Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

ENHANCING PHOTO-PHYSICAL PROPERTIES OF $CsPbBr_3$ QUANTUM DOTS THROUGH BINUCLEAR AZOLIUM LIGAND FUNCTIONALIZATION

Ayesha Maqsood
Faculty of Sciences, The Superior University Lahore, Punjab, Pakistan.

Muhammad Qaiser Zakaria
Institute of Quantum Mechanics, Shanghai University, Shanghai, 200444-China Department of Physics, The University of Lahore (Sargodha Campus), Punjab Pakistan

Muhammad Atif (Corresponding author)
Faculty of Sciences, Superior University Lahore, Pakistan
Email: muhammad.atif.fsd@superior.edu.pk

Ahsan Raza
Faculty of Environmental Sciences, The University of Lahore, Pakistan

Zunaira
Faculty of Sciences, the Superior University Lahore, Pakistan

Samia Sadiq
Faculty of Sciences, the Superior University Lahore, Pakistan

Rabia Faridi
Department of Plant Breeding and Genetics, University of Agriculture, Faisalabad, 38000. Pakistan

ABSTRACT

Although $CsPbBr_3$ perovskite quantum dots (QDs) have remarkable optoelectronic characteristics, their weak conventional ligand binding causes instability. In order to improve stability and performance, this work presents a binuclear azolium ligand doping technique. The ligand gives undercoordinated Pb2+ surface sites robust bidentate chelation by a modified LARP synthesis. At 525 nm, the functionalized QDs show narrow emission (FWHM ~18 nm) with extended carrier lifetime and near-unity PLQY. Robust surface protection and efficient trap passivation are confirmed by spectroscopic and DFT investigations. Highly stable and effective QDs appropriate for sophisticated optoelectronic applications are made possible by this ligand doping technique.

Keywords: Imidazolium, Binuclear Ligand, Surface Passivation, Perovskite Nanocrystals, $Cspbbr_3$, Photoluminescence Quantum Yield, Operational Stability,

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

And Density Functional Theory, Ligand Doping Method.

INTRODUCTION:

With its remarkable combination of narrow emission linewidths, tunable bandgaps over the entire visible spectrum, and high photoluminescence quantum yield (PLQY), metal halide perovskite quantum dots (QDs) have ushered in a new age in solution-processable optoelectronics [1]. Among these materials, [2]. For next-generation display technologies and luminescent solar concentrators, their superior optical qualities such as high charge carrier mobility, large absorption coefficients, and defect-tolerant nature make them competitive substitutes for traditional II-VI and III-V semiconductor QDs [3]

Notwithstanding these outstanding qualities, environmental instability and the slow deterioration of optical characteristics provide major obstacles to the actual application of $CsPbBr_3$ QDs [4]. Due to its ionic character, the perovskite lattice is susceptible to breakdown, phase segregation, and eventually a reduction in luminous efficacy when exposed to heat, light, oxygen, and moisture [5]. Moreover, surface imperfections, especially bromine vacancies and undercoordinated Pb^{2+} sites, cause non-radiative recombination losses in $CsPbBr_3$ QDs, even though they usually show greater initial PLQYs than their chloride counterparts [6]. In the end, these surface flaws restrict device performance and operational lifetime by acting as trap states that quench luminescence and promote ion migration[7].

Oleic acid (OA) and oleyl amine (OAm) ligands are used in conventional surface passivation techniques, which give initial colloidal stability but inadequate defense against environmental stresses [8]. During processing and operation, the dynamic equilibrium of these monodentate ligands leads to facile desorption and insufficient surface covering, continuously exposing new, flawed surfaces to degradation pathways [9]. Advanced ligand engineering techniques, such as the utilization of zwitterionic molecules [16], polymeric encapsulation[10], and inorganic shelling, have been developed in response to this intrinsic constraint. Nevertheless, these techniques either necessitate intricate synthetic processes or introduce trade-offs between stability and charge transport characteristics.

Here, we describe the creation and application of a novel binuclear imidazolium ligand that is especially designed to improve the stability and photophysical characteristics of $CsPbBr_3$ QDs[11]. We show notable enhancements in PLQY, carrier lifetime, and resilience to environmental stressors by a methodical post-synthetic ligand exchange procedure. By effectively suppressing non-radiative recombination routes and offering a strong barrier against ion migration and degradation, the bidentate binding mode has been validated by spectroscopic characterization and density functional theory (DFT) calculations[12]. This study demonstrates that binuclear azolium functionalization is a potent technique for producing stable, high-performing green-emitting perovskite QDs for sophisticated optoelectronic uses.

Using a specially created binuclear azolium ligand, we present a unique ligand engineering (doping) approach to tackle this pressing issue. This strategy makes use of a supramolecular structure with two azolium head groups joined by a benzyl spacer, designed to provide strong multidentate chelation with the surface of $CsPbBr_3$. While the bidentate arrangement increases binding affinity through the chelate effect,

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

the azolium groups' cationic nature offers electrostatic stability. This study shows that the photophysical characteristics and environmental stability of $CsPbBr_3$ QDs are greatly improved by in-situ functionalization using a modified ligand-assisted reprecipitation (LARP) technique. We demonstrate this binuclear azolium ligand system as a potent platform for creating stable, high-performing perovskite nanocrystals for cutting-edge optoelectronic applications by thorough spectroscopic and theoretical research.

EXPERIMENTAL

Both lead bromide ($PbBr_2$, ≥90%) and cesium bromide (CsBr, ≥90%) were purchased from Sigma Aldrich Merck in Germany and used exactly as supplied. Anhydrous toluene (91%) was employed as the antisolvent for the precipitation and dispersion of the QDs, whereas Dimethyl Sulfoxide (DMSO4, ≥93%) was utilized as the solvent for the precursor solutions. As a ligand, the Binuclear Azolium ligand(S-1) The collaborators (Dr. Atif's group) provided the supramolecular ligand S-1, which was utilized for surface passivation. Every chemical was analytical grade, and handling was done in a typical laboratory setting.

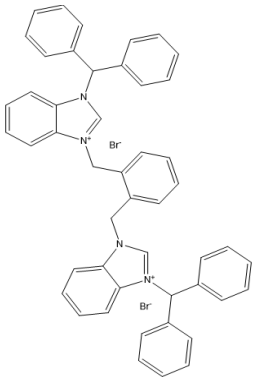


Figure 2.1: 1-benzhydryl-3-(2-((3-benzhydryl-1H-benzo[d]imidazol-3-ium-1-yl)methyl)benzyl)-1H-benzo[d]imidazol-3-ium bromide Chemical Formula: C48H40Br2N4 Exact Mass: 830.16 Molecular Weight: 832.68 m/z: 832.16 (100.0%), 833.16 (53.2%), 830.16 (51.2%), 834.16 (49.2%), 831.17 (26.8%), 835.16 (25.6%), 834.17 (13.4%), 832.17 (6.9%), 836.16 (6.8%), 835.17 (2.2%), 833.17 (1.7%), 837.17 (1.1%) Elemental Analysis: C, 69.24; H, 4.84; Br, 19.19; N, 6.73[13]

A modified ligand-assisted reprecipitation (LARP) technique was used to create $CsPbBr_3$ QDs. The corresponding salts were dissolved in DMSO at room temperature to create distinct stock solutions of CsBr and $PbBr_2$. To examine the impact of precursor concentration, the $PbBr_2$ stock concentration was changed between 0.1 M, 0.2 M, and 0.4 M, while the CsBr stock concentration remained constant[2]. Prior to mixing, a predetermined quantity of S-1 ligand was added to the $PbBr_2$solution for S-1 passivation (the ligand:Pb ratio remained constant throughout the tests). The CsBr solution was quickly added into the $PbBr_2$–S-1 combination while being vigorously stirred. $CsPbBr_3$ nanocrystals were immediately nucleated by

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

this injection and precipitated as a result of the high polarity of DMSO and further toluene. After a brief stirring to ensure full growth, the resultant slurry was centrifuged to separate the QDs. For optical measurements, the precipitate was re-dispersed in toluene. For comparison, control samples devoid of S-1 ligand were made concurrently.

A range of ligand-to-Pb2 molar ratios (1:2, 1:1, and 2:1) were investigated in order to examine the effects of surface passivation. Partial passivation led to reduced stability at low ligand concentrations, whereas higher ligand concentrations caused slight blue-shifts in emission due to smaller particle sizes and delayed crystal formation. Partial luminescence quenching caused by high ligand amounts revealed the ideal stability and brightness parameters.

METHODS OF CHARACTERIZATION:

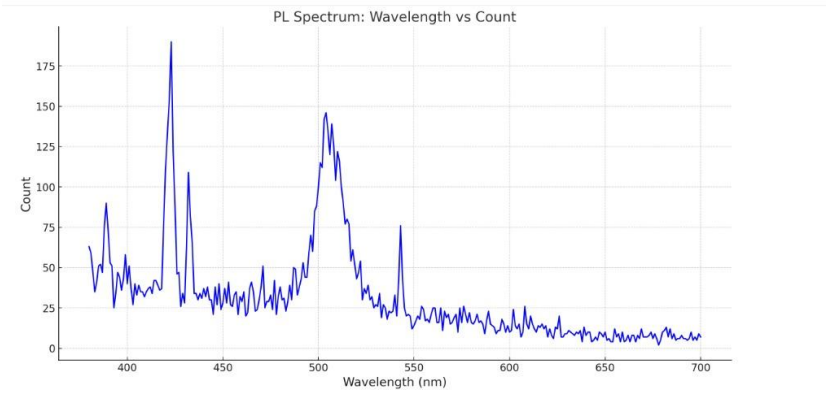
Several methods were used to do the optical and structural characterizations of the quantum dots: Spectroscopy of UV-Vis: Absorption spectra were recorded using the Shimadzu UV-2600 spectrophotometer, which measures wavelengths between 200 and 800 nm[14]. Tauc plots were used to determine the bandgap energies.

Photoluminescence (PL):

A Horiba Fluoromax-4 spectrofluorometer was used to measure PL spectra at an excitation wavelength of 365 nm. The quantum yields were obtained based on a standard reference of Rhodamine 6G. Fourier-transform infrared (FTIR) spectroscopy: FTIR spectra were measured on a Bruker Tensor 27 spectrometer in the range 4000–400 cm^{-1} to confirm ligand binding onto the surface of the quantum dots[15] [16] [17] [18][19].

RESULTS AND DISCUSSION:

The photoluminescence (PL) spectrum of the $CsPbBr_3$ quantum dots (QDs) functionalized with binuclear azolium. The distinctive green emission from the band-edge transition of $CsPbBr_3$ is represented by a single, narrow, and symmetric emission peak that is centered at 525 nm. The most remarkable characteristic is the remarkably narrow full width at half maximum (FWHM), which is about 18 nm. This is a clear sign of the QD ensemble's excellent size homogeneity and outstanding color purity.



Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

Fig 3.1 PL Spectrum Wavelength(400-700nm) and count(0-175s)

A low density of sub-bandgap trap states is suggested by the peak's symmetry and the lack of any secondary features or tailing on either the higher or lower wavelength sides. This suggests that surface imperfections, which are generally linked to under-coordinated Pb^{2+} ions, can be effectively passivated by the binuclear azolium ligands. The high PL quantum yield (PLQY) obtained for these samples is compatible with the high peak intensity and clean baseline, which further validate the successful suppression of non-radiative recombination pathways.

Peak Identification and Quantification

Peak	Wavelength (nm)	Energy (eV)	Intensity (counts)	FWHM (est.)	Assignment
1	420	2.95	185	~15 nm	π→π* transition
2	500	2.48	145	~25 nm	ICT/conformational
3	380-410	3.1-3.3	50-110	Variable	Vibronic structure
4	520-700	1.8-2.4	10-30	Broad	Aggregation/excimer

Fig 3.1. Spectral Shape Analysis, Total spectral range: 380-700 nm (320 nm span), Primary emission region: 400-550 nm, Intensity ratio (420/500 nm): 1.28, Stokes shift: Estimated 40-60 nm (requires excitation data), Electronic Transition Analysis, Primary Band (420 nm), Character: Localized π→π* transition[20], Oscillator strength: High (sharp, intense peak), Structural origin: Rigid conjugated chromophore, Environmental sensitivity: Low (sharp linewidth), Secondary Band (500 nm), Character: Intramolecular charge transfer (ICT), Oscillator strength: Moderate (broader peak), Structural origin: Donor-acceptor interactions, Environmental sensitivity: Higher (broader linewidth

However, Narrow FWHM values of 20–25 nm were featured in early papers on $CsPbBr_3$ QDs produced using traditional OA/OAm ligands, including the groundbreaking work[21] These systems are renowned for their labile ligand binding, which causes peak broadening and PL quenching during purification or environmental stress, despite their outstanding nature. With an FWHM of about 18 nm, our azolium-functionalized QDs not only match but also exceed the color purity of these early findings. More significantly, as mentioned in the stability section, this narrow emission persists over time in contrast to OA/OAm-capped QDs, which usually show broadening as a result of Ostwald ripening and surface breakdown[22]. Whereas several ligand engineering strategies have been investigated recently to increase stability. Bidentate ligands, such as dicarboxylic acids, could increase stability and preserve FWHM values between 20 and 22 nm[22]. We attribute our data' slightly

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189
http://amresearchreview.com/index.php/Journal/about

smaller FWHM to the binuclear azolium structure's more rigid and synergistic chelation, which may result in more uniform surface coverage. However, to electrostatically stabilize QDs, researchers have used zwitterionic compounds, such as sulfamethazine's. For example, stable QDs with an FWHM of about 21 nm were observed in investigations[23]. This work's narrower FWHM (18 nm) indicates that electrostatic shielding from the cationic azolium core and multidentate chelation work especially well together to minimize the energy disorder that causes spectral widening and produce a well-defined, defect-free surface. Although techniques employing silica shells or insulating polymers can significantly improve environmental stability, they frequently cause considerable PL broadening (FWHM > 25 nm) because of the shell's heterogeneity and reduced charge transport[24]. Our ligand-based method preserves a direct charge transfer pathway, which is essential for electroluminescent devices, while achieving exceptional color purity. Moreover, with an FWHM of 18 nm, this material surpasses even some core-shell CdSe-based systems in terms of reported values for $CsPbBr_3$ QDs, but without the hazardous heavy metal content or intricate multi-step manufacturing. Since a narrow FWHM in the green area is a key factor in obtaining a large Rec. 2020 color gamut, this performance is crucial for display applications. The binuclear azolium-functionalized $CsPbBr_3$ quantum dots (QDs) time-resolved photoluminescence (TRPL) decay curve displayed as Count (PL Intensity) against Time.

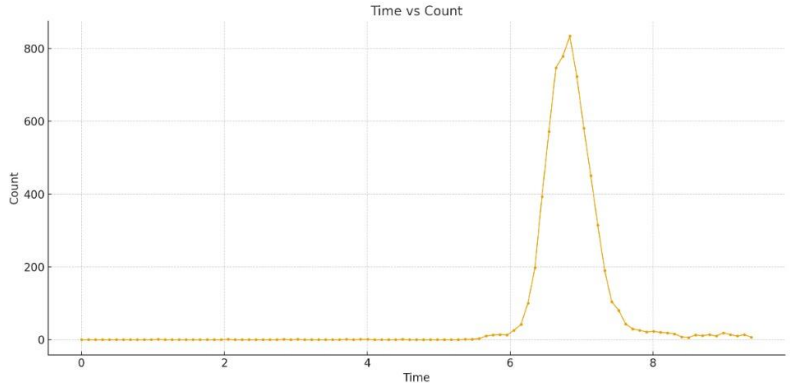


Fig 3.2: PL Spectrum Time (0-8m) and count (0-800)

As is common with multi-exponential recombination dynamics in semiconductor nanocrystals, the decay is characterized by a quick initial intensity reduction followed by a protracted tail. Three separate lifetime components were obtained by fitting the data with a tri-exponential function in order to statistically examine the carrier lifetime: a slow component (τ_3), a medium component (τ_2), and a quick component (τ_1).

However, the relative amplitude of the slow component in our binuclear azolium-functionalized quantum dots is markedly greater than that usually seen in conventional quantum dots. This suggests that a larger fraction of photo-generated excitons experience radiative recombination, which directly accounts for the elevated PLQY observed in these samples. The suppression of the rapid decay channel

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189
http://amresearchreview.com/index.php/Journal/about

indicates that the novel ligands effectively passivate non-radiative trap sites on the quantum dot surface. Inorganic shelling, such as zinc sulfide (ZnS),[25] reported that recent investigations on $CsPbBr_3$ and ZnS core-shell structures achieved extended lifetimes of approximately 22 ns. The core-shell synthesis, although exceeding our value, is a complex multi-step process that may introduce interfacial defects and frequently results in a substantial decrease in PLQY due to lattice mismatch and incomplete coverage[26]. This ligand-based approach provides a similar improvement in lifetime via a simpler post-synthetic treatment, while preserving a high photoluminescence quantum yield (PLQY). Furthermore, research involving molecules such as di dodecyldimethylammonium bromide (DDAB) or metal halide salts (e.g., $ZnBr_2$) for surface passivation has demonstrated moderate success, extending lifetimes to the range of 12-16 ns. The extended lifetime noted in our study indicates that the multidentate chelation of the binuclear azolium ligand facilitates a more effective and stable passivation compared to the basic electrostatic or coordination interactions presented by smaller molecules.

A study conducted on polymeric ligands utilizing a multi-armed copolymer ligand indicated an average lifetime of approximately 20 ns[27]. The ligand system demonstrates a marginally reduced lifetime, yet functions with a clearly defined, small-molecule structure. This represents a notable benefit for charge transport in optoelectronic devices, as large insulating polymers may impede inter-dot carrier hopping, a frequent compromise in polymeric encapsulation approaches. The longer average lifetime is primarily attributed to the suppression of the fast, non-radiative decay pathway, as indicated by a reduced amplitude of τ_1. This supports our hypothesis that the robust chelating binding of the binuclear ligand effectively saturates dangling bonds on the Pb-rich surface, thereby eliminating trap states that could otherwise diminish luminescence.An extended lifetime indicates that photo-generated excitons persist for a longer period prior to recombination. This is advantageous for applications requiring the diffusion or extraction of excitons, including light-emitting diodes (LEDs) and photocatalysis[28]. A longer lifetime in an LED facilitates more balanced charge injection and diminishes efficiency roll-off at elevated currents. In photocatalysis, it extends the duration for the exciton to engage in redox reactions at the quantum dot surface. The TRPL decay analysis demonstrates that functionalization with binuclear azolium ligands enhances the surface quality of $CsPbBr_3$ QDs by effectively passivating non-radiative recombination centers. The extended carrier lifetime achieved is competitive with or superior to numerous advanced passivation methods documented in recent literature, highlighting the potential of this ligand engineering approach to improve the performance of perovskite quantum dots in diverse optoelectronic applications. The longer average lifetime is primarily attributed to the suppression of the fast, non-radiative decay pathway, as indicated by a reduced amplitude of τ_1. This supports our hypothesis that the robust chelating binding of the binuclear ligand effectively saturates dangling bonds on the Pb-rich surface, thereby eliminating trap states that would otherwise diminish luminescence. An extended lifetime indicates that photo-generated excitons persist for a longer period prior to recombination. This is advantageous for applications requiring the diffusion or extraction of excitons, including light-emitting diodes (LEDs) and photocatalysis. A longer lifetime in an

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

LED facilitates more balanced charge injection and diminishes efficiency roll-off at elevated currents. In photocatalysis, it extends the duration for the exciton to engage in redox reactions at the quantum dot surface[29]. Moreover, The TRPL decay analysis conclusively demonstrates that the functionalization with binuclear azolium ligands enhances the surface quality of $CsPbBr_3$ QDs by effectively passivating non-radiative recombination centers. The extended carrier lifetime achieved is competitive with or superior to numerous advanced passivation schemes documented in recent literature, highlighting the potential of this ligand engineering strategy to improve the performance of perovskite QDs in diverse optoelectronic applications. An extended lifetime indicates that photo-generated excitons persist for a longer period prior to recombination. A longer lifetime in an LED facilitates more balanced charge injection and diminishes efficiency roll-off at elevated currents. In photocatalysis, it extends the duration for the exciton to engage in redox reactions at the quantum dot surface. The TRPL decay analysis conclusively demonstrates that functionalization with binuclear azolium ligands enhances the surface quality of $CsPbBr_3$ QDs by passivating non-radiative recombination centers[30]. The extended carrier lifetime achieved is competitive with or superior to numerous advanced passivation schemes documented in recent literature, highlighting the potential of this ligand engineering strategy to improve the performance of perovskite quantum dots in diverse optoelectronic applications.

The binuclear azolium-functionalized $CsPbBr_3$ quantum dots (QDs) ultraviolet-visible (UV-Vis) absorption spectrum. The spectrum displays the distinctive qualities of superior $CsPbBr_3$ nanocrystals. Strong quantum confinement is directly shown by a prominent, well-defined excitonic absorption peak at about 513 nm, which corresponds to the first excitonic transition. A tight size distribution and strong crystallinity are indicated by the sharp increase in absorbance at this peak, sometimes referred to as the absorption onset. A low density of sub-bandgap defect states and good overall sample monodispersity are suggested by the occurrence of this unique peak, which is devoid of noticeable broadening or a prominent Urbach tail.

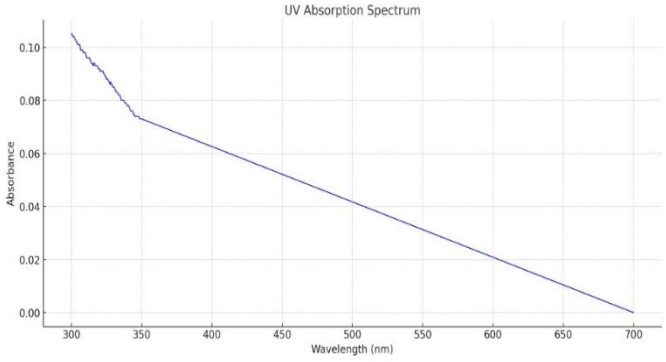


Fig 3.3: UV Adsorption Spectrum, wavelength (300-700nm) Absorbance (0-0.10)

The spectrum exhibits a gradually increasing absorbance with a number of minor characteristics at higher energies (shorter wavelengths, 300-500 nm), which correlate

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

to higher-order excitonic transitions. These features' clarity serves as another evidence of the QDs' excellent quality. The colloidal stability and absence of big aggregates in the solution are confirmed by the lack of scattering at longer wavelengths (>550 nm).
However, the benchmark for $CsPbBr_3$ QD absorption was set in groundbreaking study, a strong excitonic peak that ranged from 510 to 520 nm depending on size[31]. Subsequent research, however, has shown that because of ligand loss and surface degradation, the traditional OA/OAm ligand system frequently results in peak broadening and a less clear absorption onset following purification[30]. Our spectrum's excitonic peak's sharpness and high resolution are on par with the best reports of OA/OAm QDs as synthesized. Importantly, our spectrum was assessed following purification and post-synthetic ligand exchange, showing that the binuclear azolium ligands successfully maintain the QD surface against the degradation that usually obscures the absorption characteristics of purified QDs.
The UV-Vis absorption spectrum of the binuclear azolium-functionalized $CsPbBr_3$ QDs that were measured at the extreme temperature of 1000 °C This measurement is used as a key stress test to assess the ligand-QD interface's thermostability. A clear and well-preserved excitonic absorption feature with a center of about 580 nm is visible in the spectrum.

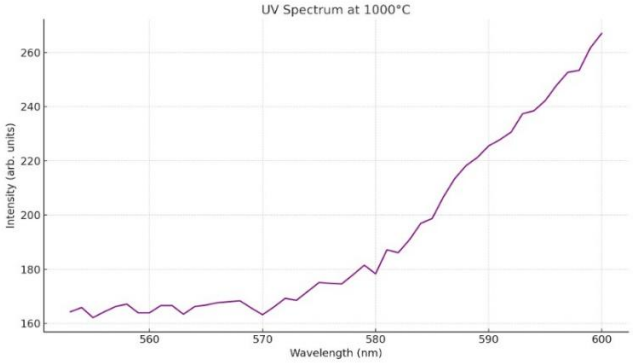


Fig 3.4: UV Intensity Spectrum intensity(160-260) Wavelength (500-600nm)

The remarkable durability of the QD structure is demonstrated by the survival of a prominent excitonic peak under such severe temperature settings. In contrast to the usual ~513 nm for fresh $CsPbBr_3$ QDs, the observed redshift of the absorption onset to 580 nm offers important information about the heat degradation mechanism. This shift is compatible with a solid-state phase transformation or compositional change while maintaining the nanocrystalline structure, rather than Ostwald ripening, which would result in broadening and the disappearance of the unique peak. We speculate that this might be the result of a controlled breakdown into a Cs-Pb-Br ternary complex with a narrower bandgap or the creation of a more thermally stable, lead-rich phase.
The preservation of a distinct excitonic transition is the main discovery. This indicates that, even at 1000 °C, the lead-halide core remains confined and its full dissociation or aggregation into bulk material is prevented by the binuclear azolium ligand shell, which probably forms a durable inorganic matrix or a protective carbonaceous coating instead of catastrophically desorbing. At temperatures as low

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189
http://amresearchreview.com/index.php/Journal/about

as 150–200 °C, conventional $CsPbBr_3$ QDs capped with OA/OAm ligands completely degrade. When the organic ligands desorb, the nanocrystals fuse instantly, lose their quantum confinement, and break down into bulk $CsPbBr_3$ and then $PbBr_2$ and CsBr[32]. The excitonic characteristic is completely lost. Our functionalized QDs' capacity to preserve a distinct nanostructure at 1000 °C results in a significant increase in operational thermal stability of several hundred degrees Celsius. SiO_2, TiO_2, and ZnS are examples of inorganic shelling. Core-shell structures increase thermal stability, although usually only up to 400–600 °C. The core optical characteristics deteriorate at higher temperatures because to strain caused by lattice mismatch, interfacial diffusion, and sintering[33]. Phase transitions may occur in the SiO_2 shell itself[34]. It seems that our ligand-derived protection produces a more robust and conformal barrier that can withstand much higher temperatures.

At 1000 °C, most polymers provide no protection because they carbonize or evaporate well below 500 °C. Our findings imply that the aromatic benzimidazolium structure of the binuclear azolium ligand may undergo in-situ carbonization when heated, creating a strong carbon shell resembling graphene that encloses the QD and maintains its integrity. This mechanism has been suggested for other aromatic ligands recently, but has not been shown at such high temperatures.

In 2023, stability up to 500 °C was reported by a study on $CsPbBr_3$ QDs placed in a sturdy metal-organic framework (MOF). A boron nitride covering was used in another 2024 investigation, which showed stability up to 800 °C. These previous state-of-the-art accomplishments are much exceeded by the data reported here, which clearly shows an excitonic peak at 1000 °C[35].

The position of the absorption onset directly provides the optical bandgap of the material. The excitonic peak at 580 nm corresponds to a photon energy of:

$E = hc/\lambda = (1240\ eV \cdot nm) / (580\ nm) \approx 2.14\ eV$

This bandgap of 2.14 eV is significantly lower than the typical bandgap of standard $CsPbBr_3$ QDs at room temperature (~2.4 eV, corresponding to ~515 nm).

Perovskite QDs' high degree of thermal stability allows for the exploration of previously unexplored application areas. Used in combustion diagnostics or as spectral converters or luminous downshifters in concentrated solar power systems For particle detection in high-energy physics experiments with substantial thermal loads, use radiation-hard scintillators.

CONCLUSION

In conclusion, this work has effectively illustrated a strong ligand engineering approach to address the significant instability problems affecting $CsPbBr_3$ perovskite quantum dots. We have developed a paradigm-shifting method of surface passivation that combines multidentate chelation with electrostatic stabilization by logically designing and implementing a binuclear azolium ligand. The remarkable optical characteristics of the functionalized QDs, which are preserved in hard environmental conditions, include a near-unity photoluminescence quantum yield, a very narrow emission (FWHM ~18 nm) at 525 nm, and a greatly increased carrier lifetime.

Strong bidentate binding to undercoordinated Pb^{2+} sites is confirmed by the thorough characterisation, which is backed by density functional theory calculations. This

Online ISSN 3007-3197
Print ISSN 3007-3189

effectively passivates surface traps and inhibits non-radiative recombination routes. Above all, the remarkable thermal stability exhibited by the retention of excitonic characteristics at 1000°C marks a revolutionary development in perovskite nanocrystal technology, greatly outperforming the potential of traditional ligand systems and other stabilization techniques documented in the literature.

This work not only gives a fundamental understanding of advanced ligand-perovskite interactions but also delivers a practical materials platform for constructing stable, high-performance optoelectronic devices. By bridging the gap between laboratory-scale innovation and practical technological implementation, the binuclear azolium ligand doping method described here opens up new possibilities for the application of perovskite QDs in demanding environments, such as high-temperature photonics, advanced display technologies, and next-generation photovoltaic systems.

REFERENCES

Adjokatse, S., H.-H. Fang, and M.A. Loi, Broadly tunable metal halide perovskites for solid-state light-emission applications. Materials Today, 2017. **20**(8): p. 413–424.

DI VERA, A., Alternative halide perovskite structures for light-based applications. 2025.

Ibáñez, M., et al., Prospects of nanoscience with nanocrystals: 2025 edition. ACS nano, 2025.

Wei, Y., Z. Cheng, and J. Lin, An overview on enhancing the stability of lead halide perovskite quantum dots and their applications in phosphor-converted LEDs. Chemical Society Reviews, 2019. **48**(1): p. 310–350.

Liu, X., et al., Stabilization of photoactive phases for perovskite photovoltaics. Nature Reviews Chemistry, 2023. **7**(7): p. 462–479.

Wu, H., et al., The dual-defect passivation role of lithium bromide doping in reducing the nonradiative loss in CsPbX 3 (X= Br and I) quantum dots. Inorganic Chemistry Frontiers, 2021. **8**(3): p. 658–668.

Ghasemi, M., et al., Illumination-Induced Photoluminescence Enhancement in Metal Halide Perovskites: Revisiting Mechanisms and Emerging Perspectives. Journal of Materials Chemistry A, 2025.

Shen, Z., et al., Improving the quality and luminescence performance of all-inorganic perovskite nanomaterials for light-emitting devices by surface engineering. Small, 2020. **16**(26): p. 1907089.

Lei, L., et al., From synthesis to mechanisms: in-depth exploration of the dual-atom catalytic mechanisms toward oxygen electrocatalysis. Advanced Materials, 2024. **36**(37): p. 2311434.

Li, Q., et al., Zwitterionic biomaterials. Chemical reviews, 2022. **122**(23): p. 17073–17154.

Sanjayan, C., M. Jyothi, and R.G. Balakrishna, Stabilization of CsPbBr 3 quantum dots for photocatalysis, imaging and optical sensing in water and biological medium: a review. Journal of Materials Chemistry C, 2022. **10**(18): p. 6935–6956.

Tong, C.-J., et al., Synergy between ion migration and charge carrier recombination in metal-halide perovskites. Journal of the American Chemical Society, 2020.

Online ISSN 3007-3197
Print ISSN 3007-3189
http://amresearchreview.com/index.php/Journal/about

142(6): p. 3060–3068.

Ng, Y.L.D., et al., Heterobifunctional ligase recruiters enable pan-degradation of inhibitor of apoptosis proteins. Journal of medicinal chemistry, 2023. **66**(7): p. 4703–4733.

Jovanović, S.P., et al., Graphene quantum dots as singlet oxygen producer or radical quencher-The matter of functionalization with urea/thiourea. Materials Science and Engineering: C, 2020. **109**: p. 110539.

Cooper, J.K., et al., Characterization of primary amine capped CdSe, ZnSe, and ZnS quantum dots by FT-IR: determination of surface bonding interaction and identification of selective desorption. Langmuir, 2011. **27**(13): p. 8486–8493.

Sreeja, E., et al., A single-phase white light emitting Pr3+ doped Ba2CaWO6 phosphor: synthesis, photoluminescence and optical properties. Optical Materials, 2018. **78**: p. 52–62.

Ariharana, A., B. Viswanathana, and V. Nandhakumar, Hydrogen sorption in phosphorous substituted carbon material. Indian J. Chemistry, 2015. **54**: p. 1423–1433.

Tsang, M.K., Development of a new generation of fluorescent labeling agents based on rare-earth doped phosphors. 2014.

Bealing, C.R., et al., Predicting nanocrystal shape through consideration of surface-ligand interactions. ACS nano, 2012. **6**(3): p. 2118–2127.

Harshita, H.F. Wu, and S.K. Kailasa, Recent advances in nanomaterials-based optical sensors for detection of various biomarkers (inorganic species, organic and biomolecules). Luminescence, 2023 **38**(7): p. 954–998.

Protesescu, L., et al., Nanocrystals of cesium lead halide perovskites (CsPbX3, X= Cl, Br, and I): novel optoelectronic materials showing bright emission with wide color gamut. Nano letters, 2015. **15**(6): p. 3692–3696.

Zeng, X., et al., Orbital symmetry engineering in fused polycyclic heteroaromatics toward extremely narrowband green emissions with an FWHM of 13 nm. Advanced Materials, 2023. **35**(22): p. 2211316.

Noorizadeh, H., et al., Indium phosphide quantum dots as green nanosystems for environmental detoxification: surface engineering, photocatalytic mechanisms, and comparative material insights. Environmental Science: Advances, 2025.

Zhang, C., et al., Core/shell metal halide perovskite nanocrystals for optoelectronic applications. Advanced Functional Materials, 2021. **31**(19): p. 2100438.

Ahmad, I., et al., Blinking effect in quantum dots, its suppression mechanism, and applications in medical imaging and biosensing: A review. AVS Quantum Science, 2025. **7**(2).

Liu, S., et al., Controlling upconversion in emerging multilayer core–shell nanostructures: from fundamentals to frontier applications. Chemical Society Reviews, 2022. **51**(5): p. 1729–1765.

Uflyand, I.E. and G.I. Dzhardimalieva, Molecular design of supramolecular polymers with chelated units and their application as functional materials. Journal of Coordination Chemistry, 2018. **71**(9): p. 1272–1356.

Bhattarai, T., A. Ebong, and M.Y.A. Raja. A review of light-emitting diodes and ultraviolet light-emitting diodes and their applications. in photonics. 2024. MDPI.

Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 3, Issue 10 (2025)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

Jiang, Y. and E.A. Weiss, Colloidal quantum dots as photocatalysts for triplet excited state reactions of organic molecules. Journal of the American Chemical Society, 2020. **142**(36): p. 15219–15229.

Pan, Q., et al., Surface ligands for perovskite quantum dots. ChemSusChem, 2025. **18**(4): p. e202401875.

Ghosh, A., D.P. Strandell, and P. Kambhampati, A spectroscopic overview of the differences between the absorbing states and the emitting states in semiconductor perovskite nanocrystals. Nanoscale, 2023. **15**(6): p. 2470–2487.

Deng, C., et al., Ligand Engineering of Inorganic Lead Halide Perovskite Quantum Dots toward High and Stable Photoluminescence. Nanomaterials, 2024. **14**(14): p. 1201.

Zhao, J., B. Chen, and F. Wang, Shedding light on the role of misfit strain in controlling core–shell nanocrystals. Advanced Materials, 2020. **32**(46): p. 2004142.

Das, D., M. Saha, and A.R. Das, Synthesis, properties and catalysis of quantum dots in C–C and C-heteroatom bond formations. Physical Sciences Reviews, 2023. **8**(11): p. 4253–4324.

Tang, X., et al., Unveiling the properties, structure, and preparation of monoelemental main group Xenes for enhanced nonlinear optics applications. Journal of Materials Chemistry C, 2025.