Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2023

Supporting Information

Pure Red CsPbBr_{0.96}I_{2.04}/SiO₂ Core/Shell Nanocrystals with

Simultaneous Efficient and High Stability for Mini-LEDs

Yixin Cai,^a Yang Yang,^a Haorui Dong,^a Tongtong Xuan, *^{acd} Xueyuan Tang, *^{ae} Rong-Jun Xie *^{abcd}

^aFujian Key Laboratory of Surface and Interface Engineering for High Performance Materials, College of Materials, Xiamen University, Xiamen 361005, P. R. China.

^bState Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen 361005, P. R. China.

^cShenzhen Research Institute of Xiamen University, Shenzhen 518000, P. R. China.

^dXiamen Key Laboratory of High Performance Metals and Materials, Xiamen University, Xiamen 361005, P. R. China.

^eKey Laboratory of High Performance Ceramics Fibers (Xiamen University), Ministry of Education, P. R. China.

*E-mail: <u>ttxuan@xmu.edu.cn</u> (T.T. Xuan), <u>xytang@xmu.edu.cn</u> (X.Y. Tang), <u>rjxie@xmu.edu.cn</u> (R.-J. Xie)



Figure S1. (a) XPS spectra of CsPbBr_{1.16}I_{1.84} NCs and CsPbBr_{0.96}I_{2.04}/SiO₂ NCs, (b)-(e) High-resolution XPS spectra of CsPbBr_{1.16}I_{1.84} NCs and CsPbBr_{0.96}I_{2.04}/SiO₂ NCs for Cs 3d, Pb 4f, I 3d and Br 3d.



Figure S2. Particle size distribution of (a) $CsPbBr_{1.16}I_{1.84}$ NCs and (b) $CsPbBr_{0.96}I_{2.04}/SiO_2$ NCs.

1	Emission peak (nm)	FWHM (nm)	A_1	$ au_1$ (ns)	A_2	$ au_2$ (ns)	$ au_{ m avg}$ (ns)
$CsPbBr_{1.16}I_{1.84}$	632	28	0.57	134.98	0.43	375.47	254.6
CsPbBr _{0.96} I _{2.04} /SiO ₂	631	27	0.37	372.32	0.63	1323.72	1158.9

 Table S1. Optical properties of the pure red NCs.



Figure S3. Photograph of NC films synthesized with different contents of APTES after aging under ambient conditions for several days.

50 µs	150 µs	250 µs	350 µs	450 µs
	· ·		+	
		<u> </u>	<u> </u>	

Figure S4. Diagram of the falling state of droplets at different times.

	Solvent	Surface tension (mN m ⁻¹)	Density (g cm ⁻³)	Viscosity (mPa s)	Contact angle ($^{\circ}$)	Z value
Ink-0	Dodecane	25.5	0.79	1.68	14.2	14.6
Ink-1	Toluene : Dodecane (V : V = 4:6)	27.1	0.83	1.21	13.2	17
Ink-2	Toluene : Dodecane (V : V = 4:6)	27.2	0.83	1.22	13.1	17

Table S2. Physical properties of the NC inks.

The Z value is an empirical formula used to evaluate the compatibility of ink with nozzle material and size, which can be expressed as the following formula:¹

$$Z = \frac{1}{Oh} = \frac{\sqrt{\gamma \rho a}}{\eta}$$

where γ is the surface tension (mN/m), ρ is the density (g/cm³), η is the viscosity (mPa·s), a is the nozzle diameter (µm), and Oh is the Ohnesorge number.



Figure S5. PL QY curves of Ink-1 and Ink-2 as a function of time under ambient conditions (25°C, 70-90% RH), and the inset shows photographs of these two inks.



Figure S6. EL spectra of the red-emitting Mini-LED prepared by using CsPbBr_{1.16}I_{1.84} NCs at different current densities from 1.67 A/cm² to 300 A/cm².

Perovskite	Method	PL Peak (nm)	FWHM (nm)	PLQY (%)	Stability	Ref.
CsPbI _{1.5} Br _{1.5} film	Hot Injection, Thermal Pressed	618	N.A.	N.A.	12 months in glovebox with Ar	2
CPBI-DMAPbX₃-OcAm NCs	Hot Injection, Post Treatment	640	N.A.	92	UV irradiation (20 μw/cm ²) for 48 hours, maintain the initial intensity of 90%, with a blueshift of 10 nm	3
KBr passivated CsPb(I _x Br ₁₋ x)3 NCs	Hot Injection, Post Treatment	N.A	N.A	95	a colloidal stability of 1 year in ambient conditions (25 °C and 40% humidity)	4
Silica-coated CPBI-Zn-K NCs	High- temperature Solid-state Reaction	631	N.A	64.5	maintain the initial intensity of 41% when heated from 303 K to 373 K	5
GAI passivated FA _x Cs _{1-x} Pb (I _y Br _{1-y}) ₃ film	In Situ	692	32	N.A	The half-lifetime of the GAI-modified PeLED was 563 min at an initial luminance of 1000 cd m ⁻²	6
Ni ²⁺ doping CsPbBrI ₂	Hot Injection	N.A	N.A	81.05	No phase separation occurred during 4 months of storage	7
KBr passivated CsPbI _{3-x} Br _x NCs	Hot Injection	641	N.A	> 90	UV irradiation (100 mw/cm ²) for 480 s, show a blueshift of 3 nm	8
This work	Hot Injection	630	27	~100	Ine nair-infetime of the CsPbBr _{0.96} I _{2.04} /SiO ₂ NC films under UV irradiation (150 mw/cm ²) was 445 min, the PLQY of which still maintained 89% of initial value after storage in air for 100 days	-

Table S3. Summary of optical properties and stability of red CsPb(Br/I)₃ NCs

Reference

- 1. S. Shi, W. Bai, T. Xuan, T. Zhou, G. Dong and R.-J. Xie, *Small Methods*, 2021, 5(3): 2000889.
- T. Zhang, L. Zhang, G. L. Zhu, D. L. Cui, Q. L. Wang, G. Lian, Z. K. Zheng and H. H. Yu, Advanced Materials Interfaces, 2022, 9, 10.
- F. X. Xu, D. J. Chen, D. C. Huang, K. Y. Xu, S. S. Liang, J. Hu, X. Y. Zhang, L. Liu, F. B. Xiong and H. M. Zhu, *Journal of Physical Chemistry Letters*, 2022, 13, 718-725.
- Y. K. Wang, K. Singh, J. Y. Li, Y. T. Dong, X. Q. Wang, J. M. Pina, Y. J. Yu, R. Sabatini, Y. Liu,
 D. X. Ma, J. Liu, Z. K. Liu, Y. Y. Gao, O. Voznyy, W. L. Ma, M. K. Fung, L. S. Liao and E. H. Sargent, *Advanced Materials*, 2022, **34**, 6.
- 5. S. Y. Tian, X. F. Zhou, C. H. Bi, X. J. Sun, M. Q. Zhang, S. X. Yang and J. J. Tian, *Advanced Optical Materials*, 2022, **10**, 8.
- Y. C. Ye, Y. Q. Li, Y. Tian, X. Y. Cai, Y. Shen, K. C. Shen, X. Y. Gao, F. Song, W. J. Wang and J. X. Tang, *Nanoscale*, 2021, 13, 340-348.
- S. P. Yang, H. W. Zhu, E. Z. Xu, J. C. Li, H. M. Yang, Y. Zhang, Z. F. Zhu and Y. Jiang, Nanotechnology, 2021, 32, 335601.
- 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, *Journal of the American Chemical Society*, 2020, 142, 2956-2967.