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# *An Overview of Perovskite Quantum Dots for Carbon Dioxide Photoreduction*

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***Abstract.*** The rising level of atmospheric $CO_2$ necessitates more efficient artificial photosynthesis methods. Perovskite quantum dots (PQDs) are promising photocatalysts because their bandgaps are easily tunable, and they feature high light absorption and efficient charge carrier mobility. This review surveys recent progress in PQD-based $CO_2$ photoreduction, covering synthesis methods, characterization techniques, and thermodynamic requirements. Among synthesis methods, the hot-injection technique is widely used as the benchmark for high-quality PQDs due to its excellent size control, whereas the ligand-assisted reprecipitation (LARP) method offers a simpler and more scalable alternative at room temperature. Characterization approaches—XRD, TEM, and XPS—are discussed for structural analysis, along with in situ FTIR for detecting surface ligands and reaction intermediates. Thermodynamic feasibility is evaluated by comparing the conduction band position of PQDs with the redox potentials of $CO_2$ reduction. Furthermore, we discuss key challenges, including moisture degradation, fast charge recombination, and Pb toxicity. Finally, future directions such as machine learning-assisted design, operando studies, and heterostructure engineering are outlined.

***Keywords:*** Perovskite quantum dots, Photocatalytic $CO_2$ reduction, Thermodynamics, Characterization

## 1. Introduction

The global energy crisis and rising atmospheric $CO_2$ concentration are two of the most pressing challenges today. $CO_2$ emissions from fossil fuel combustion have accelerated over recent decades：growth rates rose from 1.1% per year in the 1990s to over 3% per year in the early 2000s [1]. The residential sector alone accounts for about 27% of global energy consumption and 17% of $CO_2$ emissions [2]. If left unchecked, these trends will continue to drive global warming and climate change [3].

Converting $CO_2$ into value-added fuels using solar energy is a promising route to address both environmental and energy issues. Catalytic valorization of exhaust carbon has attracted considerable attention, as it can produce CO, $CH_4$, and other chemicals under mild conditions [4]. Photocatalytic $CO_2$ reduction is particularly attractive because it uses inexhaustible solar energy.

Since the pioneering work in the 1970s, various semiconductors such as $TiO_2$, CdS, and g-$C_3N_4$ have been explored for photocatalytic $CO_2$ reduction [4]. However， many of these materials are

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limited by wide bandgaps, fast charge recombination, or poor product selectivity.

Halide perovskite quantum dots (PQDs) have recently emerged as promising photocatalysts，combining tunable bandgaps, high light absorption coefficients, long carrier diffusion lengths, and high photoluminescence quantum yields. These properties make PQDs attractive for $CO_2$ photoreduction, although their stability and charge recombination remain challenges, and this review systematically summarizes the synthesis, characterization, and thermodynamics of PQDs using a literature review method, aiming to provide theoretical guidance for the rational design of highly efficient PQD-based photocatalysts.

## 2. Synthesis methods

### 2.1. Hot-injection method

#### 2.1.1. Procedure and workflow

The hot-injection method was introduced by Murray et al. in 1993. Precursors are injected rapidly into a hot coordinating solvent, which separates nucleation and growth [5]. This creates a burst of supersaturation and a brief nucleation event, followed by controlled growth (LaMer model ) [6]. For CsPbX3, cesium oleate is made by reacting $Cs_2CO_3$ with oleic acid (OA) in 1-octadecene (ODE), while $PbX_2$ is dissolved in ODE with OA and oleylamine [7, 8]. The cesium oleate solution is then injected at 140–200 °C. Nucleation is immediate,indicating $CsPbX_3$ has formed [7, 9]. After seconds to minutes, the mixture is cooled in an ice-water bath, then purified and redispersed in nonpolar solvents [8, 9].

#### 2.1.2. Effects of temperature and growth parameters

Temperature controls both nucleation density and growth rate. In $CsPbBr_3$, raising it from 100 to 180 °C enlarged average diameters from 9.9 to 12.5 nm, red-shifted the PL peak from 2.469 to 2.391 eV, and narrowed the FWHM from 150 to 90 meV [8]. Mechanistically, a higher temperature accelerates both the nucleation and growth rates, leading to a larger final QD size. This size increase weakens the quantum confinement effect, which directly causes the red-shift in the PL peak and the narrowing of the FWHM due to improved size uniformity. The optical bandgap decreased from 2.462 to 2.383 eV, and the Stokes shift decreased from 101 to 38 meV, indicating improved size uniformity and surface passivation [8]. Ligand ratios, precursor molar ratios, and halide compositions further tune size, stability, and emission across the entire visible spectrum from 410 to 700 nm [7].

Table 1. Properties of $CsPbBr_3$ PQDs made by hot injection at different temperatures [8]

| Property | 100 °C | 180 °C |
|---|---|---|
| Average diameter (nm) | 9.9 | 12.5 |
| PL peak energy (eV) | 2.469 | 2.391 |
| Optical bandgap (eV) | 2.462 | 2.383 |
| PL FWHM (meV) | 150 | 90 |
| Stokes shift (meV) | 101 | 38 |

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## 2.2. Brief overview of other methodss

### 2.2.1. Ligand-assisted reprecipitation(LARP)

Ligand-assisted reprecipitation (LARP) relies on the solubility difference of precursors between a good solvent (e.g., DMF) and a poor solvent (e.g., toluene). Principle and process: A precursor solution is injected into a vigorously stirred poor solvent containing capping ligands at room temperature, triggering rapid supersaturation and crystallization. Pros and cons: The advantages include simple operation, ambient conditions, and short reaction time, making it highly suitable for mass production. However, the rapid crystallization process often leads to lower crystallinity and poorer stability compared to the high-temperature hot-injection method [10]. It reaches PLQY up to 70% with a narrow FWHM [10].

### 2.2.2. Solvothermal method and other methods

Solvothermal methods provide good crystallinity but require high pressure and long reaction times. Other emerging methods include ultrasonication and microwave-assisted synthesis.

### 2.2.3. Summary comparison

Table 2 compares the two methods. Hot-injection offers high crystallinity and excellent size control (PLQY > 90%) [7, 8], but requires harsh conditions (high temperature, inert atmosphere) and is difficult to scale up [11]. LARP is simple, operates at room temperature, and scales easily, but provides lower stability. Consequently, hot-injection is preferred for high-performance research, while LARP is more suitable for cost-effective industrial production.

Table 2. Comparison between the hot-injection method and LARP [7, 8, 10]

| Parameter | Hot-injection | LARP |
|---|---|---|
| Reaction temperature | 140-200 °C | Room temperature |
| Atmosphere | Inert ($N_2$/Ar) | Ambient air |
| Crystallinity | High | Lower |
| Size distribution | Narrow | Broader |
| PLQY | Up to ~90% | Up to ~70% |
| Stability | High | Lower |
| Operation & scale-up | Batch, hard to scale | Simple, easier to scale |

*Note: Values for the LARP column (including the ~70% PLQY) refer to the $CH_3NH_3PbX_3$ system reported by Zhang et al. [10], the hot-injection values refer to $CsPbX_3$ [7, 8].*

## 3. Characterization methods

### 3.1. XRD: phase identification and quantitative analysis

X-ray diffraction (XRD) identifies the crystal phase of PQDs. For $CsPbBr_3$ QDs, the diffraction peaks at 14.9°, 21.1°, 26.3°, 30.4°, 37.4°, and 43.4° correspond to the (100), (110), (111), (200), (211), and (202) planes of the monoclinic perovskite structure [12]. Peak shifts indicate lattice

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contraction or halide substitution. Peak broadening estimates crystallite size [13]. The significance of XRD lies in tracking structural changes during catalytic reactions (e.g., lattice contraction). However, it only provides bulk average information and lacks surface sensitivity, requiring complementary techniques.

### 3.2. TEM-XPS: elemental valence and interfacial electron transfer analysis

Transmission electron microscopy (TEM) gives particle size and morphology. $CsPbBr_3$ QDs are cubic, about 10 nm on average, with a lattice spacing of 0.41 nm assigned to the (110) plane [12] . X-ray photoelectron spectroscopy (XPS) gives elemental valence states. The peaks at 738.6 and 724.8 eV correspond to Cs $3d_{3/2}$ and $3d_{5/2}$, and the peaks at 143.8 and 138.8 eV correspond to Pb $4f_{5/2}$ and $4f_{7/2}$ [12]. Binding energy shifts indicate electron transfer between QDs and surface species [14]. These techniques are significant because understanding the morphology and interfacial charge transfer is critical for evaluating catalytic performance. The limitation is that TEM only provides localized morphological information, while XPS requires an ultra-high vacuum environment, which may not fully reflect the real reaction conditions.

### 3.3. FTIR: ligand identification, coordination bond confirmation, and $CO_2$ adsorption intermediate detection

#### 3.3.1. Ligand identification and surface coordination

Fourier transform infrared spectroscopy (FTIR) is particularly powerful for identifying surface ligands on PQDs. Carboxylate coordination to surface metal ions is a common binding motif on nanocrystal surfaces, which is crucial for colloidal stability and surface passivation [15].

#### 3.3.2. Detection of $CO_2$ adsorption intermediates

In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) allows real-time detection of reaction intermediates. On Fe-modified $CsPbBr_3$ QDs, key intermediates such as COOH* and *CO are observed, with $CO_2$ preferentially binding at Cs sites [14]. These bands trace the stepwise conversion of $CO_2$ to CO and clarify how surface sites participate in photocatalysis [14].

### 3.4. PL: charge carrier dynamics

Photoluminescence (PL) spectroscopy reports radiative recombination and charge carrier dynamics. As-synthesized $CsPbBr_3$ QDs show a PL quantum yield of 79 ± 4% at 400 nm, with about 94% of the lowest excitonic states decaying single-exponentially (4.5 ± 0.2 ns) [16]. Steady-state PL reflects radiative recombination behavior and PL quantum yield. In contrast, time-resolved PL provides exciton lifetime, and transient absorption (TA) spectroscopy probes ultrafast exciton dissociation and charge transfer dynamics. These techniques are significant as they directly correlate photophysical properties with catalytic activity, though optical spectroscopy alone cannot distinguish surface from bulk recombination pathways.

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## 4. Thermodynamic fundamentals of $CO_2$ photocatalytic reduction

### 4.1. Multi-electron reaction pathways and reduction potentials of products

$CO_2$ is thermodynamically stable and chemically inert. Its photoreduction is an uphill process that requires substantial energy input. The single-electron reduction pathway is thermodynamically highly challenging because the formation of the $CO_2^{\bullet-}$ radical anion requires an extremely negative potential, requiring a large driving force that most unassisted photocatalysts struggle to provide. Proton-coupled multi-electron pathways are therefore favored.

At pH 0, the key reduction half-reactions and their standard potentials vs. NHE are:

$$CO_2 + 2H^+ + 2e^- \rightarrow CO + H_2O \quad E^\circ = -0.52\ \text{V}\ [17]$$

$$CO_2 + 8H^+ + 8e^- \rightarrow CH_4 + 2H_2O \quad E^\circ = -0.24\ \text{V}\ [17]$$

The water oxidation half-reaction, which supplies protons and electrons for $CO_2$ reduction, requires a valence band maximum more positive than +0.82 V vs. NHE [17]. The competing hydrogen evolution reaction (HER) must be suppressed to achieve high $CO_2$ reduction selectivity. In nonaqueous media such as ethyl acetate, the HER is efficiently inhibited, and selectivity over 99% for $CO_2$ reduction has been reported for $CsPbBr_3$ QDs [17, 18] .

### 4.2. Band-edge matching between perovskite QDs and reaction energy levels

$CO_2$ reduction requires a CBM more negative than the target potential and a VBM more positive than water oxidation. For $CsPbBr_3$ QDs, ultraviolet photoelectron spectroscopy gives a VBM of −5.5 eV vs. vacuum, and the optical bandgap is 2.43 eV [17]. The corresponding CBM is −3.1 eV vs. vacuum, or −1.03 V vs. NHE at pH 0, while the VBM is +1.4 V vs. NHE [17]. Both reductions are thermodynamically accessible: the CBM lies negative of the $CO_2$/CO and $CO_2$/$CH_4$ potentials. Water oxidation is also feasible, since the VBM sits positive of +0.82 V.

In CPB-PCN composites, the CBM of PCN is −0.60 V vs. NHE, which is thermodynamically sufficient for $CO_2$-to-CO (−0.52 V) but not for $CO_2$-to-$CH_4$ (−0.24 V) [19]. Ou et al linked this band alignment to selective CO production, reporting 148.9 μmol $g^{-1}$ $h^{-1}$—about 15 times the rate of pristine $CsPbBr_3$ QDs [19].

### 4.3. Value of bandgap tunability

Particle size determines the bandgap and band-edge positions of CsPbBr3 QDs. The average size can be adjusted from 3.8 to 11.6 nm by changing the reaction temperature. The PL lifetime varies with size: 6.6 ns for 3.8 nm, 7.8 ns for 6.1 nm, 9.7 ns for 8.5 nm, and 8.9 ns for 11.6 nm [17]. The 8.5 nm QDs exhibit the longest PL lifetime and the highest $CO_2$ reduction activity, with CO and $CH_4$ yields of 34.1 and 12.2 μmol $g^{-1}$ after 8 h, corresponding to an electron consumption rate of 20.9 μmol $g^{-1}$ $h^{-1}$ and a selectivity over 99% [17]. This is because a longer PL lifetime implies a lower non-radiative recombination rate, allowing more photogenerated electrons to participate in the surface reaction.

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### 4.4. More negative conduction band and higher electron energy

Quantum confinement in $CsPbBr_3$ QDs pushes the CBM to more negative potentials, increasing the driving force for electron transfer to $CO_2$ [17]. In $CsPbBr_3$ QD/GO composites, the Fermi level of GO is more positive than the conduction band edge of $CsPbBr_3$, making electron transfer from QDs to GO thermodynamically favorable [18]. Charge separation is therefore enhanced, and the electron consumption rate rises by 25.5% compared with pristine $CsPbBr_3$ QDs (29.8 vs. 23.7 μmol $g^{-1}$ $h^{-1}$) [18]. The PL lifetime decreases from 38.3 ns to 11.3 ns after GO introduction, confirming faster charge transfer [18].

## 5. Challenges and future research directions

### 5.1. Challenges

#### 5.1.1. Stability issues and charge recombination

PQDs are ionic and sensitive to moisture, oxygen, light, and heat. Under continuous light, CsPbBr3 QDs degrade through ligand desorption, surface trap formation, and aggregation [13]. In photocatalytic $CO_2$ reduction, water and light are both present, so long-term stability remains a major obstacle [17] . Fast charge recombination is another bottleneck. Surface defect states promote non-radiative recombination [13]. A drop in PL lifetime in QD/GO composites shows charge transfer competing with recombination [18]. In CPB-PCN composites, N–Br bonding promotes charge separation and extends the fluorescence lifetime [19] . Optimized ligand density further reduces surface defects and suppresses recombination [20] .

#### 5.1.2. Lead toxicity

Lead in $CsPbX_3$ PQDs raises environmental and health concerns for large-scale production . Lead-free alternatives such as Cu-based perovskites have been explored, but their optoelectronic properties and stability still remain inferior to those of lead-based counterparts [21].

### 5.2. Future directions

#### 5.2.1. Lead-free PQDs and surface engineering

Although still inferior to lead-based PQDs, Cu-based $Cs_2CuCl_4$, $Cs_2CuBr_4$, and $Cs_2CuBr_2Cl_2$ nanostructures reach PLQY up to 38% and retain fluorescence after 45 days in ambient conditions [21]. Surface passivation with organic ligands or inorganic shells can suppress defect states and enhance stability [15] . Ligand density engineering further boosts exciton dissociation and interparticle energy transfer, achieving a 2.26-fold improvement in CO production [20] .

#### 5.2.2. Machine learning and microfluidic synthesis

Machine learning can accelerate the discovery of optimal PQD compositions. Munyebvu et al. developed an autonomous flow platform using Bayesian optimization to simultaneously target QD size, bandgap, and size dispersity [22]. Mechanistically, this AI-guided strategy builds a surrogate model to efficiently navigate a vast parameter space, achieving multi-objective targeting in under 10 hours [22]. This directly addresses the challenges in 5.1 by replacing traditional trial-and-error

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methods, thereby improving batch-to-batch consistency and allowing for the precise design of stable PQDs.

## 6. Conclusion

This review summarized recent progress in perovskite quantum dots (PQDs) for photocatalytic $CO_2$ reduction. Hot injection gives excellent size control and high crystallinity, but it is a batch process and hard to scale up. LARP is simpler and works at room temperature, but the product has lower crystallinity and stability. XRD, TEM, XPS, FTIR, and PL are useful tools. They provide information on crystal phase, morphology, surface chemistry, and charge carrier dynamics.

Thermodynamically, $CsPbBr_3$ QDs are well placed: the conduction band is negative enough for $CO_2$-to-CO and $CO_2$-to-$CH_4$ reduction, and the valence band is positive enough for water oxidation. However, PQDs still face major challenges: they degrade easily under moisture and light, charge recombination is fast, and lead toxicity is also a serious concern. Future work should target lead-free PQDs, surface passivation, heterostructure engineering, and continuous-flow synthesis. Furthermore, as a literature review, this paper primarily focuses on summarizing the fundamental mechanisms and recent theoretical progress. It does not deeply cover other emerging synthesis methods, nor does it provide an in-depth analysis of practical issues like economic cost, industrial scale-up, and environmental impact.

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