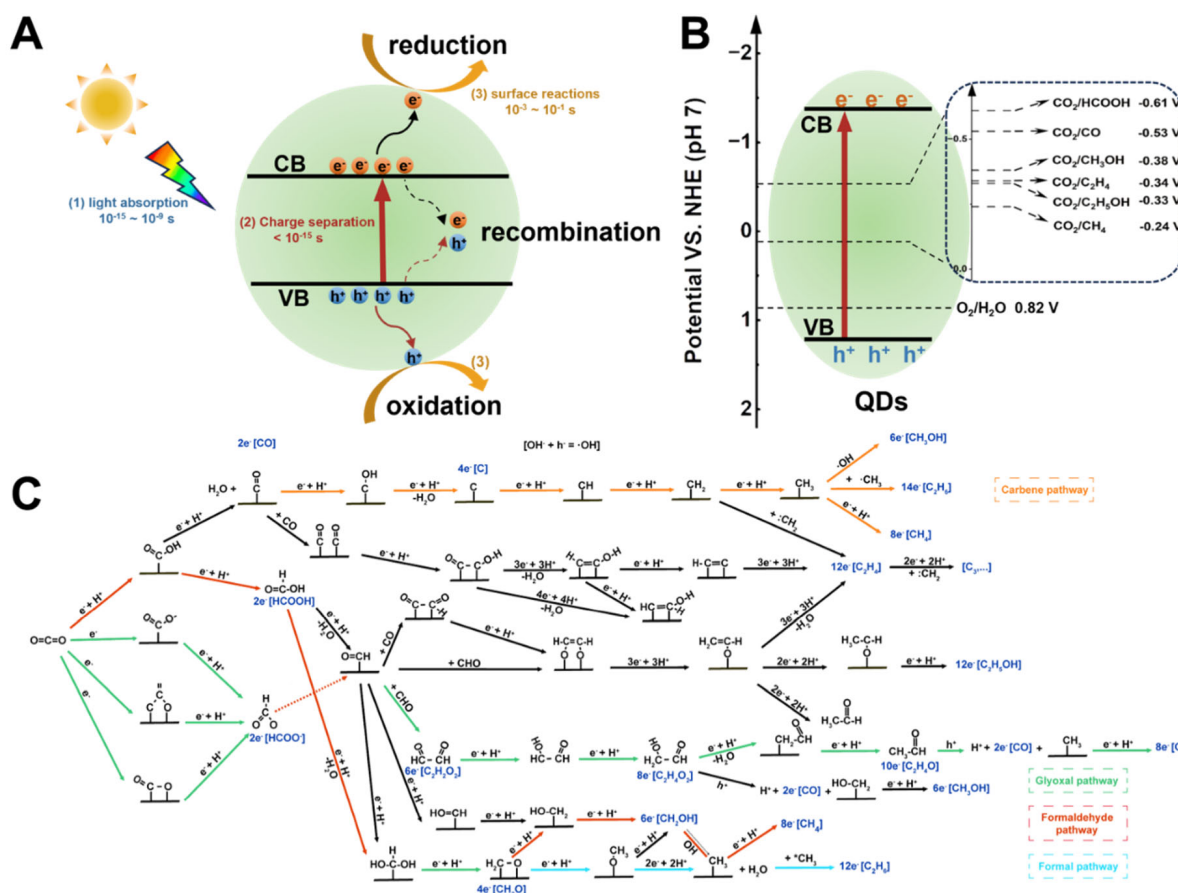


Figure 2. Schematic of the photocatalytic CO_2 reduction mechanism. (A) Key steps in the photocatalytic process on a semiconductor quantum dot (QD), with characteristic timescales for each step; (B) Redox potentials versus NHE for CO_2 reduction to various products at pH 7; (C) Proposed reaction pathways and intermediates for the formation of different CO_2 reduction products^[11]. Adapted with permission. Copyright 2024, American Chemical Society.

LIGHT-DRIVEN CO_2 REDUCTION REACTION

Principles of CO_2 reduction

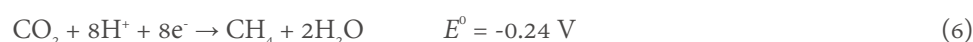
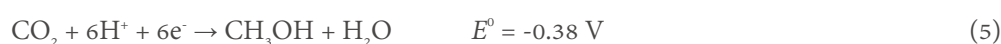
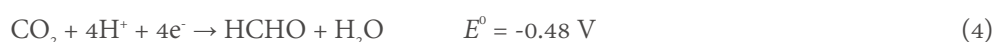
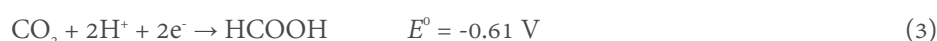
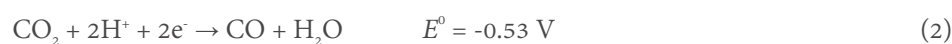
As shown in Figure 2A, the photocatalytic CO_2 reduction reaction (CO_2RR) generally involves three sequential steps that occur within a time frame of 10^{-15} to 10^{-1} seconds^[27–29]: (i) Light Absorption (10^{-15} – 10^{-9} s): A photocatalyst absorbs photons with energy exceeding its bandgap, exciting electrons from the valence band (VB) to the conduction band (CB) to generate electron-hole (e^-/h^+) pairs; (ii) Charge Separation and Migration ($< 10^{-15}$ s): the photogenerated charge carriers separate and migrate from the bulk phase to the active sites on the surface of the photocatalyst; (iii) Surface Redox Reactions (10^{-3} – 10^{-1} s): Adsorbed CO_2 molecules are reduced by electrons, while holes oxidize water or sacrificing agents. And efficient CO_2RR demands both suitable semiconductor band alignment and effective charge utilization. Thermodynamically, the CB minimum must be more negative than the CO_2 reduction potentials, while the VB maximum must be more positive than the oxidation potential of the electron donor. Kinetically, rapid charge transfer to surface active sites is critical to outcompete the rapid recombination of photogenerated electron-hole pairs, which occurs on picosecond to millisecond timescales.

The photocatalytic CO_2RR is inherently challenging. Chemically, the CO_2 molecule is linear and thermodynamically stable, with a high C=O bond dissociation energy of $750 \text{ kJ}\cdot\text{mol}^{-1}$, making it difficult to

activate^[30]. Physically, its low aqueous solubility (0.033 mol·L⁻¹ at 25 °C and 1 atm^[31]) limits mass transfer to the catalyst surface in aqueous environments. Despite these challenges, the CO₂RR proceeds through several key steps. The process initiates with the adsorption of a CO₂ molecule onto the photocatalyst surface. This is followed by a kinetically slow, one-electron reduction to form a bent *CO₂ radical anion, a step that requires a substantial energy input (ca. -1.9 V vs. NHE (Normal Hydrogen Electrode)), as given in



Subsequent proton-coupled electron transfer steps then occur, leading to the breakage of O=C=O bonds and the formation of key intermediates such as dentate (*OCHO) or carboxyl (*COOH) species. These intermediates are ultimately converted into various products such as CO, CH₄, HCOOH, and CH₃OH through divergent reaction pathways [Figure 2B], as given in



A representative network of these potential photocatalytic synthesis pathways is summarized in Figure 2C^[32-34].

Evaluation metrics for photocatalytic CO₂RR performance

The performance of a photocatalytic CO₂RR in a particulate suspension system is typically quantified using six metrics^[35]: (1) CO₂ conversion rate; (2) production rate; (3) selectivity; (4) turnover number (TON) or turnover frequency (TOF); (5) quantum efficiency and (6) solar-to-chemical (STC) conversion efficiency. The CO₂ conversion rate is defined as the ratio of reacted CO₂ to the initial CO₂ feedstock, as given in

$$\text{CO}_2 \text{ conversion rate} = \frac{\text{reacted CO}_2 \text{ (}\mu\text{ mol)}}{\text{total CO}_2 \text{ (}\mu\text{ mol)}} \quad (7)$$

This, though often omitted, is crucial for evaluating the total consumption of CO₂ across all products^[36]. It depends not only on the catalyst's intrinsic activity but also on reaction conditions such as time and total amount of CO₂ supplied^[37]. Production rate refers to the yield of a specific product (e.g., CO, CH₄, HCOOH) per unit time and per mass of catalyst, as determined by

$$\text{production rate (}\mu\text{mol} \cdot \text{h}^{-1} \cdot \text{g}^{-1}\text{)} = \frac{\text{Yield over a period time (}\mu\text{mol)}}{\text{Time (h)} \times \text{Catalyst mass (g)}} \quad (8)$$

This is the most commonly reported metric for evaluating performance in heterogeneous photocatalytic systems. In addition, when multiple products are formed during the photocatalytic process, the selectivity metric is used to measure the tendency of formation of the target product over all products, as calculated using

$$\text{Selectivity} = \frac{\text{Yield of target product } (\mu\text{mol})}{\text{Yield of all products } (\mu\text{mol})} \quad (9)$$

Unlike other metrics, a key consideration in this calculation is the inclusion of H_2 production, a common competing side reaction. For a homogenous system with a clearly defined active site, TON and TOF are used to quantify catalytic efficiency, defined as the number of product molecules generated per active site over a reaction period (TON) or per unit time (TOF), as given by

$$\text{TON} = \frac{\text{Number of reacted } \text{CO}_2}{\text{Number of active sites}} \quad (10)$$

$$\text{TOF } (\text{h}^{-1}) = \frac{\text{Number of reacted } \text{CO}_2}{\text{Number of active sites} \times \text{Time (h)}} \quad (11)$$

While straightforward for homogeneous catalysts with well-defined active sites, accurately determining the number of active sites poses a significant challenge in heterogeneous systems. Quantum efficiency is an important metric to measure the effectiveness of a photocatalyst in converting incident photons into chemical energy. Generally, the apparent quantum efficiency (AQE), which is based on the total incident photon flux, is widely used due to its practical measurability^[38], as given in

$$\begin{aligned} \text{AQE} &= \frac{\text{Number of electrons used for } \text{CO}_2 \text{ reduction}}{\text{Number of incident photons}} \\ &= \frac{\sum \mu (\text{Amount of Product} \times (\mu \text{ mol}) \times \text{Electron Numbers required to reduce } \text{CO}_2 \text{ to } x)}{\text{Light intensity } (\text{W} \cdot \text{m}^{-2}) \times \text{Irradiation area } (\text{m}^2) \times \text{Time (s)}} \\ &\div \frac{\text{Plank constant } (\text{J} \cdot \text{s}) \times \text{Light speed } (\text{m} \cdot \text{s}^{-1})}{\text{wavelength (m)}} \end{aligned} \quad (12)$$

Calculating AQE requires knowing the number of electrons needed to form a given product (e.g., 2 for CO or HCOOH, 8 for CH_4). Finally, STC conversion efficiency evaluates the overall efficiency of converting the full spectrum of solar energy into chemical energy stored in the products, as given by

$$\text{STC efficiency} = \frac{\sum ((\text{Yield of } x (\mu \text{ mol}) \times \text{Gibbs free energy change of } \text{CO}_2 \text{ to } x (\text{kJ} \cdot \text{mol}^{-1})))}{\text{Light intensity } (\text{W} \cdot \text{m}^{-2}) \times \text{Irradiation area } (\text{m}^2) \times \text{Time (s)}} \quad (13)$$

This is the most comprehensive metric for assessing practical solar fuel generation, though it is currently reported in only a limited number of studies^[39].

Beyond these qualitative metrics, a comprehensive assessment of a catalyst's overall performance must also include its stability and recyclability. The challenge of distinguishing between different degradation mechanisms in QD photocatalysts requires a coordinated characterization approach that correlates temporal performance changes with microscopic structural evolution^[40]. For instance, operando X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) can differentiate between active site poisoning (evidenced by surface oxidation state changes) and bulk structural degradation (revealed through coordination environment analysis)^[41]. When coupled with time-resolved photoluminescence (PL) spectroscopy, these techniques help distinguish whether performance loss originates from increased surface trap states (photo-corrosion) or altered charge separation dynamics (interface degradation in heterostructured QDs)^[42]. Ion migration pathways, particularly critical in perovskite QDs, can be tracked through secondary ion mass spectrometry (SIMS) depth profiling combined with *in-situ* electrical measurements^[43]. The temporal correlation between halide redistribution (detected by SIMS) and photocurrent decay patterns helps identify whether performance degradation stems from compositional instability or morphological changes.

To distinguish dominant degradation pathways, a systematic approach is often applied to correlate degradation kinetics with environmental conditions^[44]. Rapid performance loss under illumination (hours) typically indicates photochemical degradation, while gradual decline over weeks suggests ion migration or chemical poisoning^[45]. For example, comparing stability under dry CO₂ versus humid CO₂ environments can isolate moisture-induced degradation from CO₂-specific effects, while reversibility tests (thermal annealing or chemical treatment) distinguish between permanent structural changes and recoverable surface poisoning.

Furthermore, optimizing photocatalytic systems requires balancing these metrics, as enhancing one often comes at the expense of another^[35]. For instance, while increasing light intensity can enhance production rates, CO₂ conversion, and TON/TOF, it typically reduces both quantum efficiency and STC conversion efficiency due to heightened charge recombination losses. Beyond technical performance metrics, techno-economic analysis (TEA) is crucial for evaluating the commercial viability of photocatalytic CO₂RR systems^[46]. Key economic parameters, including the cost of catalyst production, capital expenditure (CAPEX), and operating expenses (OPEX), are fundamentally determined by the technical performance metrics achieved under solar irradiation^[47-49]. Furthermore, the inherent intermittency of sunlight and the costs associated with large-scale photoreactor installations present unique economic challenges for photocatalytic CO₂RR systems^[50-52]. Therefore, optimizing technical metrics such as performance under low-light conditions and long-term catalyst durability is not merely a scientific goal but an economic imperative to minimize the levelized cost of solar fuel production.

ADVANCES IN QD-BASED PHOTOCATALYTIC CO₂ CONVERSION SYSTEMS

As stated, photocatalytic CO₂ reduction generally includes three essential steps: light absorption, charge separation/migration and surface redox reactions. Furthermore, given the low concentration of CO₂, the efficient capture and adsorption of CO₂ molecules on the catalyst surface are critical prerequisites for high performance. This section details recent advances in enhancing the overall efficiency of QD-based photocatalytic CO₂RR. We will examine key strategies focused on: Broadening and intensifying light absorption, suppressing charge carrier recombination, and facilitating CO₂ adsorption and activation at active sites [Table 1].

Strategies to enhance light absorption

Absorbing photon energy to generate charge carriers is the initial step of the photocatalytic CO₂RR process^[53]. The visible spectrum (400-800 nm) encompasses approximately 50% of solar emission energy. Thus, the performance of QD-based photocatalysts depends critically on extending their absorption edge

Table 1. Various parameters associated with CO₂RR catalyzed by QDs

Photocatalyst	Surface loading	Reactant	Sacrificial agent	Gas species	Gas evolution rate	Light source	Reaction duration	Efficiency	Ref.
CsPbBr ₃	None	Gas-solid phase reaction		CO/CH ₄	75.50/4.02 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	5 h	AQE = 4.47% (420 nm)	[56]
CdS	Cu	water		CO/CH ₄	30.3/5.90 μmol·g ⁻¹ ·h ⁻¹	λ > 400 nm, 100 mW·cm ⁻²	8 h	AQE = 0.03% (420 nm)	[57]
CuInS ₂	Co	water		CO	15.24 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp			[58]
CdS	Ni			CO/CH ₄	9.38/1.83 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	12 h		[59]
Cu _{0.05} Zn _{2.95} In ₂ S ₆	CQDs	water/acetonitrile	TEOA	CO	70.69 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp			[60]
CdSe	g-C ₃ N ₄	water		CH ₄	47 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	5 h		[61]
CdS	Cu	acetonitrile		CO/H ₂	0.12/0.21 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	6 h		[62]
ZnIn ₂ S ₄	BP	KCO ₃		H ₂ /CO	15.0/27.2 μmol	300 W Xe lamp	4 h		[63]
CuInS ₂	Zn	water	ascorbic acid	CO	535.3 μmol·g ⁻¹ ·h ⁻¹	380 < λ < 780 nm, 100 mW cm ⁻²	120 h	AQY = 0.32% (400 nm)	[64]
g-C ₃ N ₄	CQDs	water vapor		CO/CH ₄	79.2/2.7 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp		AQY = 0.02% (420 nm)	[65]
CsPbBr ₃	Bi ₂ WO ₆	EA/water		CO	251.5 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	2 h		[68]
CsPbBr ₃	TiO ₂	acetonitrile/water	BIH	CO	9.02 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	4 h		[69]
g-C ₃ N ₄	BiVO ₄	water		CO/CH ₄	5.19/4.57 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	6 h		[70]
g-C ₃ N ₄	CQDs			CO/CH ₄	5.88/2.92 μmol·g ⁻¹ ·h ⁻¹			AQE = 0.076%	[71]
CuInS ₂	TiO ₂	water vapor		CH ₄ /CH ₃ OH	2.5/0.86 μmol·g ⁻¹ ·h ⁻¹	350 W Xe lamp	3 h		[72]
CdSe	CdS	water		CO/H ₂	495/401.25 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	8 h		[73]
CsPbBr ₃	TiO ₂	ethyl acetate/water		CO	145.28 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	4 h	QE = 0.126% (420 nm)	[75]
CsPbBr ₃	ZnO	water	TEOA	CO	85.55 μmol·g ⁻¹ ·h ⁻¹	Xe lamp	4 h		[76]
Cs ₃ Bi ₂ Br ₉	SnO ₂	acetonitrile/water		CH ₄	1.78 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	12 h		[77]
Bi	CsPbBr ₃ QDs	water vapor		CO/CH ₄	31.55/43.11 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	5 h		[78]
CsPbBr ₃	ferrocene carboxylic acid (FCA) ligand	water vapor		CO/C ₂ H ₄	132.8/1.6 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	5 h	QE = 0.072%	[82]
CsPbBr ₃	Ni(tpy)	water		CO/CH ₄	1724 μmol·g ⁻¹	300 W Xe lamp	4 h		[83]
CsPbBr ₃	Ru	CO ₂		CO	28.12 μmol·g ⁻¹	300 W Xe lamp	6 h		[85]
CdSe	Carbonic	20 mM NaHCO ₃	TEA	CO	47.3 μmol·g ⁻¹ ·h ⁻¹	300 W Xe lamp	4 h		[86]

CdS QDs/NC	Co(bpy)32+ (bpy = 2,2'-bipyridine) a	acetonitrile/water		CO	5120 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	300 W Xe lamp	5 h	[87]
CdSe	PEI-LA	water	TEOA	CO	4.98 $\text{mmol}\cdot\text{g}^{-1}$	blue LED lamp ($\lambda_{\text{max}} = 450\text{ nm}$)	6 h	[88]
CsPbBr ₃	MOF	water vapor		CH ₄	29.63 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	100 W Xe lamp	3 h	EQE = 0.035% (386 nm) [89]
Cs ₂ AgBiBr ₆	Ce-UiO-66-H	water		CO	309.01 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	300 W Xe lamp	2 h	[91]
Cs ₃ Bi ₂ Br ₉	Bi-MOF	water		CO/CH ₄	572.24/35.502 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	300 W Xe lamp	2 h	[92]
CsPbBr ₃	COF	water		CO/CH ₄	5.15/1.713 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	300 W Xe lamp	8 h	[95]
CdS/BN	Ti ₃ C ₂	water		CO/CH ₄	1.45/0.44 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	300 W Xe lamp	5 h	[96]

into this region and maximizing their absorption efficiency. This section reviews key strategies for enhancing the light-harvesting capabilities of QDs, including ion doping^[54], size modulation^[55], localized surface plasmonic resonance effect^[56], and others.

Introducing foreign atoms into the host lattice of QDs is a powerful method to tailor their physicochemical and photoelectronic properties. Doping could be categorized into three different primary types: metal doping (e.g., with transition metals such as Cu^[57], Co^[58], Ni^[59]), non-metal doping (e.g., with N^[60], P^[61], S, C), and co-doping (simultaneous introduction of different elements). These doping methods enable precise modulation of the host's energy level, creating intermediate states that extend the photon absorption of the QDs into the visible light region, thereby enhancing light utilization. Among these approaches, metal atom doping leverages the introduction of d-orbital states to alter the host's energy levels, enabling tailored electronic properties. For example, Zhang *et al.* synthesized Cu-doped CdS QDs through a hot-injection method followed by cation exchange, where Cu dopants were introduced into the CdS lattice at varying nominal Cu/Cd molar ratios (0.125% to 2%)^[57]. The Cu doping introduced intermediate energy levels within the bandgap that enabled sub-bandgap photon absorption, thus extending the light absorption spectrum into the visible region [Figure 3A]. Compared to the pristine CdS QDs, the PL emission intensity of Cu:CdS QDs exhibited a considerable enhancement (~40 times) higher than that of the pristine CdS QDs. Photocatalytic evaluation revealed that under visible-light irradiation, the optimally Cu:CdS QDs exhibited CO and CH₄ production rates of 30.3 and 5.9 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$, respectively, whereas pristine CdS showed negligible activity^[57]. Also, Gao *et al.*^[62] introduced Cu doping into CdS QDs (Cu:CdS QDs) at varying concentrations (0.125% to 0.184%) via a one-pot method. Distinguished from prior studies on Cu:CdS, this study employs a Cu-doping strategy that serves a dual purpose: enhancing light harvesting and promoting charge separation via Cu-induced electron enrichment. The incorporated copper also acts as an active site for CO₂ adsorption and activation. This dual contribution significantly improves visible-light utilization and promotes syngas formation with a tunable CO/H₂ ratio. Under visible light illumination ($\lambda > 420\text{ nm}$), the optimal Cu:CdS QDs (0.036% molar ratio Cu of CdS) achieved synergistic photocatalytic performance with 96.4% benzylamine conversion and tunable syngas production (CO/H₂ ratios from 2:1 to 1:2), where CO and H₂ yields reached 7.20 and 12.34 μmol after 6 h while simultaneously producing 31.54 μmol of dibenzyl amine with > 99% selectivity. In addition to Cu, other metals have similar properties: Yang *et al.*^[58] synthesized Co-doped CuInS₂ (Co/CuInS₂) nanoflowers via an oil-bath method followed by high-temperature calcination. Ultraviolet-visible (UV-vis) diffuse

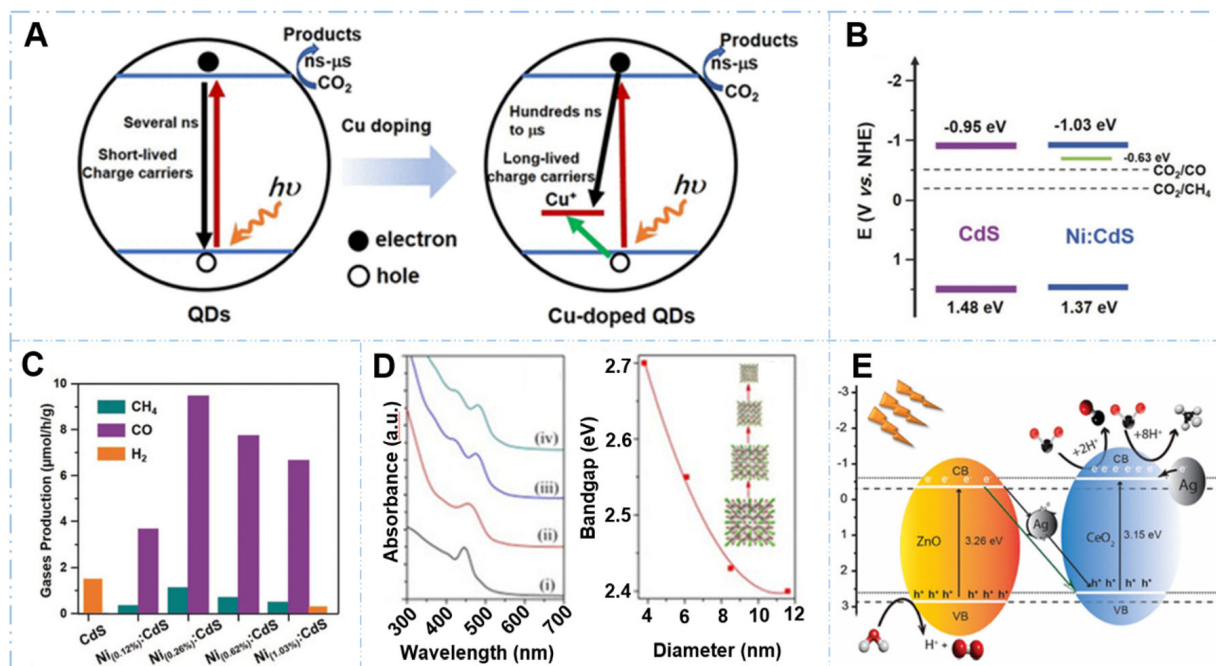


Figure 3. Strategies for enhancing the light absorption of QDs. (A) Cu doping in CdS QDs extends the light absorption range and improves charge separation^[57]. Reproduced with permission from ref.^[57]. Copyright 2024, American Chemical Society; (B and C) Ni doping increases the light utilization efficiency of CdS QDs^[59]. Reproduced with permission from ref.^[59]. Copyright 2018, John Wiley and Sons; (D) Size-dependent tuning of the absorption spectrum in CsPbBr₃ QDs^[55]. Reproduced with permission from ref.^[55]. Copyright 2017, John Wiley and Sons; (E) Enhanced absorption in a CeO₂-ZnO QD system through the localized surface plasmon resonance (LSPR) effect of Ag nanoparticles^[56]. Reproduced with permission from ref.^[56]. Copyright 2021, American Chemical Society.

reflectance spectra (DRS) analysis revealed that Co doping did not significantly alter the absorption in the UV and near-infrared regions but notably enhanced it across the visible spectrum. Further data and electrochemical measurements indicated a shift in band positions and a narrowing of the bandgap from 1.52 to 1.41 eV, which corroborates the observed enhancement in visible-light absorption. Consequently, under 300 W Xenon (Xe) lamp irradiation, the Co/CuInS₂ catalyst achieved a CO production rate of 15.24 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$, which is four-fold over the pristine CuInS₂. Similarly, Wang *et al.*^[59] reported Ni²⁺-doped CdS QDs for CO₂ photoreduction. While linear sweep voltammetry (LSV) indicated a marginally narrowed bandgap (from 2.43 to 2.40 eV) post-doping, the primary function of Ni was revealed by PL and Electron Spin Resonance (ESR): serving as an electron-enriching center that promotes carrier separation and enhances light utilization. This modification endowed the typically H₂-producing CdS with high activity for photocatalytic CO₂ reduction to CO and CH₄ [Figure 3B and C].

While metal doping can enhance light absorption through bandgap engineering, non-metal doping offers a complementary strategy by primarily modifying the VB structure. For instance, Yang *et al.*^[60] synthesized nitrogen-doped carbon QDs (NCQDs) from corn straw biomass using tryptophan as the nitrogen source to achieve high pyridine-nitrogen content (17.56%), which were then used to modify Cu_{0.05}Zn_{2.95}In₂S₆ photocatalysts (CZIS@CQDs-T). The NCQD modification enhanced light harvesting efficiency to over 70% and improved photon conversion in the 370–410 nm region through up-conversion of low-energy photons to high-energy photons. The optimized CZIS@CQDs-T photocatalyst, under a 300 W Xe lamp irradiation, achieved a CO production rate of 70.69 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ with nearly 100% selectivity, representing a 4.77-fold enhancement over the unmodified material. Also, Raziq *et al.*^[61] developed CdSe QDs coupled with phosphorus-doped graphitic carbon nitride (CdSe/P-CN) nanocomposites through a facile thermal treatment and wet chemical approach, where phosphorus atoms substituted carbon sites in the graphitic

carbon nitride ($g\text{-C}_3\text{N}_4$) lattice. Phosphorus doping significantly narrowed the bandgap from 2.7 eV (pristine $g\text{-C}_3\text{N}_4$) to 2.2 eV (P-CN), while coupling with CdSe QDs extended the visible-light absorption range from 450 to 700 nm. Under a 300 W Xe lamp irradiation, the optimized 4CdSe/P-CN composite achieved exceptional performance with $47 \mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ conversion rate for CO_2 reduction to methane, representing a 6.71 and 4.7-fold enhancement over the CN and P-CN, respectively. In summary, the strategic selection of dopant type, concentration, and lattice position enables precise tuning of the optical properties of QDs, making ion doping a highly attractive route for developing efficient photocatalysts for CO_2 reduction under solar irradiation.

Furthermore, the light absorption characteristics of QDs can be precisely tuned via the quantum confinement effect by controlling their physical dimensions. For instance, Hou *et al.*^[55] systematically tuned the bandgap of perovskite CsPbBr_3 QDs by varying their size from 3 to 12 nm [Figure 3D]. The optimized QDs with a diameter of 8.5 nm exhibited exceptional photocatalytic performance under 300 W Xe lamp irradiation, achieving > 99% selectivity for CO_2 reduction to CO and CH_4 and an electron consumption yield of $20.9 \mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$. Beyond quantum size effects, localized surface plasmon resonance (LSPR) offers a powerful alternative mechanism to enhance light absorption. In plasmonic QDs, the collective oscillations of free charge carriers at the metal-semiconductor interface generate intense localized electromagnetic fields, dramatically amplifying photon absorption, particularly in noble metal-decorated QD systems. For example, Mahyoub *et al.*^[56] synthesized Ag-CeO₂-ZnO (AgCZ) through hydrothermal and photo-deposition methods, where Ag nanoparticles (NPs, 3 wt% optimal loading) were uniformly dispersed on the CeO₂-ZnO composite surface [Figure 3E]. The surface plasmon resonance (SPR) effect of Ag NPs dramatically extended light absorption from the UV region into the visible spectrum. The optimized 3AgCZ photocatalyst achieved exceptional CO_2 reduction performance with CH_4 production rate of $302 \mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ and 89.3% selectivity under simulated sunlight. In summary, these strategies, when combined with appropriate heterostructure engineering and morphological design synergistically, have proven highly effective for enhancing the light-harvesting capability of QDs in photocatalytic CO_2 reduction.

Strategies to improve charge separation

To achieve high quantum efficiency for QD-photocatalyzed CO_2 reduction, it is crucial to separate electrons from holes and facilitate their migration to surface active sites for subsequent reactions^[14]. A significant challenge arises from the fact that charge carrier lifetimes in QDs typically range from picoseconds to nanoseconds [Figure 2A], a timescale comparable to that of recombination. Researchers have developed various ways to drive effective charge transfer in QDs through heterojunction construction^[63], defect engineering^[64], *etc.*

Heterojunction construction is to combine two or more semiconductors through hydrothermal, *in-situ* growth or other synthesis methods^[65]. Based on the arrangement of the components' energy band structures, photocatalyst heterojunctions can be classified as type I (straddling), type II (staggered), type III (broken-gap), Z-scheme, and S-scheme heterojunctions^[66,67]. This section will detail the application of three typical heterostructures: type II, Z-scheme, and S-scheme heterojunctions in enhancing charge transfer for photocatalytic CO_2 reduction.

Type II heterojunctions are formed between two semiconductors with a staggered band alignment [Figure 4A]. This configuration creates a built-in electric field at the interface that drives the spatial separation of photogenerated electrons and holes into opposite materials, effectively suppressing recombination and prolonging carrier lifetimes. A representative example is the work by Han *et al.*^[63], who constructed a heterostructure between black phosphorus QDs and ZnIn_2S_4 nanosheets (BP/ZIS) via ultrasonic-assisted self-assembly. This heterojunction significantly enhanced charge-carrier separation,

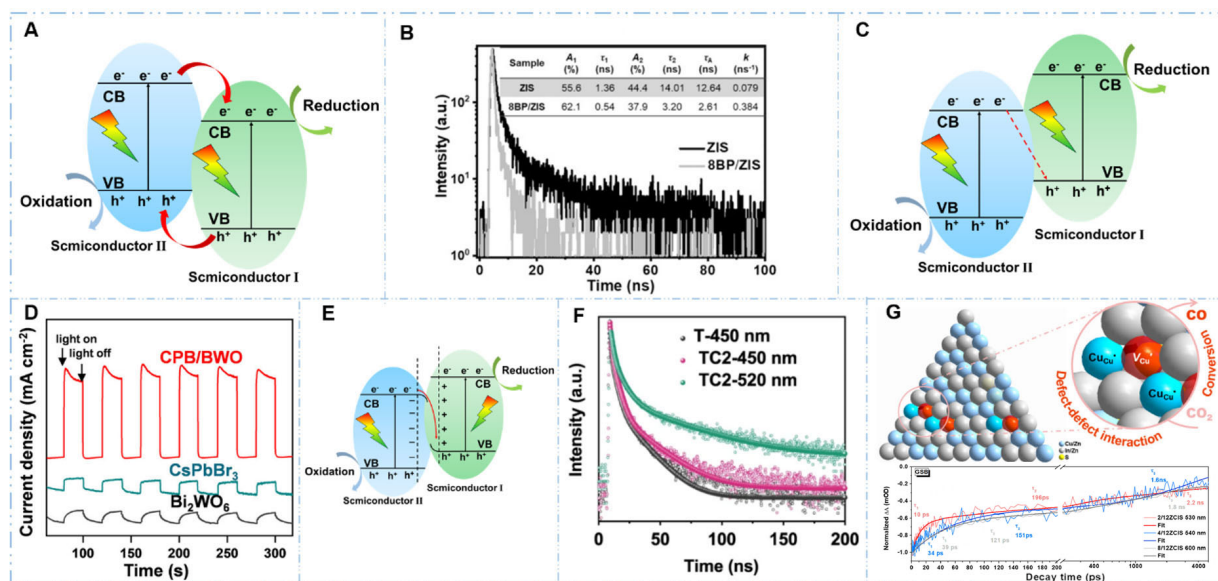


Figure 4. Strategies for enhancing charge separation and transfer in QDs. (A) A schematic representation of type II heterojunction; (B) Transient absorption spectra demonstrating improved charge separation by forming type II heterojunction^[63]. Reproduced with permission from ref.^[63]. Copyright 2021, John Wiley and Sons; (C) A schematic representation of Z-scheme heterojunction; (D) Photocurrent response (I-t curve) showing enhanced photocurrent by Z-scheme heterojunction engineering^[68]. Reproduced with permission from ref.^[68]. Copyright 2020, American Chemical Society; (E) A schematic representation of S-scheme heterojunction; (F) Transient absorption spectra confirming prolonged carrier lifetime by constructing S-scheme heterojunction^[69]. Reproduced with permission from ref.^[69]. Copyright 2020, Xu *et al.*^[69]; (G) Cu defect engineering improved charge separation in CuInS QDs, as evidenced by transient absorption spectroscopy^[64]. Reproduced with permission from ref.^[64]. Copyright 2023, American Chemical Society.

evidenced by a four-fold increase in charge transfer rate and prolonged carrier lifetimes compared to pristine ZnIn₂S₄ [Figure 4B]). Under visible light ($\lambda > 420$ nm) irradiation, the optimized 8 wt%. BP loading on ZIS (8BP/ZIS) photocatalyst achieved tunable syngas production with CO/H₂ ratios adjustable from 1:6 to 2:3, alongside 95% benzylamine conversion with 94% selectivity toward N-benzylidene benzylamine formation and an apparent quantum yield of 6.5% at 465 nm.

While type II heterojunctions are effective in promoting the separation of photogenerated charge carriers, thermodynamic analysis reveals that they will decrease the overall redox abilities of photocatalysts^[70]. An alternative strategy, inspired by natural photosynthesis [Figure 4C]^[71,72], is the Z-scheme heterojunction, which achieves the desired charge separation without compromising redox ability. In this configuration, photogenerated electrons in the CB of one semiconductor recombine with holes in the VB of the other semiconductor (via conductive mediators or direct interfacial contact). This strategic recombination selectively removes charge carriers with weaker redox potential, thereby preserving the most potent electrons and holes in their original components, resulting a system that achieves spatial charge separation while maintaining strong driving forces for both reduction and oxidation reactions. For instance, Wang *et al.*^[68] synthesized a direct Z-scheme heterojunction by growing 0D CsPbBr₃ (CPB) QDs on 2D Bi₂WO₆ (BWO) nanosheets through an *in-situ* growth strategy for visible-light-driven CO₂ photoreduction. The band positions of Bi₂WO₆ and CsPbBr₃, determined by UV-Vis DRS and VB XPS tests, reveal a favorable band alignment between the two semiconductors, which is suitable for the formation of a Z-scheme heterojunction. This heterojunction formation significantly enhanced charge-carrier separation and transfer efficiency, as evidenced by PL quenching and a robust photocurrent response [Figure 4D]. The optimized CPB/BWO composite achieved a product yield of 503 $\mu\text{mol}\cdot\text{g}^{-1}$ under visible-light illumination ($\lambda > 400$ nm), representing a 9.5-fold enhancement over pristine CsPbBr₃ QDs. In another example, Zhang *et al.* engineered hybrid CdSe/CdS QDs with Z-scheme band alignment heterostructure through an oil bath

method, creating a cooperative photoredox system that simultaneously reduced CO_2 while selectively oxidizing thiol^[73]. The heterostructure formation established an internal electric field (IEF) at the CdSe/CdS interface that significantly enhanced photoinduced charge carrier separation and transfer efficiency, as confirmed by PL quenching, electrochemical impedance spectroscopy, and transient photocurrent measurements. The optimized CdSe/CdS QDs achieved simultaneous production of tunable syngas ($3.96 \text{ mmol}\cdot\text{g}^{-1} \text{ CO}$ and $3.21 \text{ mmol}\cdot\text{g}^{-1} \text{ H}_2$) with CO/H_2 ratios adjustable from 1:4 to 5:4, alongside highly selective disulfide synthesis ($8.05 \text{ mmol}\cdot\text{g}^{-1}$) after 8 h of visible light irradiation^[73].

The S-scheme heterojunctions are comprised of two closely bound photocatalysts, an oxidation photocatalyst (OP) and a reduction photocatalyst (RP), and the RP possesses higher CB, VB, and Fermi level than the OP [Figure 4E]^[74]. Before light irradiation, Fermi level equilibration generates an IEF at the RP/OP interface, pointing from RP to OP. This causes the CB and VB of RP to bend upward, while the CB and VB of OP bend downward. As a result, photogenerated electrons from the CB of OP can recombine with holes in the VB of RP, and electrons in the CB of RP and holes in the VB of OP are driven from the interior toward the surface^[75,76]. This mechanism preserves electrons with strong reduction capability in the RP's CB and holes with strong oxidation capability in the OP's VB, enabling efficient spatial charge separation while maintaining high redox potentials for enhanced photocatalytic performance^[77,78]. For example, Xu *et al.*^[69] synthesized a unique S-scheme heterojunction by integrating CsPbBr₃ QDs with TiO₂ nanofibers through electrostatic self-assembly. The potential S-scheme heterojunction between CsPbBr₃ QDs and TiO₂, first indicated by their band positions from UV-Vis DRS and VB XPS test, was then confirmed by *in-situ* XPS. Under illumination, the composite (TC2) showed a 0.3 eV positive BE shift for Ti 2p/O 1s and a 0.5 eV negative shift for Cs 3d/Pb 4f/Br 3d, validating the S-scheme electron transfer from the TiO₂ CB to the CsPbBr₃ VB. The heterojunction formation significantly enhanced charge carrier transfer efficiency through the establishment of an IEF at the interface, as evidenced by time-resolved PL measurements [Figure 4F]. Under UV-vis light irradiation, the optimized TiO₂/CsPbBr₃ hybrid achieved a CO₂ photoreduction rate of $9.02 \text{ }\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ with 95% CO selectivity, corresponding to 1.92-fold and 1.83-fold enhancements over pristine TiO₂ nanofibers ($4.68 \text{ }\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$) and pristine CsPbBr₃ QDs ($4.94 \text{ }\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$), respectively. Similarly, Zhang *et al.* constructed a Bi/CsPbBr₃ QD S-scheme heterojunction photocatalyst via an *in-situ* growth method^[78]. The heterojunction formation significantly enhanced charge carrier dynamics through a strong Cs-Bi interaction at the interface, as evidenced by time-resolved PL spectra, electrochemical impedance spectra, and steady-state PL. The hybrid system achieved optimal CO₂ photoreduction performance with yields of $157.76 \text{ }\mu\text{mol}\cdot\text{g}^{-1}$ for CO and $215.56 \text{ }\mu\text{mol}\cdot\text{g}^{-1}$ for CH₄ after 5 h of under UV-vis light irradiation without sacrificial agents, representing 16.84-fold and 2.45-fold enhancements, respectively, compared to pristine CsPbBr₃ QDs. Additionally, Wang *et al.*^[79] verified the mechanism of S-scheme heterojunction by *in situ* XPS test. They fabricated TiO₂ hollow spheres (HSS) by template method and then deposited ZnIn₂S₄ on the surface of TiO₂ to obtain composite materials. After the coupling of TiO₂ and ZnIn₂S₄, due to the high Fermi level of ZnIn₂S₄, the free electrons in ZnIn₂S₄ RP were transferred to TiO₂ OP, resulting in the decrease and increase of the binding energy of elements in TiO₂ and ZnIn₂S₄, respectively. However, under illumination, the photogenerated electrons in TiO₂ CB are transferred to ZnIn₂S₄ VB, causing the elements in TiO₂ and ZnIn₂S₄ to shift toward higher and lower binding energies, respectively, resulting in opposite binding energy displacements. The following activity tests have shown that, under a 300 W Xe lamp, the hybrid system total CO₂ photoreduction conversion rates have increased by 2.75 and 4.43 times compared with the pristine ZnIn₂S₄ and TiO₂, respectively, attaining $18.32 \text{ }\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$. In summary, these heterojunction systems effectively enhance charge separation by establishing IEFs at the semiconductor interfaces through band alignment engineering to achieve optimal performance for photocatalytic CO₂ reduction reactions.

While heterojunction engineering effectively enhances charge separation through interfacial electric fields and band alignment optimization, the intrinsic electronic structure of individual semiconductor components also plays a critical role in the charge separation process. Defect engineering, by intentionally introducing structural deficiencies (e.g., oxygen or metal vacancies), can modify band structures and provide additional charge trapping or detrapping sites, suppressing charge recombination, to enhance photocatalytic performance^[80,81]. For instance, Cai *et al.*^[64] synthesized Cu-deficient CuInS₂ QDs (ZCIS QDs) by precisely controlling the Cu/In ratio to manipulate copper defect states [Figure 4G]. Femtosecond transient absorption spectroscopy confirmed that this defect engineering significantly enhanced charge carrier dynamics. The optimally deficient QDs (2/12ZCIS with Cu/In ratio of 2/12) achieved a high photocatalytic activity for CO₂ reduction to CO with a rate of 400–500 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$, which was 24-fold enhancement compared to the stoichiometric 8/12ZCIS QDs. In summary, both heterojunction construction (Type II, Z-scheme, S-scheme) and intrinsic defect engineering are powerful strategies for suppressing electron-hole recombination. By ensuring that a greater number of photoexcited carriers reach the catalyst surface, these methods are fundamental to driving efficient CO₂ activation and reduction.

Strategies to improve surface chemical reactions

The ultimate determinant of photocatalytic efficiency and product selectivity lies in the surface-mediated processes that occur after charge carriers arrive. These processes, including CO₂ adsorption, activation, and multi-electron and proton transfer, are governed by the local chemical environment, the atomic configuration of active sites, and the ability to stabilize key reaction intermediates. Consequently, significant research efforts are dedicated to engineering the QD surface to enhance these critical steps. This section reviews prominent strategies, such as surface ligand modification^[82] and cocatalyst loading^[83], which are designed to optimize surface reaction kinetics and steer product distribution.

Among these approaches, surface modification directly tailors the chemical and electronic properties of the QD surface where catalysis occurs. By introducing specific ligands, functional groups, or dopants, these modifications can modulate CO₂ binding affinity, alter surface charge, and create specific active sites that facilitate electron transfer to adsorbed reactants. For example, Du *et al.*^[82] modified CsPbBr₃ QDs with ferrocene carboxylic acid (FCA) ligands that grafted onto the QD surface through Cs atom coordination [Figure 5A]. The FCA ligands significantly enhanced CO₂ adsorption and activation, reducing the adsorption energy to -2.5256 eV (approximately half that of pristine QDs). The sandwich structure of ferrocene created natural CO₂ capture sites, and *in situ* Diffuse reflectance infrared fourier transform spectroscopy (DRIFTS) measurements combined with Density functional theory (DFT) calculations confirmed that these strengthened CO₂-surface interactions and favorable binding configurations facilitate subsequent electron transfer to the activated CO₂ molecules [Figure 5B]. The activity test showed that the FCA-modified CsPbBr₃ exhibited an impressive CO₂ to CO conversion rate of 132.8 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ under the 300 W Xe lamp irradiation, which is approximately ninefold higher than that of pristine CsPbBr₃ QDs. Furthermore, surface engineering can stabilize key reactive intermediates through coordination interactions and steric effects, thereby lowering activation barriers and directing product selectivity toward desired reduction pathways. For instance, Sahm *et al.*^[84] functionalized ZnSe QDs with imidazolium-terminated thiol ligands (MEMI) that not only passivated surface Zn sites to suppress competing hydrogen evolution but also created a favorable secondary coordination sphere for CO₂ reduction. The positively-charged imidazolium ligands stabilized the key $\text{*CO}_2^{\delta-}$ radical intermediate through π -p orbital interactions and hydrogen bonding, lowering the activation barrier for the rate-determining electron transfer step (0.77 eV) and enhancing CO production by 4-fold and selectivity by 13-fold compared to pristine ZnSe QDs under the UV-filtered simulated solar light ($\lambda > 400\text{ nm}$).

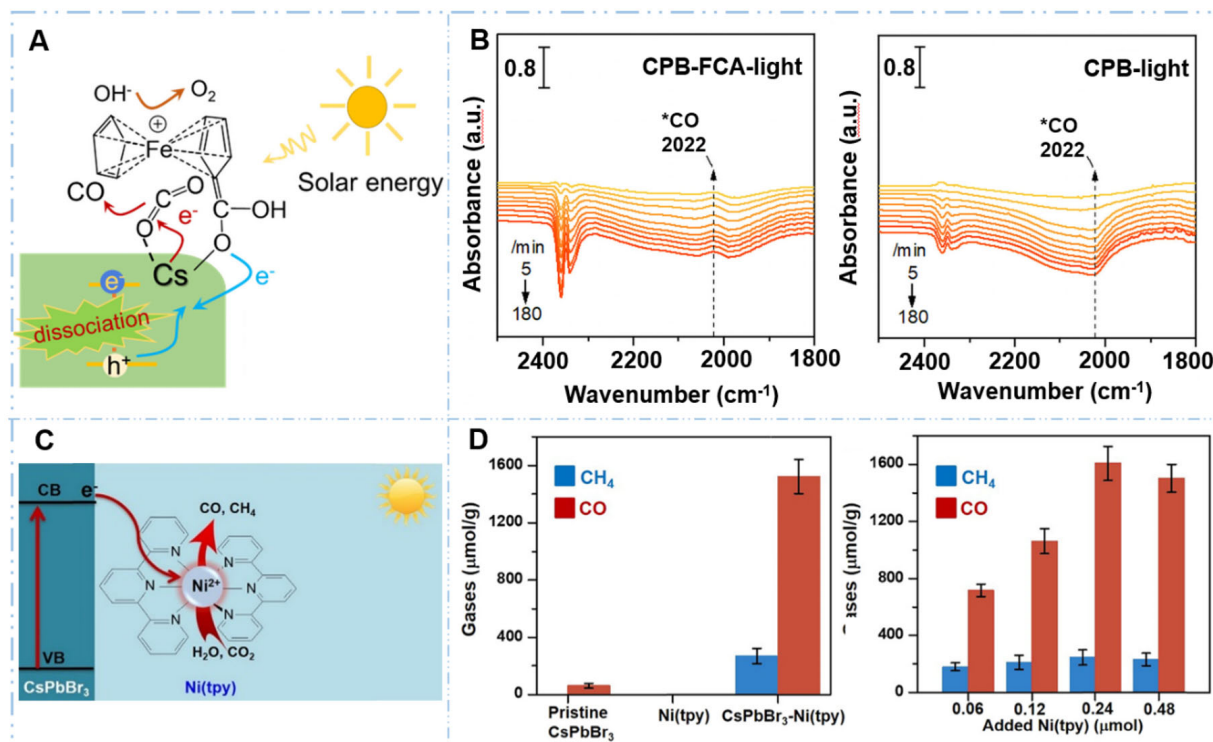


Figure 5. Strategies enhancing surface reaction kinetics in QDs. (A and B) Surface reaction kinetics of CsPbBr₃ QDs were improved through surface ligand modifications of ferrocene carboxylic acid^[82]. Reproduced with permission from ref.^[82]. Copyright 2024, National Academy of Sciences; (C and D) The surface reaction kinetics of CsPbBr₃ QDs were improved through loading Ni(tpy) molecular catalyst as cocatalyst^[83]. Reproduced with permission from ref.^[83]. Copyright 2020, American Chemical Society.

Surface modification focuses on optimizing the intrinsic active sites of QDs through chemical engineering, while cocatalyst loading aims to introduce external active centers with distinct catalytic functionalities. These cocatalysts, typically metals^[85], metal oxides or molecular complexes^[83], provide additional reaction sites and can spatially separate oxidation and reduction processes, thereby enabling tandem catalytic pathways. For example, Yu *et al.* decorated CsPbBr₃ perovskite QDs with dispersed Ru NPs (~1.5 nm) as cocatalysts, which served as active centers for CO₂ reduction and significantly enhanced CO production to 28.12 μmol·g⁻¹·h⁻¹ under simulated visible-light irradiation^[85]. This activity is approximately fourfold and 1.6-fold higher than that of CsPbBr₃ QDs and Ru NPs, respectively. The Ru NPs provided highly active sites with superior CO₂ adsorption capacity (-1.516 eV) and dramatically lowered the activation energy barrier for forming the rate-limiting *COOH intermediate from 1.23 to 0.68 eV, thereby accelerating the surface catalytic kinetics as evidenced by DFT calculations and *in situ* Fourier transform infrared (FTIR) spectroscopy, validating the mechanism by which the metal cocatalyst optimizes the CO₂ reduction pathway. Also, Chen *et al.*^[83] immobilized cationic Ni(terpyridine) metal complexes onto CsPbBr₃ perovskite QDs through electrostatic interactions with surface PF₆⁻ anions, creating spatially separated catalytic centers for CO₂ reduction [Figure 5C]. The metal complex cocatalysts provided dedicated active sites with optimized coordination environments for multi-electron CO₂ conversion, achieving 100% selectivity toward CO and CH₄ production while completely suppressing the competing hydrogen evolution reaction (HER, Figure 5D). In conclusion, strategies to enhance surface reactions, whether through intrinsic surface modification with conjugated or ionic ligands, or the extrinsic loading of cocatalysts, all converge on a common goal of optimizing the binding energies of key intermediates and reducing the kinetic barriers for the complex multi-step process of CO₂ reduction.

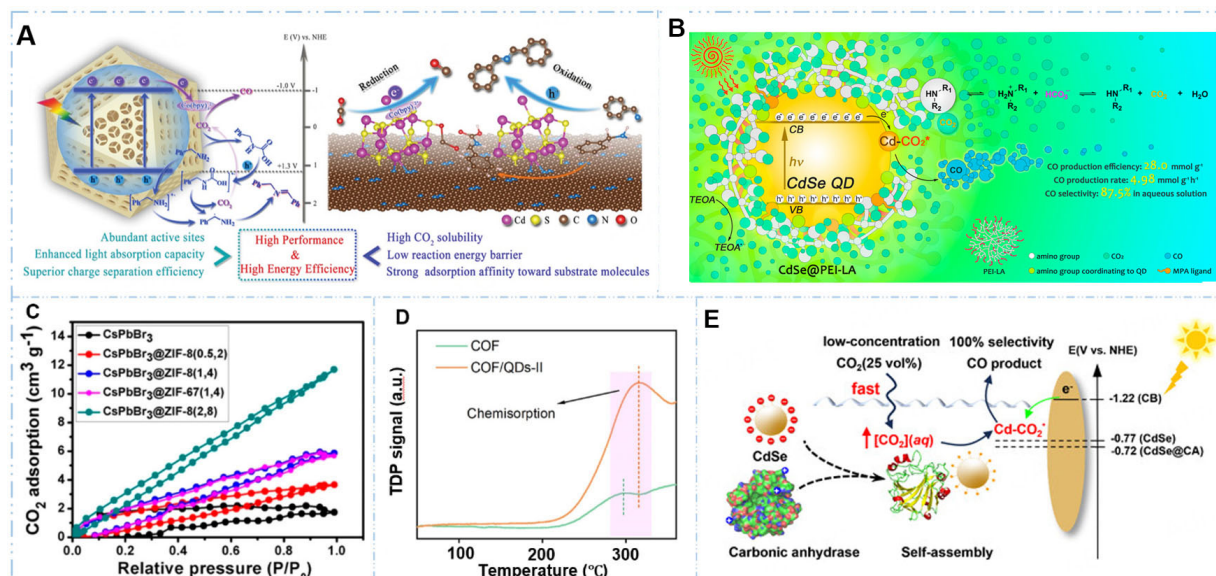


Figure 6. Strategies to integrate CO₂ capture with utilization (CCU). (A) Integration of QDs with porous carbon-based materials^[87]. Reproduced with permission from ref.^[87]. Copyright 2021, John Wiley and Sons; (B) Integration of QDs with amine-based polymers^[88]. Reproduced with permission from ref.^[88]. Copyright 2022, American Chemical Society; (C) Integration of QDs with MOFs^[89]. Reproduced with permission from ref.^[89]. Copyright 2018, American Chemical Society; (D) Integration of QDs with COFs^[95]. Reproduced with permission from ref.^[95]. Copyright 2024, American Chemical Society; (E) Integration of QDs with carbonic anhydrase enzyme^[86]. Reproduced with permission from ref.^[86]. Copyright 2025, John Wiley and Sons.

Capture and conversion of CO₂ molecules

Although strategic optimizations of photon absorption, charge separation, and surface reactions have substantially improved the performance of photocatalytic CO₂ reduction in laboratory settings, its translation to real-world scenarios is hampered by a critical issue: the substrate concentration problem^[86]. Most laboratory studies employ pure CO₂ or saturated CO₂ streams to maximize conversion rates, yet real-world CO₂ sources, whether atmospheric air at 420 ppm or industrial flue gas at 4%-15%, present severely diluted, multicomponent streams. At these low concentrations, mass transfer limitations, unfavorable thermodynamics, and competitive adsorption (especially from H₂O) severely reduce photocatalytic efficiency. This situation has spurred the development of integrated carbon CCU systems. These systems aim to synergistically combine selective CO₂ capture with photocatalytic conversion in tandem configurations, enabling these processes to work synergistically rather than sequentially. To facilitate CO₂ concentration and adsorption, researchers are incorporating QDs with various high-affinity capture materials, such as porous carbon-based materials^[87], amine-based materials^[88], MOFs^[89-92], COFs^[93-96], enzymes^[86], and others^[97], to create hybrid architectures that enhance overall CCU efficiency.

Porous carbons combine high surface area, tunable pore structure, strong and selective CO₂ adsorption, facile regeneration, and excellent stability, establishing them as versatile and cost-effective platforms for carbon capture technologies. Wang *et al.*^[87] synthesized CdS QDs supported on 3D ordered macroporous N-doped carbon (3DOM CdS QD/NC) through an *in situ* transformation strategy [Figure 6A]. Under visible light irradiation, the resulting photocatalyst achieved an exceptional CO production rate of 5,210 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ using benzylamine oxidation as the coupled oxidation reaction and maintained 34% activity (1,780 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$) even under a diluted CO₂ atmosphere (10% CO₂ in N₂). The 3DOM structure addresses the carbon capture challenge through multiple mechanisms confirmed by experimental and computational methods: Brunner-Emmet-Teller (BET) measurements revealed high surface area (144.4 m²·g⁻¹) for CO₂ adsorption, *in situ* DRIFTS spectroscopy demonstrated enhanced formation and stabilization of the critical *COOH intermediate on the carbon-supported CdS surface, and DFT calculations quantified a significant reduction in CO₂ activation energy barrier from 0.94 eV (pristine CdS) to 0.67 eV (CdSQD/NC) through

strong S-O covalent bonding, collectively enabling the porous carbon framework to serve dual functions of concentrating dilute CO₂ near photocatalytic active sites and lowering kinetic barriers for conversion.

Amine-functionalized porous polymers, ranging from linear polyethylenimine to porous organic frameworks with primary, secondary, or tertiary amine functionalities, enable integrated CCU platforms by selectively capturing CO₂ from dilute gas mixtures through strong amine-CO₂ interactions while simultaneously serving as solid supports for QDs, thereby creating bifunctional materials that concentrate and convert CO₂ within a single architecture. Wu *et al.*^[88] encapsulate CdSe QDs in an amphiphilic polymer (polyethylenimine-lauric acid (PEI-LA)) through electrostatic interactions and surface coordination to form CdSe@PEI-LA assemblies [Figure 6B]. The resulting system achieved a CO production efficiency of 28.0 mmol·g⁻¹ with 87.5% selectivity under visible light irradiation, representing 57-fold and 1.5-fold enhancements, respectively, compared to pristine CdSe QDs. The PEI-LA polymer addresses CO₂ capture through multiple mechanisms as evidenced by CO₂ solubility measurements showing 66.7% increased CO₂ dissolution in water at optimized PEI-LA concentration and FTIR spectroscopy confirming reversible chemisorption through carbamate formation between amino groups and CO₂.

In CCU systems, MOFs function as both CO₂ adsorbents and support matrices for QDs, where post-synthetic modification or *in situ* synthesis strategies incorporate QDs into MOF pores or surfaces to create bifunctional materials that capture dilute CO₂ from ambient or industrial sources, concentrate it within the porous network near photocatalytic QD sites, and enable photocatalytic conversion under mild conditions. Kong *et al.*^[89] synthesized core@shell nanocomposites by *in situ* coating zeolitic imidazolate framework (ZIF-8 or ZIF-67) shells onto CsPbBr₃ perovskite QDs through direct growth. The as-synthesized photocatalysts achieved electron consumption rates of 15.5 and 29.6 μmol·g⁻¹·h⁻¹ for CsPbBr₃@ZIF-8 and CsPbBr₃@ZIF-67, respectively, representing 1.39-fold and 2.66-fold improvements over pristine CsPbBr₃. The ZIF shells provide enhanced CO₂ absorption capacity through the microporous framework structure to create high local concentrations near photocatalytic sites in integrated CCU systems with capacity reaching 5.93 cm³·g⁻¹, which was a 3.68-fold increase compared to QDs alone [Figure 6C]. In addition, Ding *et al.* synthesized a bifunctional composite by *in situ* embedding lead-free double perovskite Cs₂AgBiBr₆ QDs into C₄₈H₂₄Ce₆O₃₂ (Ce-UiO-66-H) MOF through solvothermal growth^[91]. The optimized 20% Cs₂AgBiBr₆ QDs loading on the Ce-UiO-66-H (20CABB/UiO-66) composite achieved a CO production rate of 309.01 μmol·g⁻¹·h⁻¹ under simulated solar light irradiation using a 300 W Xe lamp, with a CO₂ conversion efficiency of 19.41%, representing 2.1-fold and 2.7-fold improvements over pristine Cs₂AgBiBr₆ and Ce-UiO-66-H, respectively. The enhanced performance stems from porous crystalline frameworks can optimize CO₂ capture capacity (58.8 cm³·g⁻¹) through defect-engineered high surface area (620.2 m²·g⁻¹), compared to 483.4 m²·g⁻¹ for pristine MOF, providing concentrated CO₂ molecules near photocatalytic sites for efficient conversion. Subsequently, the same research group^[92] synthesized a novel bifunctional composite by *in situ* growing Cs₃Bi₂Br₉ QDs on Bi-MOF nanosheets. The optimized 3 wt% Cs₃Bi₂Br₉ QDs loading on Bi-MOF (3CBB/Bi-MOF) composite achieved a CO production rate of 572.24 μmol·g⁻¹·h⁻¹ under the irradiation of a 300 W Xe lamp, which was over 2-fold higher than the physical mixture, with over 98% CO selectivity. The 3CBB/Bi-MOF composite provides CO₂ adsorption sites with binding energy of -0.208 eV calculated by DFT, compared to -0.114 eV for Cs₃Bi₂Br₉, demonstrating that the MOF component concentrates CO₂ molecules near photocatalytic QD sites. It is noteworthy that in this Bi-MOF structure, QDs grow *in situ* on the surface of the Bi-MOF nanosheets and share Bi atoms with the framework. This atomic sharing not only improves the dispersion of QDs on the nanosheets but also increases the number of reactive active sites for CO₂ molecule adsorption. Furthermore, the shared atomic configuration helps reduce Coulombic electrostatic repulsion, thereby accelerating the separation of photogenerated electrons and holes and lowering the activation energy for charge carrier migration during photocatalysis.

While MOFs provide effective platforms for integrating CO₂ capture and photocatalytic conversion with QDs, the emerging class of COFs offers an alternative strategy featuring metal-free, fully covalent architectures with tunable porosity and nitrogen-rich functional groups that can enhance CO₂ chemisorption. For instance, He *et al.*^[95] synthesized Triphenylamine (TPA)-COF/CsPbBr₃ QD hybrid materials by electrostatic self-assembly. The optimized COF/QDs-II composite achieved CO and CH₄ production rates of 41.2 and 13.7 μmol·g⁻¹, respectively, over 8 h under a 300 W Xe arc lamp without any cocatalyst or scavenger, representing substantial improvements over bare COF and QDs. The reasons could be attributed to the enhanced CO₂ chemisorption of COF/QDs, as evidence by desorption peaks shifting to higher temperatures compared to pristine COF [Figure 6D], indicating stronger CO₂-catalyst interactions, and DFT calculations quantified that QD surfaces provide more negative adsorption energies (-0.41 eV) than COF (-0.16 to -0.19 eV), demonstrating that anchoring QDs onto COF augments CO₂ activation capability at catalytic sites. Cheng *et al.*^[96] designed a 5 nm porous COF cage to serve as a nanoreactor for the *in situ* growth of QDs, thereby preventing their aggregation. Transmission electron microscope (TEM) images revealed that the synthesized ZnSe QDs were exclusively sized between 3 and 5 nm, confirming successful spatial confinement. This COF framework thus creates a tailored microenvironment that concentrates reactants and guides interfacial charge transfer along an S-scheme gradient. As a result, the COF/ZnSe heterostructure achieves a CO generation rate of 128.3 μmol·g⁻¹·h⁻¹, while synchronously delivering 95.1% conversion of 1-phenylethanol to 1-phenylethanone under the irradiation of a 300 W Xe lamp with an Air Mass (AM) 1.5G filter.

Natural photosynthesis utilizes light and atmospheric CO₂ to synthesize carbohydrates for sustaining life on Earth^[98]. During the dark reaction, various enzymes^[99,100] were involved in the process to concentrate CO₂ for subsequent reactions. Carbonic anhydrase (CA), as one of the most active enzymes, could catalyze the quick interconversion between aqueous form CO₂ and HCO₃⁻ ($k = 10^6$ s⁻¹), thus facilitating CO₂ concentration process^[101-103]. For example, our research group^[86] designed and synthesized a self-assembled biohybrid system consisting of CdSe QDs with CA. At 100% CO₂ concentration, this system achieved a CO₂ conversion rate of 47.3 μmol·g⁻¹·h⁻¹, which was 3.5-fold higher than the bare CdSe QDs. Even under simulated flue gas conditions (15% CO₂), the CdSe@CA system still maintained a CO₂ conversion rate of 8.2 μmol·g⁻¹·h⁻¹ [Figure 6E]. This effectiveness is attributed to CA's ability to increase CO₂ solubility in water, allowing for the rapid accumulation of CO₂ in its aqueous form, which serves as the reaction substrate. In conclusion, these diverse CCU integration efforts, spanning from porous carbon to MOFs, COFs and enzymes as platforms for QDs anchoring, collectively represent ongoing efforts to overcome the substrate concentration barrier and advance photocatalytic CO₂ reduction from controlled laboratory settings toward practical application scenarios.

CONCLUSION AND OUTLOOK

In conclusion, QDs have emerged as powerful photocatalysts for CO₂ reduction, with significant progress achieved through systematic engineering. Key advancements include the expansion of light-harvesting capabilities via doping, size/composition control, and plasmonic enhancement; the suppression of charge recombination through sophisticated heterostructures (Type-II, Z-scheme, S-scheme); and the optimization of surface reactions using tailored ligands and cocatalysts to improve selectivity and kinetics. A critical recent realization is that high performance under pure CO₂ conditions does not translate to real-world applications, where dilute sources such as air (~420 ppm) or flue gas (4%-15%) impose severe mass-transfer limitations. This has spurred the development of integrated CCU systems, where QDs are combined with adsorbents such as MOFs, COFs, or enzymes to concurrently concentrate and convert CO₂, bridging a vital gap between laboratory research and practical deployment.

Despite this promising trajectory, several formidable challenges must be addressed to realize the commercial viability of QD-based photocatalytic CO₂ reduction:

(1) **Low quantum efficiency and economic viability:** Solar-to-fuel conversion efficiencies typically remain below <1%, far from the ~10% threshold for economic competitiveness. Breakthroughs are needed to mitigate thermalization losses, enhance infrared photon utilization, improve charge separation, and lower the high overpotentials of multi-electron reactions.

(2) **Competition from hydrogen evolution:** The HER is a major selectivity challenge due to its overlapping potential with CO₂ reduction. The goal is to realize a universal efficiency of ≥90% for CO₂ reduction products. Suppressing HER requires precise engineering of surface sites, the local pH environment, and CO₂ concentration at the catalyst interface.

(3) **Limited product value:** Current systems predominantly yield low-value two-electron products, CO and HCOOH, rather than more commercially valuable multi-electron products such as CH₄, CH₃OH, or C²⁺ hydrocarbons. Steering selectivity toward more valuable multi-carbon products (e.g., CH₄, CH₃OH, C²⁺) necessitates overcoming significant kinetic barriers for C-C coupling and deep reduction through precise control of proton-coupled electron transfer and intermediate stabilization.

(4) **Oxidation half-reaction limitations:** Coupled with the CO₂ reduction reaction, the oxidation half-reaction, typically water oxidation to O₂ or sacrificial agent decomposition, suffers from sluggish kinetics due to the four-electron/four-proton transfer process or results in wasting photogenerated holes and generating undesirable byproducts. Consequently, identifying alternative oxidation reactions that can utilize these holes to produce value-added chemicals, such as selective organic oxidations (benzyl alcohol to benzaldehyde) or biomass upgrading reactions, has emerged as a critical research priority for developing economically viable and sustainable photocatalytic CO₂ conversion systems.

(5) **Challenges in carbon capture integration:** While bifunctional materials combining CO₂ adsorption and photocatalytic conversion show promise in laboratory demonstrations, significant challenges remain in integrating these processes at scale, including regeneration energy requirements for adsorbents, heat management during exothermic adsorption, and maintaining photocatalytic activity in the presence of impurities from real flue gas streams. Beyond the technical hurdles, a critical gap exists in realistic energy balance assessment. Current research predominantly reports photocatalytic conversion efficiencies under isolated conditions, failing to account for the substantial energy overhead of complete adsorption-conversion-regeneration cycles, including cooling for enhanced CO₂ capture, illumination for conversion, and thermal regeneration. Future work must prioritize calculating net energy ratios (NER) - the energy content of produced fuels divided by total cycle energy input - with comprehensive techno-economic analyses that account for carbon abatement costs alongside product value.

The development of dynamic systems that can cycle between capture and conversion modes without performance degradation, while operating under realistic temperature and pressure conditions, represents a major engineering hurdle for practical CCU deployment. Particularly given the insufficient attention to long-term cyclic stability under realistic operating conditions, most studies examine < 10 idealized cycles, while practical deployment requires stable operation over thousands of cycles with multiple degradation pathways including thermal stress from temperature cycling, chemical poisoning from real flue gas contaminants (SO_x, NO_x, particulates), and photochemical degradation from prolonged UV exposure. Future research must adopt standardized testing protocols that better reflect industrial conditions, including extended cycling with realistic cycle times, real flue gas compositions rather than pure CO₂, and continuous

monitoring of both capture capacity and photocatalytic activity throughout operation.

(1) Environmental and toxicity concerns: Many high-performance QDs (e.g., CdSe, CsPbBr₃) contain toxic heavy metals. The development of environmentally benign, high-efficiency alternatives, such as heavy metal-free perovskites (e.g., Cs₃Bi₂Br₉) and organic semiconductors, represents a critical direction for sustainable photocatalytic technologies, though these alternatives often suffer from reduced charge mobility and photostability compared to their counterparts. The development of non-toxic QDs (free of Cd, Pb, *etc.*) must meet two key criteria: compliance with the U.S. Environmental Protection Agency Toxicity Characteristic Leaching Procedure (EPA TCLP) standard for leaching toxicity, and a benchmarked AQE reaching > 70% of that achieved by heavy-metal-based control samples.

(2) Long-term stability: Operational instability due to moisture, active site poisoning, ion migration pathways, surface reconstruction, photodegradation products photocorrosion and ion migration, particularly in perovskite QDs, remains a critical barrier. Achieving thousands of hours of stable operation requires advanced encapsulation and passivation strategies that do not compromise catalytic activity or charge transfer.

Despite these multifaceted challenges, QDs-based photocatalytic CO₂ reduction, particularly when integrated with carbon capture technologies, represents a highly promising pathway for sustainable carbon management. Overcoming these hurdles through interdisciplinary collaboration will be essential to transform innovative laboratory demonstrations into scalable, economically viable technologies capable of mitigating global climate change.

DECLARATIONS

Authors' contributions

Wrote the first version of the manuscript: Wu, P.; Liu, Y.; Guo, Z.

Contributed to the revision of the manuscript: Wu, P.; Liu, Y.; Yang, J.; Hong, J.; Song, N.; He, J.; Guo, Z.; Liang, M.

Availability of data and materials

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Conflicts of interest

All authors declared that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

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