Supporting Information

In-Situ Dual-Site Passivation of All-Inorganic Perovskite Quantum Dots Using Zwitterionic Taurine for Enhanced Defect Resistance

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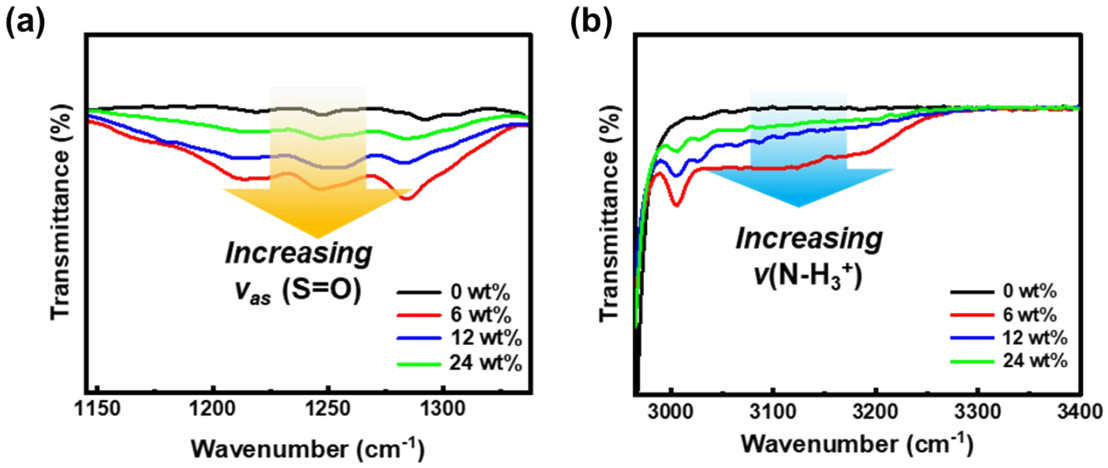

Fig. S1. FT-IR spectra of taurine-$CsPbBr_3$ PQDs with varying taurine concentrations (0, 6, 12, and 24 wt%), showing (a) the asymmetric stretching vibration of sulfonate groups ν_{as}(S=O) and (b) the stretching vibration of ammonium groups ν(N–H_3^+).

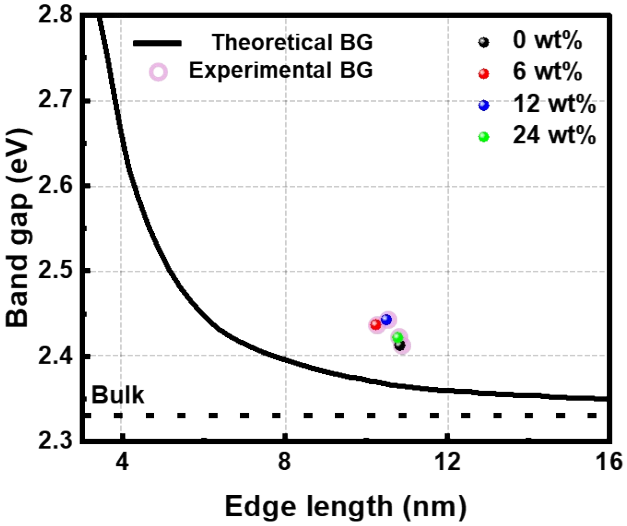

Fig. S2. Size-dependent bandgap evolution of $CsPbBr_3$ PQDs in quantum confinement. (Solid line: theoretical bandgap, symbols: experimental bandgap)

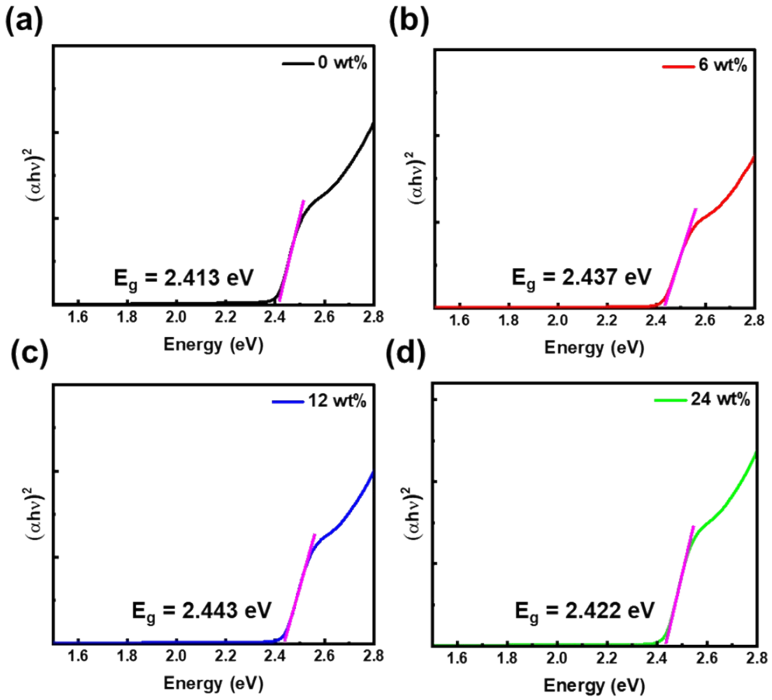

Fig. S3. Tauc plots for optical bandgap determination of $CsPbBr_3$ PQDs with different taurine concentrations (0, 6, 12 and 24 wt%).

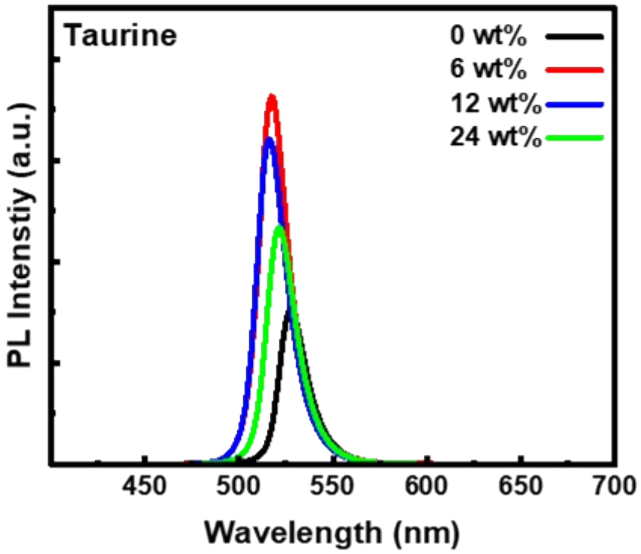

Fig. S4. PL spectra of taurine–$CsPbBr_3$ PQDs with different taurine contents (0, 6, 12, and 24 wt%).

Fig. S5. UV-vis absorption and PL spectra of rhodamine B in ethanol used for relative QY calculations.

Fig. S6. PL intensity gradient of rhodamine B solutions in ethanol for relative QY determination.

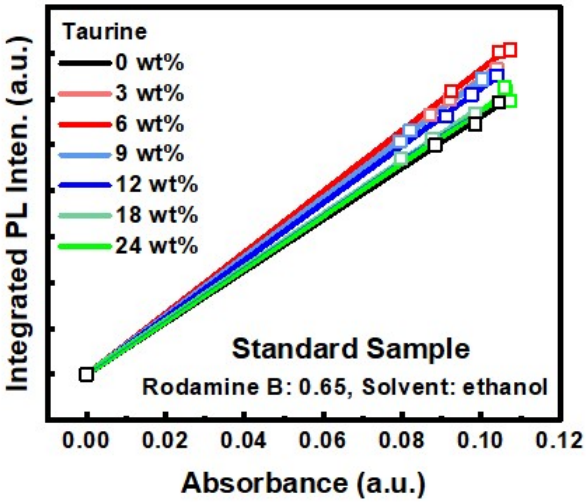

Fig. S7. Relative QY analysis used to optimize taurine concentration in $CsPbBr_3$ PQDs.

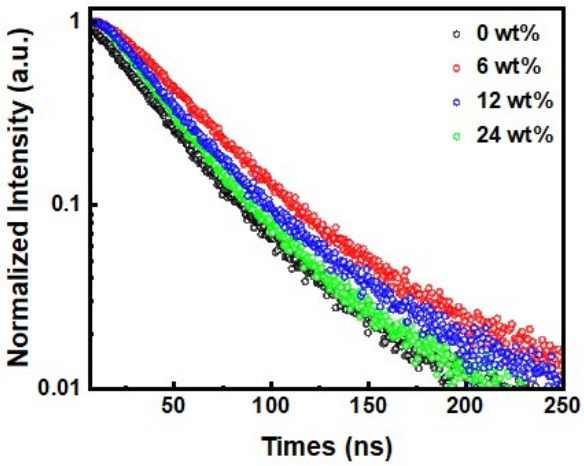

Fig. S8. Time-resolved photoluminescence (TRPL) decay curves of $CsPbBr_3$ PQDs with different taurine concentrations (0, 6, 12, and 24 wt%).

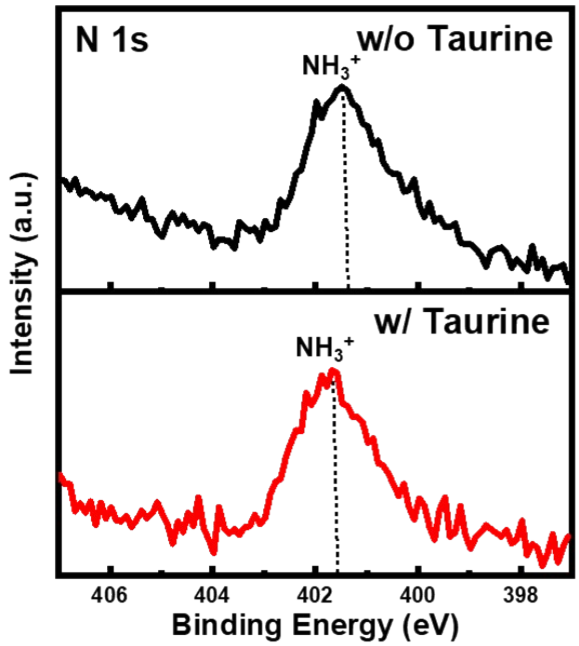

Fig. S9. XPS spectra of $CsPbBr_3$ PQDs with 0 and 6 wt% taurine of N 1s.

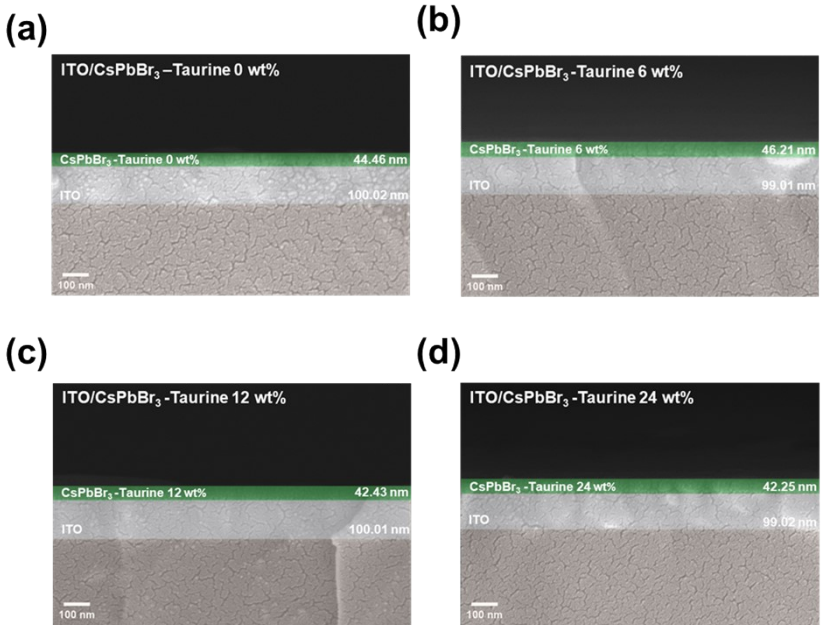

Fig. S10. FE-SEM cross-sectional images of taurine–$CsPbBr_3$ PQD films with varying taurine concentrations: (a) 0, (b) 6, (c) 12, and (d) 24 wt%.

Table S1. XRD diffraction peak positions (2θ, °) of $CsPbBr_3$ PQDs with different taurine concentrations corresponding to the (100), (110), (200), (211), and (220) lattice planes.

Taurine	Lattice Plane 2θ (°)				
	(100)	(110)	(200)	(211)	(220)
0 wt%	15.04	21.49	30.36	37.33	43.47
6 wt%	15.33	21.58	30.65	37.73	43.80
12 wt%	15.24	21.56	30.67	37.64	43.78
24 wt%	15.19	21.53	30.72	37.78	43.78

Table S2. PL peak position and FWHM of $CsPbBr_3$ PQDs with varying taurine concentrations.

Taurine	PL peak position (nm)	FWHM (nm)
0 wt%	527.6	19.98
6 wt%	517.3	17.27
12 wt%	516.6	18.59
24 wt%	521.2	20.03

Table S3. Parameters used for the relative QY calculation of rhodamine B.

Sample	Refractive index	Gradient (F/A)	Quantum yield
Rhodamine B	1.370	0.98×10^5	0.650

Table S4. Summary of QY calculation parameters for taurine concentration.

Taurine	Solvent	Refractive Index	Gradient (F/A)	Quantum Yield
0 wt%	Hexane	1.375	1.13×10^5	72.3%
3 wt%	Hexane	1.375	1.28×10^5	82.0%
6 wt%	Hexane	1.375	1.33×10^5	86.7%
9 wt%	Hexane	1.375	1.29×10^5	83.6%
12 wt%	Hexane	1.375	1.25×10^5	81.1%
18 wt%	Hexane	1.375	1.16×10^5	76.1%
24 wt%	Hexane	1.375	1.15×10^5	75.0%

Table S5. Surface energies of $CsPbBr_3$ PQDs films with varying taurine concentrations, determined using the Owens–Wendt method.

Taurine	γ^p [mJ/m^2]	γ^d [mJ/m^2]	γ [mJ/m^2]
0 wt%	11.82	43.98	55.79
6 wt%	8.89	42.08	50.97
12 wt%	11.56	42.95	54.50
24 wt%	11.98	43.09	55.07

Table S6. Summary of synthesis methods and optoelectronic properties of taurine-based and reported zwitterionic ligand based-$CsPbBr_3$ QDs.

Materials	**QY**	**Air stability**	**Water or polar stability**	**Trap density [# cm^{-3}]**	**Reference**
4-bromo-butyric acid (BBA)	86.4%	-	95.03% (DIW-after 60 h)	-	*Angew. Chem. Int. Ed.* **2022**, 61, e202116702
3-(N,N-dimethyloctadecyl ammonio) propane sulfonate (ASC 18)	92%	84.3% (after 24 h)	76% (ethanol-after 100 min)	-	*Chem.Eng. J.* **2024**, 498, 155515
zwitterionic sulfobetaine (ZSB)	70.2%	80% (after 400 h)	-	-	*Chem.Eng. J.* **2024**, 481, 148127
3-(decyldimethylammonio) propanesulfonate (DLPS)	98%	82% (after 240h)	-	2.03×10^{20}	*ACS Appl. Mater. Interfaces* 2024, 16, 10389−10397
Taurine	86.7%	71% (after 396 h)	92.8% (DIW-after 60 h)	5.21×10^{16}	**This work**

Reference

1. J. R. Martins, V. Krivenkov, C. R. Bernardo, P. Samokhvalov, I. Nabiev, Y. P. Rakovich and M. I. Vasilevskiy, Statistical Analysis of Photoluminescence Decay Kinetics in Quantum Dot Ensembles: Effects of Inorganic Shell Composition and Environment, J Phys Chem C, 2022, 126, 20480–20490.