

Supporting Information

Surface ligand engineering of pure-red perovskite nanocrystals with enhanced stability by diphenylammonium halide molecules

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Table S1. Resistivity and conductivity of the pristine, DPAI-, and DPABr-modified NC films.

Perovskite film	NC	Resistivity (ρ, $\Omega\cdot\text{cm}$)	Conductivity (σ, $\text{S}\cdot\text{cm}^{-1}$)
pristine		6.44×10^6	1.55×10^{-7}
DPAI-modified		3.26×10^5	3.07×10^{-6}
DPABr-modified		4.27×10^5	2.34×10^{-6}

The band gap of the $\text{CsPbBr}_x\text{I}_{3-x}$ NC films was determined using the Tauc plot method, as expressed in the following equation (1):

$$(\alpha h\nu)^{\frac{1}{n}} = B(h\nu - E_g) \quad (1)$$

where α is the absorption coefficient, $h\nu$ represents the photon energy, B is a proportionality constant, and E_g is the bandgap. The parameter n corresponds to the type of semiconductor; for the direct-gap $\text{CsPbBr}_x\text{I}_{3-x}$ NCs, $n = 1/2$.

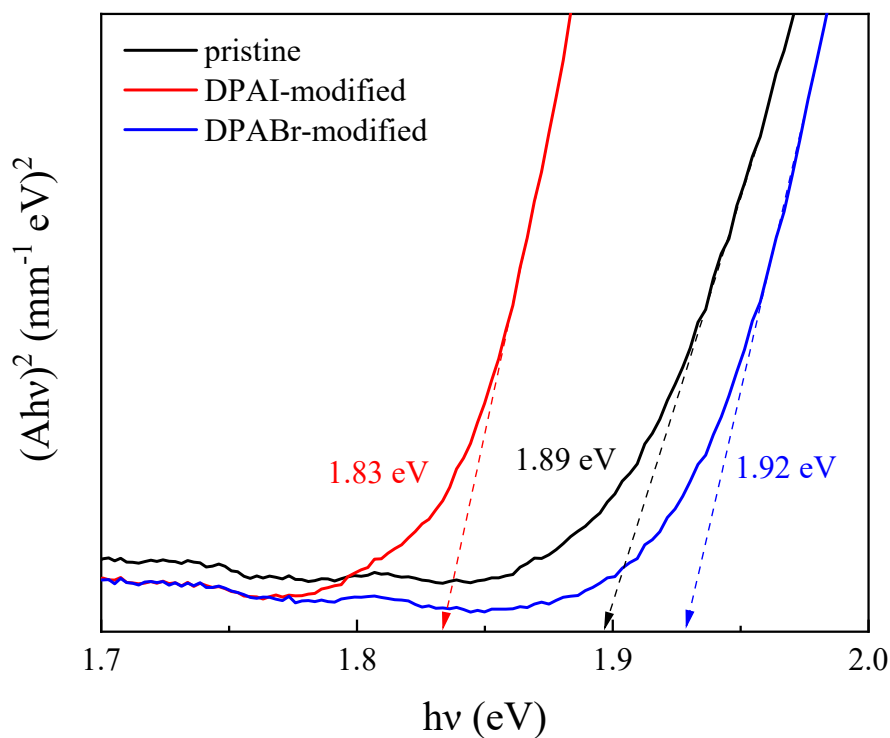


Fig. S1 Tauc plot of the pristine, DPAI-, and DPABr-modified NCs.

The PL decay curves of the CsPbBr_xI_{3-x} NC films were analyzed using a bi-exponential decay model, as described by the following equation (2):

$$f(t) = A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right) \quad (2)$$

where A_1 and A_2 are the amplitudes corresponding to the decay components with lifetimes τ_1 and τ_2 , respectively. The τ_{avg} was calculated using the weighted contribution of each component, as described by the following equation (3):

$$\tau_{\text{ave}} = \frac{A_1 \tau_1^2 + A_2 \tau_2^2}{A_1 \tau_1 + A_2 \tau_2} \quad (3)$$

Table S2. Carrier lifetime parameters of TR-PL decay curves of the pristine, DPAI-, and DPABr-modified NCs.

Sample	τ_1 (ns)	A_1 (%)	τ_2 (ns)	A_2 (%)	τ_{avg} (ns)
pristine	4.07	19.15	14.38	80.85	8.76
DPAI-modified	6.23	21.72	15.87	78.28	10.22
DPABr-modified	5.11	23.02	16.85	76.98	10.94

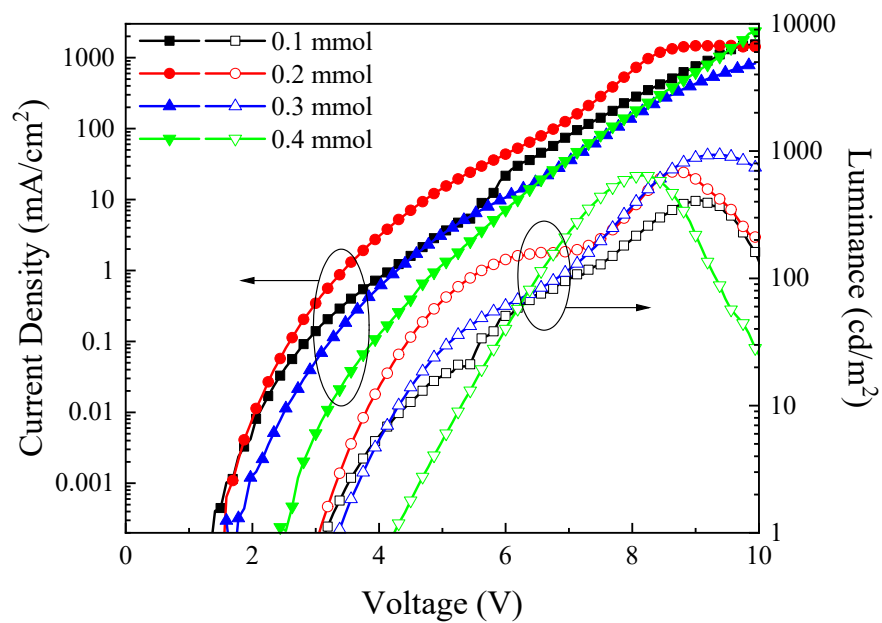


Fig. S2 J – V – L curves of DPAI-modified PeLEDs using different molar concentrations of DPAI from 0.1 to 0.4 mmol.

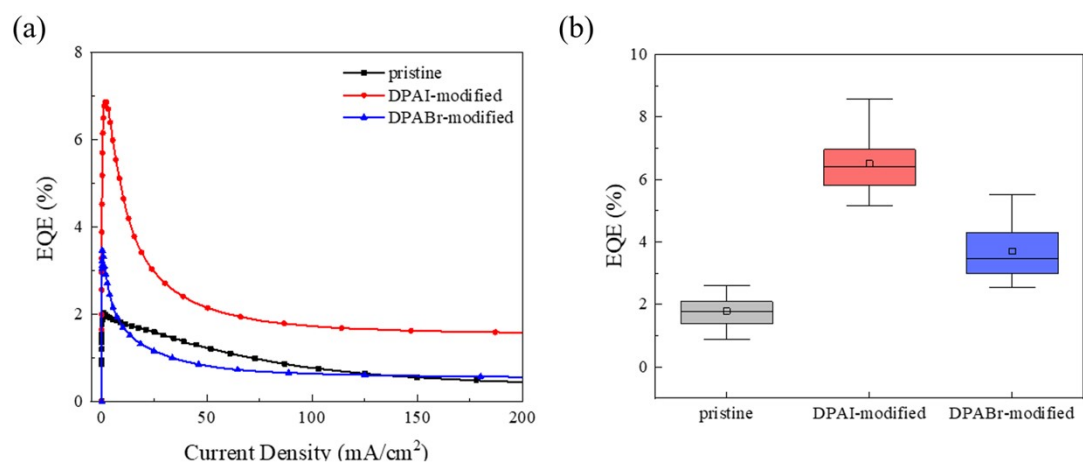


Fig. S3 (a) EQE– J curves and (b) EQE statistical distribution of the pristine, DPAI-, and DPABr-modified devices.

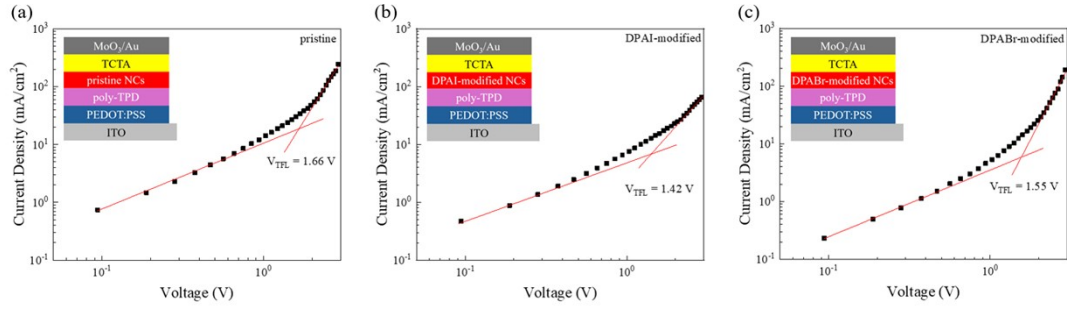


Fig. S4 SCLC characteristics for the (a) pristine, (b) DPAI-, and (c) DPABr-modified devices. The insets show the structure of the hole-only devices based on different perovskite NCs.

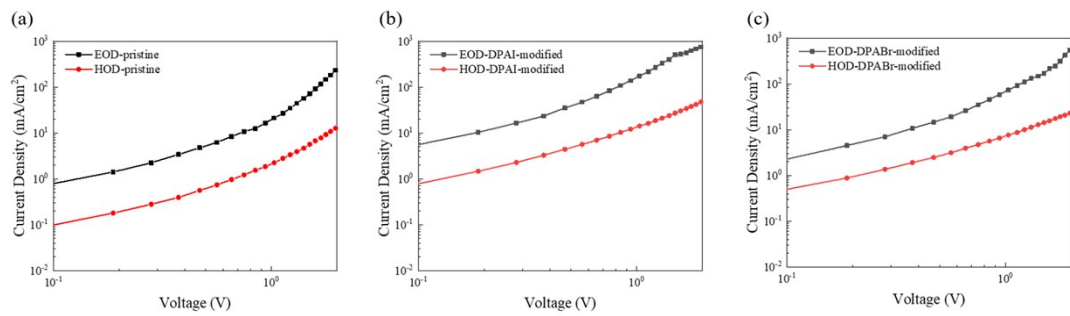


Fig. S5 J - V characteristics of the electron-only and hole-only devices based on the (a) pristine, (b) DPAI-, and (c) DPABr-modified NCs.

Table S3. An overview of the performance for red PeLEDs from previous literature and our work.

Year	perovskite	EL (nm)	$L_{\max}$ (cd/m ²)	EQE (%)	T_{50} stability	Refs.
2018	CsPbI ₃ with IDA	688	748	5.02	–	[1]
2018	CsPb(Br/I) ₃ with An-HI	645	794	14.1	180 min @ 100 cd/m ²	[2]
	CsPb(Br/I) ₃ with OAM-I	653	500	21.3	5 min @ 100 cd/m ²	
2020	CsPbBr _x I _{3-x} with TrDAI	637	255	6.36	540 s @ 4.1 V	[3]
2020	CsPbBr _x I _{3-x} with KBr	637	2,671	3.55	50 s @ 100 cd/m ²	[4]
2021	CsPbBr _x I _{3-x} with In ³⁺	639	423	11.2	–	[5]
2021	KI-exchanged CsPbI ₃	640	870	23	10 h @ 200 cd/m ²	[6]
2021	β-CsPbI ₃ with PMA	689	618	17.8	317 h @ 30 mA/cm ²	[7]
2022	CsPb(I _x Br _{1-x}) ₃	642	–	24.4	20 h @ 200 cd/m ²	[8]
2023	CsPb(Br/I) ₃ with benzenesulfonate	640	1510	23.5	97 min @ 100 cd/m ²	[9]
2023	CsPbI _{3-x} Br _x	637	2653	21.8	70 min @ 150 cd/m ²	[10]

2024	PEA ₂ Cs _{n-1} Pb _n (Br/I) _{3n+1} Br/I ratio = 0.38	668	3024	30.08	47.7 h @ 140 cd/m ²	[11]
	PEA ₂ Cs _{n-1} Pb _n (Br/I) _{3n+1} Br/I ratio = 0.60	656	2401	32.14	60 h @ 250 cd/m ²	
	PEA ₂ Cs _{n-1} Pb _n (Br/I) _{3n+1} Br/I ratio = 0.66	648	1231	29.04	43.7 h @ 270 cd/m ²	
2024	CsPbBr _x I _{3-x}	636	1621	21.2	240 min @ 130 cd/m ²	[12]
2024	CsPbI ₃ with TOP	685	906	21.23	40 min @ 100 cd/m ²	[13]
2025	CsPbBr _x I _{3-x} with DPAI	665	913	6.9	800 s @ 5 V	This work
	CsPbBr _x I _{3-x} with DPABr	654	562	3.5	488 s @ 5 V	

Table S4. Carrier mobility and μ_e/μ_h ratio of the pristine, DPAI-, and DPABr-modified electron-only and hole-only devices.

Sample	Electron Mobility (cm²/Vs)	Hole Mobility (cm²/Vs)	μ_e/μ_h Ratio
pristine	1.69×10^{-4}	2.95×10^{-5}	5.73
DPAI-modified	4.64×10^{-4}	1.25×10^{-4}	3.71
DPABr-modified	2.92×10^{-4}	5.96×10^{-5}	4.90

References

1. J. Pan, Y. Shang, J. Yin, M. De Bastiani, W. Peng, I. Dursun, L. Sinatra, A. M. El-Zohry, M. N. Hedhili, A.-H. Emwas, O. F. Mohammed, Z. Ning and O. M. Bakr, *J. Am. Chem. Soc.*, 2018, **140**, 562–565.
2. T. Chiba, Y. Hayashi, H. Ebe, K. Hoshi, J. Sato, S. Sato, Y.-J. Pu, S. Ohisa and J. Kido, *Nat. Photonics*, 2018, **12**, 681–687.
3. Y. S. Shin, Y. J. Yoon, K. T. Lee, W. Lee, H. S. Kim, J. W. Kim, H. Jang, M. Kim, D. S. Kim, G.-H. Kim and J. Y. Kim, *ACS Appl. Mater. Interfaces*, 2020, **12**, 31582–31590.
4. J.-N. Yang, Y. Song, J.-S. Yao, K.-H. Wang, J.-J. Wang, B.-S. Zhu, M.-M. Yao, S. U. Rahman, Y.-F. Lan, F.-J. Fan and H.-B. Yao, *J. Am. Chem. Soc.*, 2020, **142**, 2956–2967.
5. X. Zhou, J. Zhang, X. Tong, Y. Sun, H. Zhang, Y. Min and Y. Qian, *Adv. Opt. Mater.*, 2022, **10**, 2101517.
6. Y.-K. Wang, F. Yuan, Y. Dong, J.-Y. Li, A. Johnston, B. Chen, M. I. Saidaminov, C. Zhou, X. Zheng, Y. Hou, K. Bertens, H. Ebe, D. Ma, Z. Deng, S. Yuan, R. Chen, L. K. Sagar, J. Liu, J. Fan, P. Li, X. Li, Y. Gao, M.-K. Fung, Z.-H. Lu, O. M. Bakr and L.-S. Liao, *Angew. Chem. Int. Ed.*, 2021, **60**, 16164–16170.
7. H. Li, H. Lin, D. Ouyang, C. Yao, C. Li, J. Sun, Y. Song, Y. Wang, Y. Yan, Y. Wang, Q. Dong and W. C. H. Choy, *Adv. Mater.*, 2021, **33**, 2008820.
8. Y.-K. Wang, K. Singh, J.-Y. Li, Y. Dong, X.-Q. Wang, J. M. Pina, Y.-J. Yu, R. Sabatini, Y. Liu, D. Ma, J. Liu, Z. Liu, Y. Gao, O.

- Voznyy, W. Ma, M.-K. Fung, L.-S. Liao and E. H. Sargent, *Adv. Mater.*, 2022, **34**, 2200854.
9. J. Zhang, T. Zhang, Z. Ma, F. Yuan, X. Zhou, H. Wang, Z. Liu, J. Qing, H. Chen, X. Li, S. Su, J. Xie, Z. Shi, L. Hou and C. Shan, *Adv. Mater.*, 2023, **35**, 2209002.
 10. M. Xie, J. Guo, X. Zhang, C. Bi, X. Sun, H. Li, L. Zhang, D. Binks, G. Li, W. Zheng and J. Tian, *Adv. Funct. Mater.*, 2023, **33**, 2300116.
 11. S.-C. Feng, Y. Shen, X.-M. Hu, Z.-H. Su, K. Zhang, B.-F. Wang, L.-X. Cao, F.-M. Xie, H.-Z. Li, X. Gao, J.-X. Tang and Y.-Q. Li, *Adv. Mater.*, 2024, **36**, 2410255.
 12. H.-W. Duan, F. Zhao, S.-N. Li, J.-L. Pan, W.-S. Shen, S.-M. Li, Q. Zhang, Y.-K. Wang and L.-S. Liao, *Adv. Funct. Mater.*, 2024, **34**, 2310697.
 13. H. Cheng, Y. Zheng, Y. Lou, M. Sun, G. Zhang, H. Wang, T. Wu, Y. Bai and Y. Shao, *Adv. Electron. Mater.*, 2025, **11**, 2400334.