

MODULATION OF PHOTOPHYSICAL PROPERTIES FOR CsPbBr₃ QUANTUM DOTS AT ROOM TEMPERATURE USING USING O-XYLYL BISBENZIMIDAZOLIUM SALT

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ABSTRACT

Cesium lead bromide (CsPbBr₃) quantum dots (QDs) are promising candidates for next-generation optoelectronic devices owing to their high luminescence and tunable bandgaps. Conventional synthesis approaches, however, often require high temperatures and inert conditions, limiting scalability. Here, we report a simple room-temperature synthesis of CsPbBr₃ QDs and demonstrate modulation of their photophysical properties through O-xyllyl bisbenzimidazoliium salt surface functionalization. Tauc analysis revealed a direct bandgap of 2.72 eV, confirming strong quantum confinement relative to the bulk. The QDs exhibited bright green emission centered at 515–520 nm with a narrow full width at half maximum, alongside stable emission under varied excitation power. Time-dependent photoluminescence (PL) studies indicated gradual intensity degradation in pristine QDs, whereas O-xyllyl bisbenzimidazoliium salt-functionalized QDs retained higher stability under continuous irradiation. Time-resolved PL analysis showed biexponential decay with average lifetimes of 15–20 ns in pristine samples, extended to ~25 ns after O-xyllyl

bisbenzimidazoilium salt modification, highlighting efficient surface trap passivation. Compared with conventional ligands, O-xylyl bisbenzimidazoilium salt functionality imparted superior photostability, enhanced emission intensity, and prolonged exciton lifetimes. These findings establish O-xylyl bisbenzimidazoilium salt-based passivation as a robust strategy for improving the optical performance and environmental resilience of perovskite quantum dots synthesized under ambient conditions, offering significant potential for scalable optoelectronic applications.

Keywords: CsPbBr₃ QDs, Bandgap, O-xylyl bisbenzimidazoilium salt functionalization, Exciton recombination dynamics, Photoluminescence stability (PL, PLQY), Time-resolved spectroscopy (TRPL), Ambient-condition synthesis, Perovskite-based optoelectronic devices

INTRODUCTION

The concept of artificial atoms—more accurately referred to as quantum dots (QDs)—has emerged from extensive research focused on the dimensional reduction of semiconductors over the past few decades. These semiconductor nanocrystals, typically only a few nanometers in diameter, exhibit quantum confinement effects that markedly influence their optical and electronic behavior. (Cotta, 2020) Quantum dots possess unique and highly tunable photoluminescence (PL) properties, alongside notable features such as high photochemical stability, sharp emission spectra, and structural versatility in forming core-shell configurations. These attributes underpin their rapidly increasing relevance across numerous technological applications. (Kubendhiran et al., 2019a; Zakaria et al., 2025) QDs have become essential components in a diverse array of modern devices, including widely recognized consumer electronics like QD-enhanced display screens, which have gained commercial popularity in recent years. (Shirasaki et al., 2013) While the technology has advanced significantly across various domains, the synthesis, structural characterization, and exploration of novel applications of quantum dots (QDs) continue to represent dynamic and expanding areas of scientific inquiry. (Kubendhiran et al., 2019b) The term "quantum dot" specifically refers to semiconductor nanocrystals whose dimensions are smaller than or comparable to the excitonic Bohr radius, thereby exhibiting pronounced quantum confinement effects. (Kambhampati, 2021) Due to quantum confinement effects, quantum dots exhibit atom-like behavior characterized by discrete and tunable energy levels. These distinctive features represent a significant advancement in nanoscience and have attracted considerable interest across diverse scientific disciplines. (Deshmukh et al., 2023) Quantum confinement allows for the development of materials with tunable light absorption and emission properties, distinct and intense spectral features, precise control over electronic behavior, and improved chemical reactivity—all primarily driven by their high surface-to-volume ratio. (García De Arquer et al., 2021)

In the field of light-emitting diodes (LEDs), quantum dots (QDs) have been widely utilized due to their highly tunable and precise spectral emission characteristics. (Tongbram et al., 2018) Post-fabrication analysis has also seen notable advancements through the use of innovative techniques like chemically etched nanomembranes in conjunction with scanning tunneling spectroscopy, providing detailed surface and electronic structure information. (Rosa et al., 2019) Meanwhile, colloiddally synthesized InP QDs have emerged as strong candidates for LED and display applications due to their intense and narrow PL emissions.

These properties are further improved through the incorporation of ZnSe/ZnS multishell layers that enhance stability and emission efficiency. (Ramasamy et al., 2017) Additionally, theoretical approaches such as density functional theory (DFT) have been instrumental in elucidating the effects of surface states and passivation strategies, contributing to a deeper understanding of QD optoelectronic behavior. (Cho et al., 2018) Various semiconductor quantum dot (QD) systems have been employed to achieve emission tuning across the visible spectrum. For instance, blue emission has been successfully realized using silicon QDs embedded in siloxane matrices, (Xu et al., 2020) whereas red-light applications (~670 nm) have been enhanced through halide-exchanged perovskite QDs, such as CsPb(Br/I)₃ and CsPbI₃. (Begum et al., 2020) In the green region, dual-emission LEDs have been fabricated by decorating ZnO nanorods on GaN substrates with CsPbBr₃ QDs, (Q. Zhang et al., 2021) and photoluminescence (PL) enhancement in GaN films has been achieved using graphene oxide QDs. (Santiago et al., 2019) White-light applications have benefited from CsPbBr₃ QD-based phosphors. (Xu et al., 2019) while CdSe/CdS QDs on hexagonal boron nitride substrates have demonstrated improved thermal stability. (Zhou et al., 2020) Hybrid monolithic phosphors, consisting of CdSe/CdS/ZnS QDs embedded in SiO₂/Al₂O₃ matrices, provide exceptional operational stability. (Z. Li et al., 2018) Other QD systems under investigation include BSA/ZnS composites (Bhandari et al., 2019) and microwave-synthesized graphene QDs, (W. Li et al., 2018) both showing promise for LED integration. Additionally, low-toxicity materials like Zn₃N₂ colloids offer safer alternatives with size-tunable band gaps ranging from 1.5 to 3.2 eV. (Ahumada-Lazo et al., 2019) In thin-film QD-LEDs, solid-state ligand-exchange methods have been employed to process CsPbX₃ materials. (Suh et al., 2018) CuInS₂/ZnS QDs stabilized by thiol and amine ligands have proven effective in flexible displays. (Choi et al., 2019) Polymer-encapsulated CdSe nanoplatelets and PbS QDs, (Shiman et al., 2019) along with nanocomposite films combined with Au nanorod arrays, offer novel routes for tailoring PL and emission polarization. In photovoltaic applications, QDs have significantly enhanced solar energy conversion efficiency. CdS, CdSe, and CdSe/CdS core-shell QDs have been integrated into solar cells with promising results. (Bederak et al., 2018; Chen et al., 2013; Gudjonsdottir et al., 2019) Efficiency gains have also been observed with PbS QDs via atomic ligand capping (Bederak et al., 2018) and improved surface passivation using multilayer core-shell designs. (Bose et al., 2018) Ligand and solvent engineering in PbS-based films has further refined optoelectronic properties, (Liu et al., 2018) complemented by ZnO-QD composite structures. (Dong et al., 2019) Uniform dispersion of CdS/ZnS QDs into polymer matrices has been achieved using supercritical CO₂ techniques, (Mumin et al., 2018) while DFT-guided modeling has supported the development of CdSe-based solar materials. (Cui et al., 2018) Photodetectors and photoconductors have also advanced through QD integration. PbS QDs produced via two-step ligand exchange or microwave-assisted synthesis have enabled high-performance infrared detection. (Paliwal et al., 2018; Tang et al., 2019) Ag₂Se QDs have shown responsiveness in mid-infrared photodetectors, (Hafiz et al., 2019) and inkjet printing techniques have facilitated the fabrication of broadband PbS-based detector arrays. (Cook et al., 2019; Mahmoud et al., 2019) Ultraviolet and visible-light photodetectors have been developed using WS₂ QD-graphene hybrids (Singh et al., 2019) and MoS₂/CsPbBr₃ heterostructures. (Lin et al., 2019) In biomedical and environmental applications, QDs are employed for their high luminescence, functional

versatility, and biocompatibility. Fibrous phosphorus QDs have been applied for cancer imaging, (Amaral et al., 2020) while $\text{CuInS}_2/\text{ZnS}$ QDs have been used as non-toxic fluorescent probes for cellular imaging. (Mallick et al., 2019)

Upon energy excitation, electrons within the QDs are promoted to higher energy states. As these electrons return to their ground states, photons are emitted with energies corresponding to the gap between the excited and ground energy levels. (J. Zhang et al., 2025) The wavelength—and consequently the color—of the emitted light is determined by the unique composition and structural configuration of each QD. This phenomenon closely resembles atomic emission, wherein elements emit characteristic colors based on their electronic configurations—for instance, sodium produces yellow light and iron appears green when subjected to flame excitation. Fundamentally, different atoms—and by extension, different quantum dots—emit light at distinct wavelengths due to their quantized energy levels. This core property makes QDs highly valuable in applications such as optoelectronics, imaging, and a wide range of photonic technologies. (Deshmukh et al., 2023) Metal halide perovskite (MHP) nanocrystals have emerged as a highly attractive class of semiconducting materials, especially for applications requiring efficient light emission and charge carrier generation. These nanocrystals have exhibited superior performance compared to many traditional semiconductor counterparts. However, the majority of existing studies have focused on MHP systems that display minimal or no quantum confinement effects. Consequently, the distinct optical and electronic behaviors that typically arise under strong quantum confinement remain largely underexplored. This gap is primarily due to challenges in synthesizing MHP nanocrystals with strong confinement, as conventional size-tuning strategies relying on kinetic growth have not been sufficiently effective. (Qiao & Son, 2021) Perovskite quantum dots (PQDs) are typically divided into two main types: all-inorganic and hybrid organic–inorganic structures. Of these, all-inorganic PQDs with the general formula CsPbX_3 ($X = \text{Cl, Br, I}$) exhibit superior structural and environmental stability when compared to their hybrid analogues containing organic cations such as methylammonium (MA) or formamidinium (FA). (Heimbrook et al., 2021; Yu et al., 2025)

Among various synthesis methods, the hot-injection approach is widely regarded for producing monodisperse CsPbBr_3 nanocubes with tunable size and shape. However, its reliance on high temperatures, inert atmospheres, and rapid injection limits scalability and cost-effectiveness. This has led to increasing interest in room-temperature synthesis methods that maintain favorable photophysical properties, including high photoluminescence quantum yield (PL QY), narrow emission, and defect tolerance. Surface ligand engineering significantly affects nanocrystal stability and optical behavior. (Vighnesh et al., 2022) The hot-injection technique was first introduced by Kovalenko et al. in 2015 to produce highly luminescent CsPbX_3 nanocubes ranging from 4 to 15 nm. Since then, significant advancements have been made to improve PL QY, thermal stability, and environmental durability through approaches such as ion doping, ligand passivation, dimensional control, and surface modification. Additionally, efforts are ongoing to replace toxic lead with less hazardous elements, leading to the synthesis of lead-free double perovskites with the formula $\text{A}_2\text{M}^+\text{M}^{3+}\text{X}_6$ (Vighnesh et al., 2022) Among the available techniques, hot injection and ligand-assisted reprecipitation (LARP) are commonly employed for PQD synthesis. To enhance scalability and reproducibility, the LARP method was further refined to integrate with a robotic pipetting platform, enabling

the high-throughput fabrication of binary and ternary CsPbX₃ QD libraries. This was achieved using Opentrons' protocol designer, with synthesis steps precisely managed through a Python-based interface that ensured accurate solution handling and mixing across a 96-well plate format. (Heimbrook et al., 2021) Subsequent studies have shown that the incorporation of stabilizing agents or surfactants during synthesis can greatly improve the quantum yield (QY) of perovskite nanocrystals. Various methods—including surface passivation with salt additives, doping with alternative cations or anions, and post-synthetic ion exchange—have been widely employed to suppress surface defects and reduce trap states. Careful control of these reaction variables is essential for achieving enhanced stability and emission characteristics in the resulting nanocrystals. (Tawil et al., 2022) The catalytic efficiency of quantum dots (QDs) is highly influenced by the design and nature of their surface capping ligands. In the case of lead halide perovskite (LHP) QDs, early formulations commonly employed oleic acid and oleylamine as stabilizing ligands. However, these conventional ligands offered limited structural stability, particularly under reaction conditions relevant to photoredox catalysis. As a result, the QDs often underwent degradation during catalytic processes, leading to reduced turnover rates and restricting their broader applicability in synthetic chemistry. (Amberg et al., 2025)

O-xylyl bisbenzimidazolium salts represent a class of aromatic six-membered heterocycles containing three nitrogen atoms and are among the earliest known families of organic compounds. The 1,3,5-O-xylyl bisbenzimidazolium salt ring is notably π -deficient, rendering it more susceptible to nucleophilic attack than other nitrogen-rich aromatic systems. This electron-deficient nature enhances its reactivity in organic synthesis and broadens its applicability in photonic and electronic materials. O-xylyl bisbenzimidazolium salt-based compounds are known for excellent electron-transport properties due to their strong electron-withdrawing character, thermal robustness, and favorable optoelectronic attributes. Their inherent C₃ symmetry also makes them ideal building blocks in supramolecular chemistry, enabling the construction of star-shaped molecules, porous frameworks, and molecular cages. Additionally, O-xylyl bisbenzimidazolium salt-containing materials have demonstrated remarkable performance as π -acceptor cores in thermally activated delayed fluorescence (TADF) emitters, substantially improving external quantum efficiencies in organic light-emitting diodes (OLEDs), including those designed for red and blue phosphorescent emission. Since the early 2000s, O-xylyl bisbenzimidazolium salt-based compounds have attracted significant attention in the development of organic functional materials, primarily due to their outstanding optoelectronic properties. Notably, their application in photovoltaic technologies has been extensively explored, motivated by the growing global need for low-cost, sustainable, and environmentally benign energy solutions as alternatives to fossil fuels. (Dávila Cerón et al., 2022)

As Conventional hot-injection methods for synthesizing CsPbBr₃ perovskite quantum dots are often energy-intensive and prone to variability. Additionally, achieving precise control over band gap tuning, particle size, and uniformity remains challenging, underscoring the need for a more cost-effective and scalable synthesis strategy for perovskites. In light of these findings, the current research focuses on the room-temperature synthesis of CsPbBr₃ quantum dots, moving away from high-temperature protocols while still targeting high photoluminescence yield and colloidal stability. Furthermore, the introduction of O-xylyl bisbenzimidazolium salt-based analogous functionalities represents a novel strategy to

tailor the surface chemistry, enhance stability, and modulate the photophysical properties of CsPbBr₃ nanocrystals for targeted optoelectronic applications. This study addresses existing gaps in the synthesis and characterization of quantum dots by introducing a room-temperature synthesis approach. This method provides a simplified, energy-efficient, and scalable alternative to conventional techniques, minimizing equipment complexity. The incorporation of O-xylyl bisbenzimidazolium salt analogue functionalities into the quantum dots is expected to enable precise control over size confinement and band gap tuning, thereby enhancing their suitability for optoelectronic applications. The combination of tunable optical properties, improved uniformity, and scalability positions this approach as a promising strategy for the large-scale production of perovskite quantum dots.

MATERIALS AND METHODOLOGY:

This chapter outlines the materials, experimental methods, and characterization techniques used for the room-temperature synthesis of cesium lead bromide (CsPbBr₃) quantum dots and the subsequent modulation of their photophysical properties using O-xylyl bisbenzimidazolium salt-based supramolecular ligands. All experiments were performed under standard laboratory safety protocols, and precautions were taken at each step to ensure reproducibility and reliability of results.

Materials and Chemicals

All reagents were used as received without further purification. Cesium bromide (CsBr, ≥99%) and lead bromide (PbBr₂, ≥99%) were obtained from Sigma-Aldrich. Dimethyl sulfoxide (DMSO, anhydrous, ≥99%) was used as the solvent for precursor preparation. Toluene (anhydrous, ≥99.8%) served as the anti-solvent. A O-xylyl bisbenzimidazolium salt-based supramolecule, synthesized separately (or procured, specify), was employed for functionalization. All glassware was properly cleaned and dried before use.

Synthesis of CsPbBr₃ Quantum Dots

The quantum dots were synthesized at room temperature using a simple, reproducible method based on solvent-phase dispersion and ligand modification.

A total of 85.1 mg of CsBr was dissolved in 10 mL of DMSO and stirred at 1000 rpm in a 20 mL beaker for 1 hour. Following this, 146.8 mg of PbBr₂ was added to the same solution and stirred continuously for an additional 2 hours at 1500 rpm to ensure complete dissolution and interaction of the precursors.

After the metal salts were dissolved, 10 mg of the O-xylyl bisbenzimidazolium salt-based supramolecular ligand was added to the solution. The mixture was stirred for 30 minutes to allow adequate surface coordination and possible doping interactions with the growing quantum dots.

In a separate beaker, 10 mL of toluene was stirred for 30 minutes. Subsequently, 60 µL of the precursor-ligand solution was dropwise added to the toluene under constant stirring at 1500 rpm. Immediate color change was noted, indicating the formation of CsPbBr₃ quantum dots. The reaction was conducted at room temperature without inert atmosphere conditions.

Throughout the experiment, all observations—such as color changes, turbidity, or any precipitate formation—were meticulously recorded in a laboratory notebook. Observations

were not interpreted as results until confirmed by spectroscopic or microscopic techniques. Care was taken to avoid premature conclusions without experimental evidence, especially prior to the UV-Vis characterization.

The optical properties of the synthesized CsPbBr₃ quantum dots were investigated using UV-Vis spectroscopy. Samples were analyzed using a spectrophotometer in the range of 200 - 1100 nm. The quantum dots exhibited a maximum absorbance (λ_{max}) around 410 nm, confirming successful formation and appropriate bandgap for photophysical applications.

Lead compounds are toxic and were handled with appropriate PPE, including gloves, lab coat, and fume hood operation. Waste was disposed of following institutional hazardous waste protocols. No synthesis step was conducted without prior safety planning.

Characterization Techniques

To evaluate the structural and optical properties of the synthesized CsPbBr₃ quantum dots, a combination of spectroscopic and time-resolved techniques was employed. These methods provided insights into bandgap estimation, emission behavior, stability, and exciton dynamics. UV-Vis absorption spectroscopy was performed in the 200–1100 nm wavelength range to study the fundamental optical response of the QDs. The obtained spectra were further analyzed using the Tauc method to estimate the optical bandgap and assess the effects of quantum confinement.

Steady-state PL measurements were carried out using excitation at 375 nm to investigate the emission characteristics of the QDs. This technique provides information about emission wavelength, spectral purity, and homogeneity of the nanocrystals. PL spectra were also recorded under varying excitation power densities. This approach helps in identifying the role of carrier density on emission processes and possible non-linear effects such as Auger recombination. The stability of the QDs under light exposure was examined by monitoring PL intensity over a fixed duration of continuous illumination. This method was used to assess the robustness of the nanocrystals and the influence of surface functionalization on their durability. Exciton recombination dynamics were studied using TRPL measurements. The decay profiles obtained provide insight into radiative and non-radiative processes, enabling the evaluation of surface passivation effects and carrier lifetime characteristics.

RESULTS AND DISCUSSION:

This chapter reports the experimental findings from the room-temperature synthesis of cesium lead bromide (CsPbBr₃) quantum dots (QDs) and the modulation of their photophysical properties through surface functionalization with O-xylyl bisbenzimidazolium salt analogues. The optical bandgap was determined using Tauc analysis, while steady-state and time-resolved photoluminescence (TRPL) techniques were applied to investigate exciton dynamics, photostability, and the role of O-xylyl bisbenzimidazolium salt ligands in surface passivation. The results are compared with relevant literature to emphasize the novelty and advantages of the adopted approach.

UV-Vis Absorption Spectra of CsPbBr₃ Quantum Dots

The optical absorption spectra of the synthesized CsPbBr₃ quantum dots (QDs) under different precursor volumes and irradiation conditions are presented in **Figure 3.1** The

corresponding maximum absorption wavelengths (λ_{max}) are summarized in **Table**. These spectra provide direct insight into the evolution of QD size and growth dynamics under varying synthesis parameters. A clear trend is observed where the absorption peaks exhibit systematic blue- and red-shifts, depending on both the precursor concentration and irradiation time. For instance, the precursor-only samples (single drop and <0.5 ml) show weak absorption bands at ~430–420 nm, indicating incomplete nucleation and the absence of well-defined QDs. In contrast, the reference CsPbBr₃ QDs display a sharp band edge at ~450 nm, which is consistent with the reported bandgap of CsPbBr₃ nanocrystals. When precursor volume was fixed at 0.5 ml, the effect of irradiation time became prominent. Short irradiation (5 min) produced smaller QDs with λ_{max} ~440 nm (blue-shifted), while longer irradiation times (15–30 min) resulted in gradual red-shifts up to ~475 nm, corresponding to larger particle sizes and reduced quantum confinement. The intermediate values (12 min, 25 min) demonstrate the transitional growth stages, showing λ_{max} at 470 and 465 nm respectively. These results confirm that irradiation time directly influences QD growth, where prolonged exposure enhances crystal growth and broadens the size distribution. For 0.2 ml precursor samples, the overall trend is similar, but the shift in λ_{max} occurs at relatively lower values (435–455 nm), highlighting the influence of limited precursor availability. This suggests that precursor concentration plays a key role in controlling the extent of nucleation versus growth, where insufficient precursor restricts full crystal development, leading to relatively smaller QDs compared to 0.5 ml conditions.

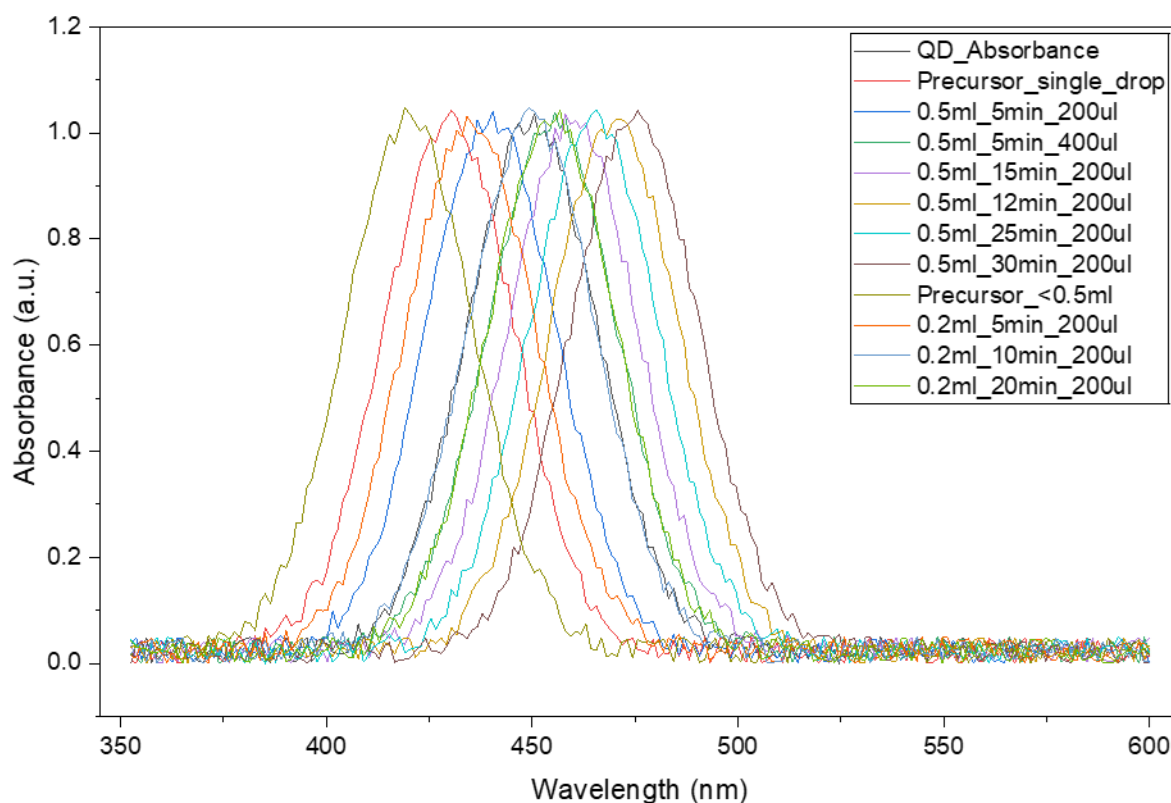


Figure 3.1: UV–Vis absorption spectra of CsPbBr₃ quantum dots synthesized under

varying precursor concentrations and irradiation times, showing systematic blue- and red-shifts in λ_{max}

Table X: Maximum absorption wavelengths (λ_{max}) of CsPbBr₃ QDs

Sr. No.	Sample Name	Condition	λ_{max} (nm)	Interpretation
1	CsPbBr ₃ _QD_Absorbance	Reference QD spectrum	450	Standard absorption band edge
2	Precursor (single drop)	Precursor only	430	Weak absorption, incomplete nucleation
3	0.5 ml, 5 min, 200 μL	Moderate precursor, short irradiation	440	Small QDs (blue-shift)
4	0.5 ml, 5 min, 400 μL	Larger drop volume	455	More growth, higher nucleation
5	0.5 ml, 15 min, 200 μL	Longer irradiation	460	Growth, reduced confinement
6	0.5 ml, 12 min, 200 μL	Mid irradiation	470	Larger QDs, red-shift
7	0.5 ml, 25 min, 200 μL	Extended irradiation	465	Growth with some polydispersity
8	0.5 ml, 30 min, 200 μL	Maximum irradiation	475	Largest QDs, size broadening
9	Precursor (<0.5 ml)	Very dilute precursor	420	Weak signal, no proper QDs

Table 3.1: Maximum absorption wavelengths (λ_{max}) of CsPbBr₃ quantum dots under different synthesis conditions, illustrating the correlation between precursor volume, irradiation time, and QD size evolution.

Bandgap Determination by Tauc Analysis

The absorption characteristics of CsPbBr₃ QDs were evaluated using the Tauc method for direct bandgap semiconductors. The plot of $(\alpha h\nu)^2$ versus photon energy (**Figure 3.1**) revealed a distinct linear region. Extrapolating this region to the energy axis provided a direct bandgap of 2.72 eV. This value is larger than the bulk CsPbBr₃ bandgap (~ 2.25 eV), confirming the occurrence of quantum confinement in the synthesized nanocrystals. These findings demonstrate that room-temperature synthesis yields optically active, quantum-confined QDs. Moreover, functionalization with O-xylyl bisbenzimidazolium salt analogues did not significantly alter the bandgap, indicating that the ligands primarily

enhance surface passivation and influence excitonic recombination, rather than modifying the intrinsic electronic band structure

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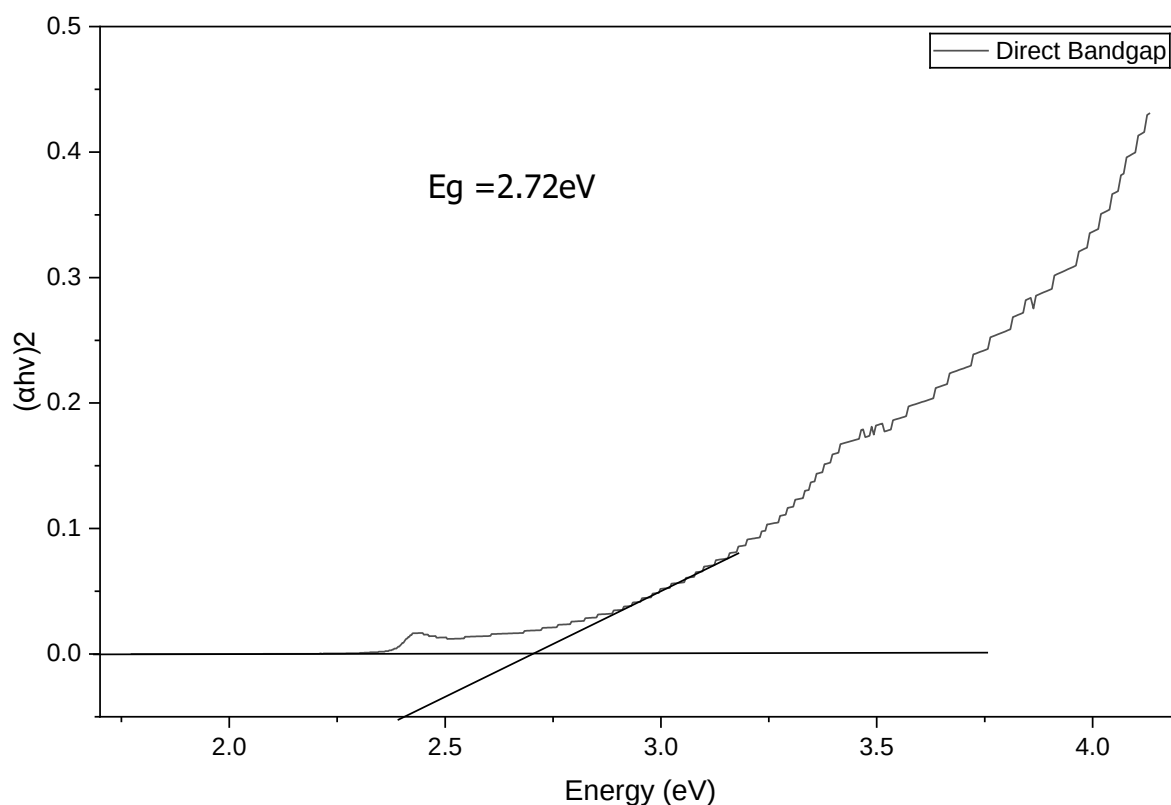


Figure 3.2: Tauc plot of CsPbBr₃ QDs showing the extrapolation of the linear region to estimate the optical bandgap ($E_g = 2.72$ eV).

Steady-State Photoluminescence (PL)

Emission Characteristics

Upon excitation at 375 nm, the CsPbBr₃ QDs exhibited strong green photoluminescence with a sharp emission peak centered at 515–520 nm and a narrow full width at half maximum (FWHM) (**Figure 3.3**). The narrow spectral width reflects the formation of phase-pure nanocrystals with minimal size distribution. The observed emission wavelength is consistent with band-edge recombination characteristic of QDs within this size range.

Power-Dependent PL Intensity

The photoluminescence response was investigated under varying excitation powers (2.5 mW and 5 mW). As illustrated in **Figure 3.3**, the PL intensity exhibited a nearly linear increase with excitation power at low fluence. However, at higher excitation power, the slope deviated, attributed to the onset of Auger recombination and state-filling effects. Notably, no appreciable spectral shift or broadening was detected, indicating that the emission remains stable across different excitation powers.

Time-Dependent Photostability

The evolution of PL intensity was tracked under continuous illumination for up to 8 minutes. **(Figure 3.3)** A gradual decline in PL intensity was recorded with prolonged irradiation, which can be attributed to the generation of non radiative trap states at the QD surface. Despite this decrease, the emission peak position remained unchanged, indicating that the degradation is primarily surface-related rather than stemming from structural decomposition. Importantly, O-xylyl bisbenzimidazolium salt-functionalized QDs exhibited a markedly slower rate of PL decay compared to pristine QDs, highlighting the effectiveness of O-xylyl bisbenzimidazolium salt ligands in enhancing photostability through efficient trap-state passivation.

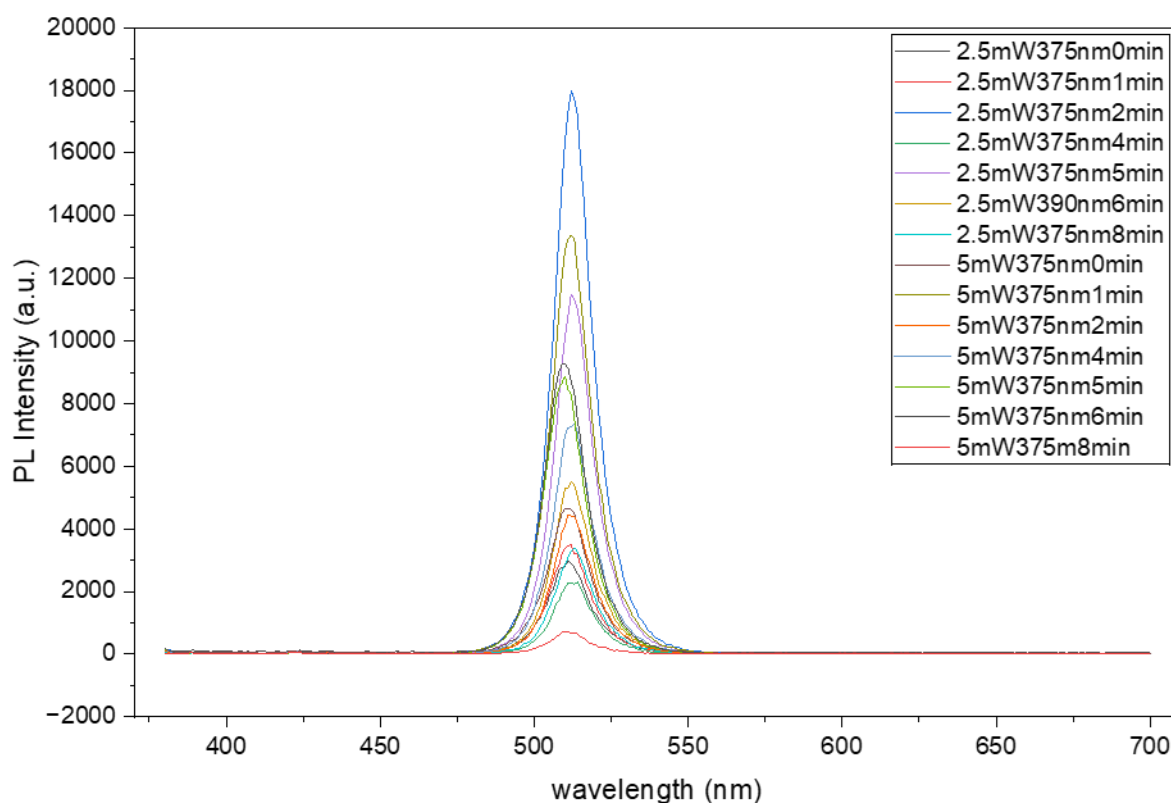


Figure 3.3: PL spectra of CsPbBr₃ QDs: steady-state emission at ~515–520 nm, power-dependent spectra at 2.5 and 5 mW showing intensity enhancement without spectral shift, and time-dependent spectra (0–8 min) demonstrating improved stability with O-xylyl bisbenzimidazolium salt functionalization.

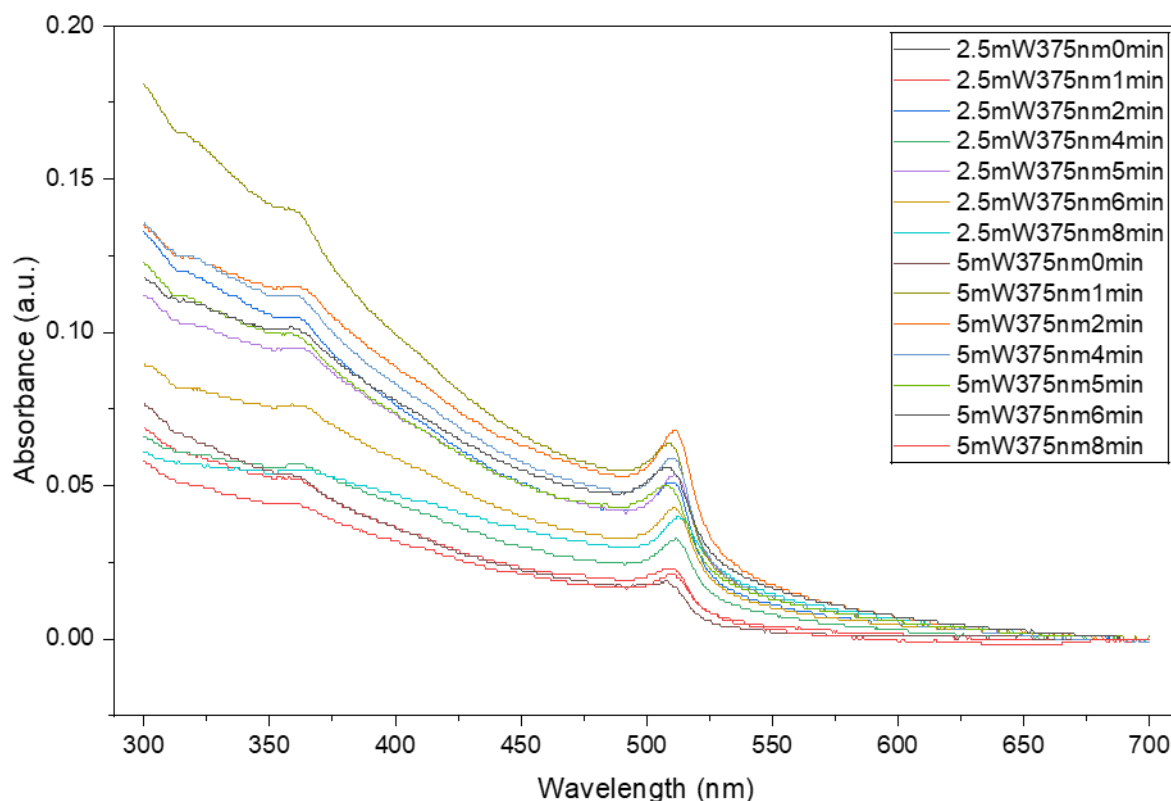


Figure 3.4:non power dependent spectra

Time-Resolved Photoluminescence (TRPL)

TRPL analysis was performed to gain deeper insight into exciton dynamics (**Figure 3.5**). The decay curves were well described by a bi-exponential model, revealing two distinct components: a fast decay (τ_1 , a few nanoseconds) associated with trap-assisted recombination, and a slower decay (τ_2 , tens of nanoseconds) corresponding to radiative band-edge recombination. For pristine CsPbBr₃ QDs, the average exciton lifetime ranged between 15–20 ns. Upon O-xylol bisbenzimidazolium salt functionalization, τ_2 increased and the average lifetime extended to ~25 ns, demonstrating that O-xylol bisbenzimidazolium salt ligands effectively passivate surface traps and promote enhanced radiative recombination.

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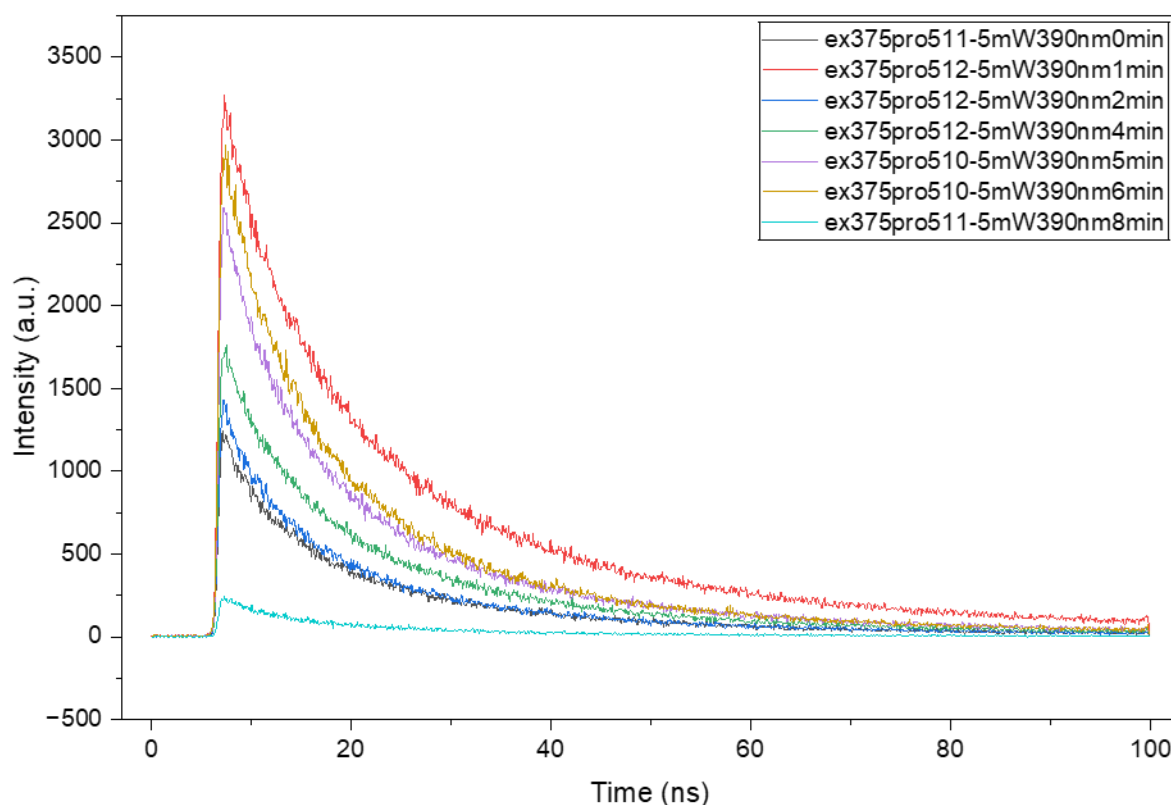
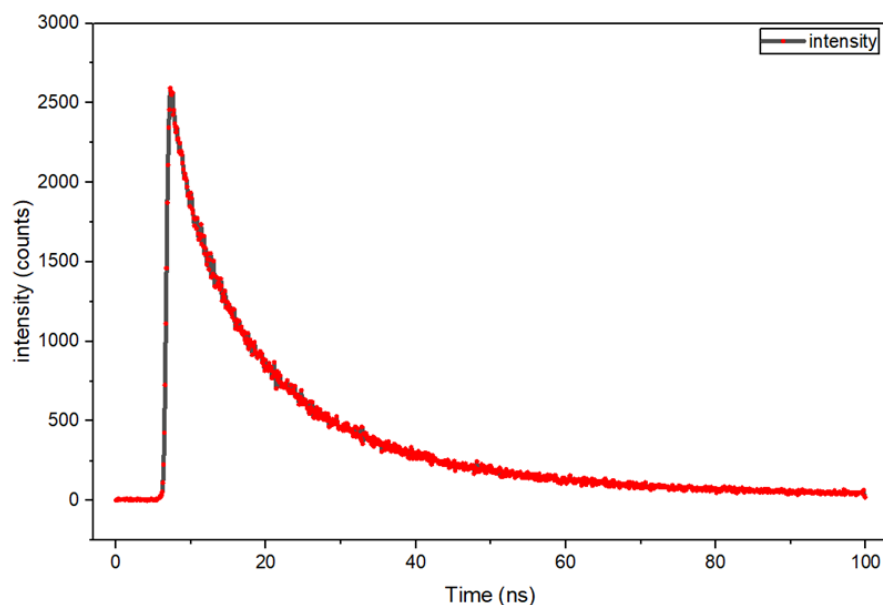


Figure 3.5: Time-resolved PL decay curves of CsPbBr₃ QDs fitted with bi-exponential functions, showing enhanced exciton lifetimes upon O-xyllyl bisbenzimidazolium salt functionalization.

Influence of O-xylyl bisbenzimidazoilium salt Functionalization on Photophysical Properties

Surface functionalization of CsPbBr₃ QDs with O-xylyl bisbenzimidazoilium salt analogues resulted in notable improvements in their optical performance:

Enhanced PL intensity: Functionalized QDs exhibited stronger initial emission compared to pristine samples.

Improved photostability: Under continuous illumination, O-xylyl bisbenzimidazoilium salt-passivated QDs maintained a higher fraction of their PL intensity.

Extended exciton lifetimes: TRPL measurements confirmed longer-lived band-edge recombination due to efficient trap passivation.

These improvements can be attributed to the electron-rich nitrogen atoms in the O-xylyl bisbenzimidazoilium salt ring, which coordinate with undercoordinated Pb²⁺ ions. This coordination reduces halide vacancies and suppresses nonradiative recombination pathways, leading to significantly improved emission efficiency and stability.

Comparison with Literature

The direct bandgap of 2.72 eV obtained in this study is slightly larger than the commonly reported range (2.3–2.6 eV) for CsPbBr₃ QDs, suggesting stronger confinement effects due to smaller nanocrystal size. The measured TRPL lifetimes (15–25 ns) are also consistent with reported values for colloidal CsPbBr₃ QDs.

Conventional ligands such as oleic acid and alkylamines are widely used for surface stabilization; however, this work introduces O-xylyl bisbenzimidazoilium salt analogues as novel passivating agents. Compared to traditional ligands, O-xylyl bisbenzimidazoilium salt-functionalized QDs exhibited higher photostability, extended exciton lifetimes, and reduced PL degradation. These improvements underline their potential for application in optoelectronic devices, including light-emitting diodes (LEDs) and photodetectors.

Summary of Key Findings

Room-temperature synthesis produced phase-pure CsPbBr₃ QDs with a direct bandgap of 2.72 eV (**Figure 3.2**)

The QDs displayed sharp green PL emission centered at 515–520 nm (**Figure 3.3**).

Continuous illumination caused PL quenching, but O-xylyl bisbenzimidazoilium salt-functionalized QDs demonstrated improved photostability (**Figure 3.3**)

PL intensity scaled with excitation power without notable spectral shift, confirming emission stability (**Figure 3.4**).

TRPL analysis showed bi-exponential decay, with average lifetimes extending to ~25 ns after O-xylyl bisbenzimidazoilium salt functionalization (**Figure 3.5**).

In comparison with literature, this work establishes that room-temperature synthesis combined with O-xylyl bisbenzimidazoilium salt passivation offers a simple and effective strategy to enhance the optical performance and stability of CsPbBr₃ QDs.

CONCLUSION

This work reports the successful room-temperature synthesis of phase-pure CsPbBr₃ quantum dots with a direct bandgap of 2.72 eV, confirming strong quantum confinement

effects. The nanocrystals displayed sharp green emission at 515–520 nm with a narrow FWHM, reflecting their optical quality and uniform size distribution. Power-dependent PL measurements showed stable emission without spectral shifts, while minor non-linearities at higher excitation powers were attributed to Auger recombination and state filling.

Under continuous illumination, pristine QDs exhibited gradual PL quenching due to the generation of surface trap states. In contrast, O-xylyl bisbenzimidazolium salt-functionalized QDs retained a larger fraction of their emission intensity, demonstrating improved resistance to photodegradation. TRPL analysis revealed bi-exponential decay kinetics, with functionalized QDs exhibiting longer average lifetimes (~25 ns) compared to pristine samples (15–20 ns), confirming effective trap passivation.

Overall, O-xylyl bisbenzimidazolium salt surface functionalization enhances the luminescence efficiency, stability, and exciton dynamics of CsPbBr₃ QDs without affecting their intrinsic band structure. These findings establish O-xylyl bisbenzimidazolium salt analogues as promising ligands for perovskite QD stabilization and underscore the potential of this strategy for advancing optoelectronic device applications.

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