

Electronic Supporting Information

**Deep-Blue Narrow-Band Emissive Cesium Europium Bromide Perovskite**

**Nanocrystals with Record High Emission Efficiency for Wide-Color-Gamut Backlight**

**Displays**

Xu Li,<sup>a,†</sup> Bibo Lou,<sup>b,†</sup> Xu Chen,<sup>a,\*</sup> Meng Wang,<sup>a</sup> Huifang Jiang,<sup>a</sup> Shuailing Lin,<sup>a</sup> Zhuangzhuang Ma,<sup>a</sup> Mochen Jia,<sup>a</sup> Yanbing Han,<sup>a</sup> Yongtao Tian,<sup>a</sup> Di Wu,<sup>a</sup> Wen Xu,<sup>c</sup> Xinjian Li,<sup>a</sup> Chonggeng Ma<sup>b</sup> and Zhifeng Shi<sup>a\*</sup>

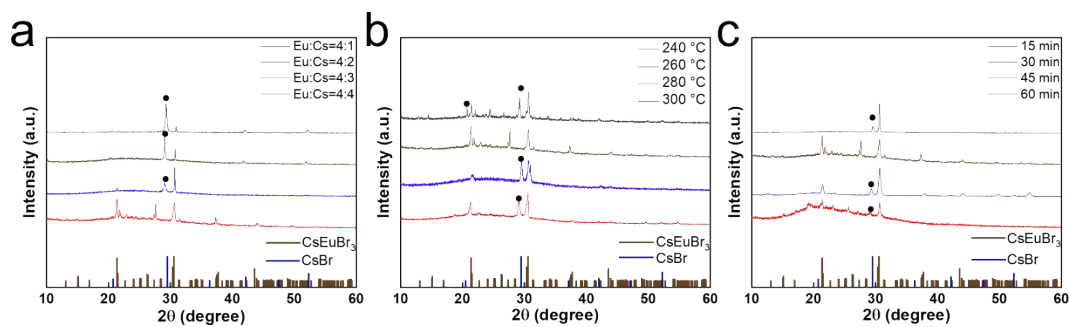
<sup>a</sup>Key Laboratory of Material Physics, Ministry of Education, School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450052, China.

<sup>b</sup> School of Optoelectronic Engineering & CQUPT-BUL Innovation Institute, Chongqing University of Posts and Telecommunications, Chongqing 400065, P.R. China.

<sup>c</sup>Key Laboratory of New Energy and Rare Earth Resource Utilization of State Ethnic Affairs Commission, School of Physics and Materials Engineering, Dalian Minzu University, Dalian 116600, China.

<sup>†</sup>These authors contributed equally: X.L. and B.L.

\*Corresponding author. E-mail: shizf@zzu.edu.cn; xchen@zzu.edu.cn



**Fig. S1** XRD results of CsEuBr<sub>3</sub> NCs synthesized under different conditions: (a) Addition ratio of Eu/Cs (45 min at 280 °C). (b) The reaction temperature for 45 min reaction time (Eu/Cs=4:1). (c) Reaction time at 280 °C (Eu/Cs=4:1).

In order to explore the synthesis conditions for obtaining pure phase CsEuBr<sub>3</sub> NCs, we characterized CsEuBr<sub>3</sub> NCs synthesized under different conditions using XRD. The results showed that the ratio of Eu/Cs was 4:1, and the XRD was pure phase after reacting at 280 °C for 45 min.

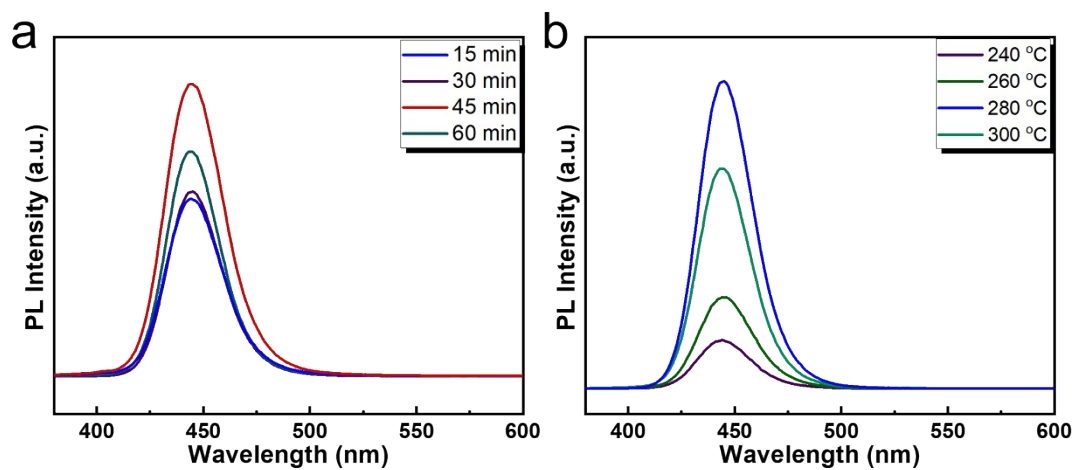


Fig. S2 (a) PL for different reaction time. (b) PL at the different reaction temperatures.

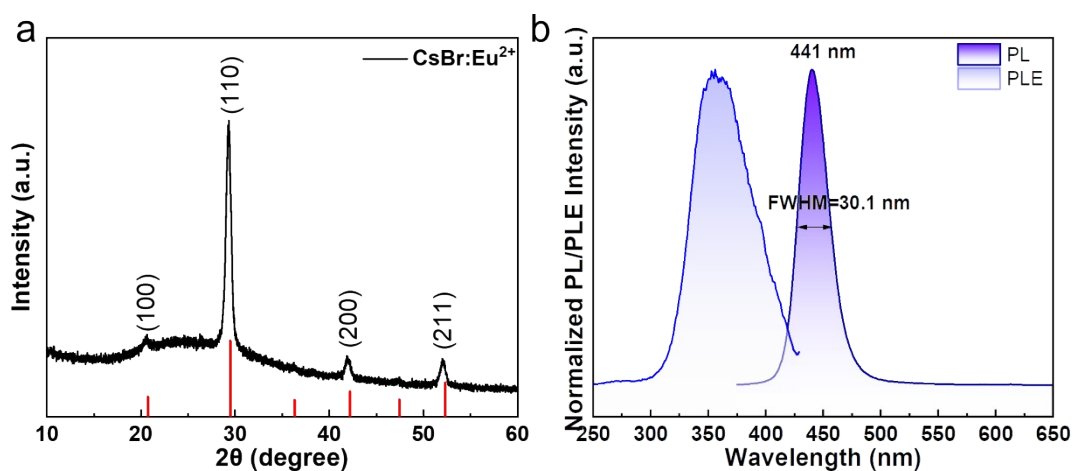
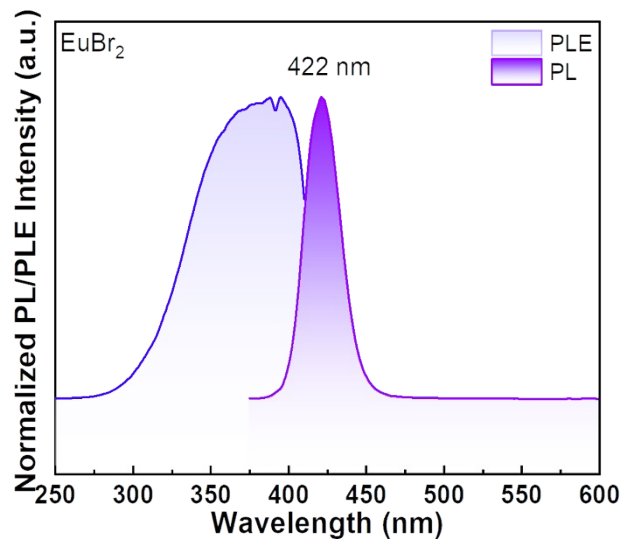


Fig. S3 (a) XRD, (b) PL and PLE of CsBr:Eu<sup>2+</sup> NCs.

The XRD pattern of CsBr:Eu<sup>2+</sup> NCs in Fig. S3a is consistent with the standard cards of CsBr (PDF# 061-071-495), and the PL spectrum of CsBr:Eu<sup>2+</sup> NCs with an emission peak at 441 nm in Fig. S3b.



**Fig. S4** PL and PLE of EuBr<sub>2</sub>.

The huge difference between EuBr<sub>2</sub> and CsEuBr<sub>3</sub> NCs can rule out the influence of EuBr<sub>2</sub> on luminescence.

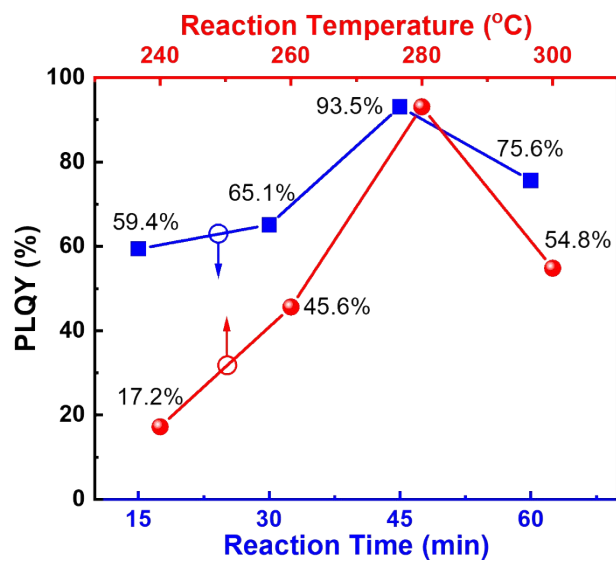
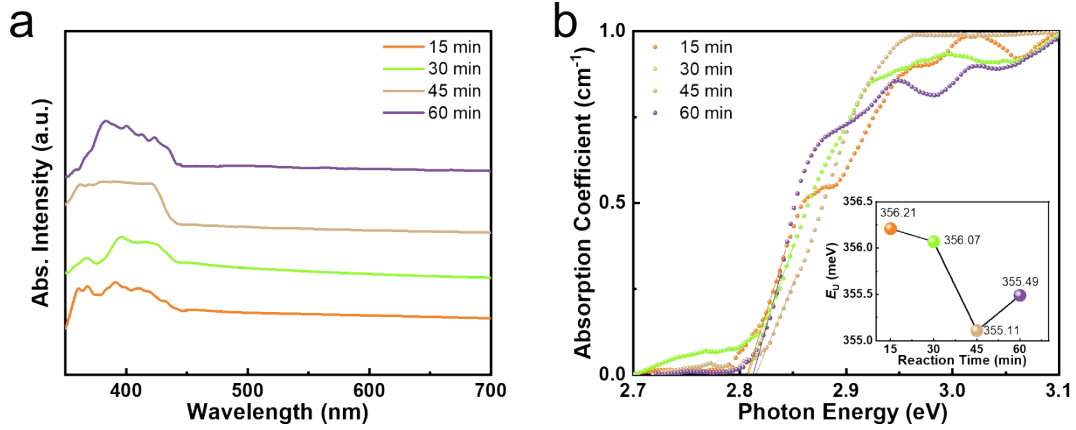


Fig. S5 PLQY variation of CsEuBr<sub>3</sub> NCs synthesized with varying conditions of the reaction

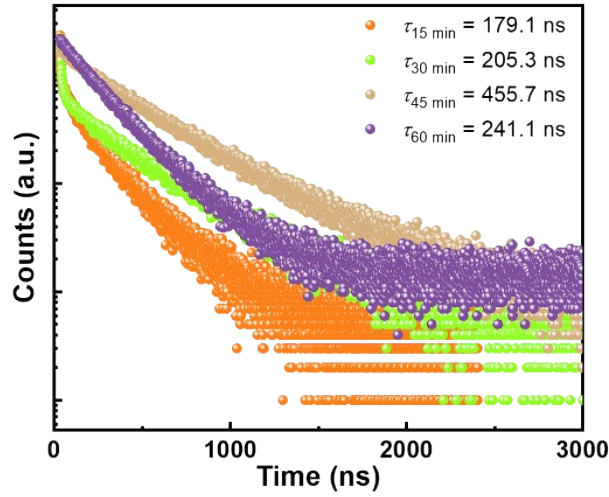


**Fig. S6** (a) UV-vis absorption spectra of the NCs prepared at 280 °C with various reaction times. (b) decay of CsEuBr<sub>3</sub> NCs for different reaction times. (c) Urbach energies in different reaction time.

The change in the Urbach energies ( $E_U$ ) is related to the change in defect density. The larger the  $E_U$ , the larger the density of defect states. According to the formula,

$$\alpha(E) = \alpha_0 \exp \left[ \sigma(T) \frac{E - E_0}{k_B T} \right] \quad \backslash * \text{MERGEFORMAT (1)}$$

where  $\alpha(E)$  is the absorption coefficient as a function of photon energy  $E$ ,  $E_0$ , and  $\alpha_0$  are the characteristic parameters of the material,  $\sigma(T)$  is the steepness factor,  $k_B$  is the Boltzmann constant, and  $T$  is the absolute temperature. The  $E_U$  is defined as  $E_U = k_B T / \sigma(T)$ . When the reaction time increases from 15 min to 45 min,  $E_U$  decreases from 356.21 to 355.11 meV. When the reaction time further increases to 60 min,  $E_U$  decreases to 355.49 meV. When the reaction time is 45 min, the corresponding  $E_U$  of CsEuBr<sub>3</sub> NCs is the smallest, indicating that the defects are the least at this time. The results are consistent with the PL, PLQY, and TRPL characterization. The results show that as the reaction time increases, the electron disorder and defect density in the NCs will increase, and the optimal reaction time is beneficial for reducing the defect density of CsEuBr<sub>3</sub> NCs.



**Fig. S7** TRPL of CsEuBr<sub>3</sub> NCs for different reaction times.

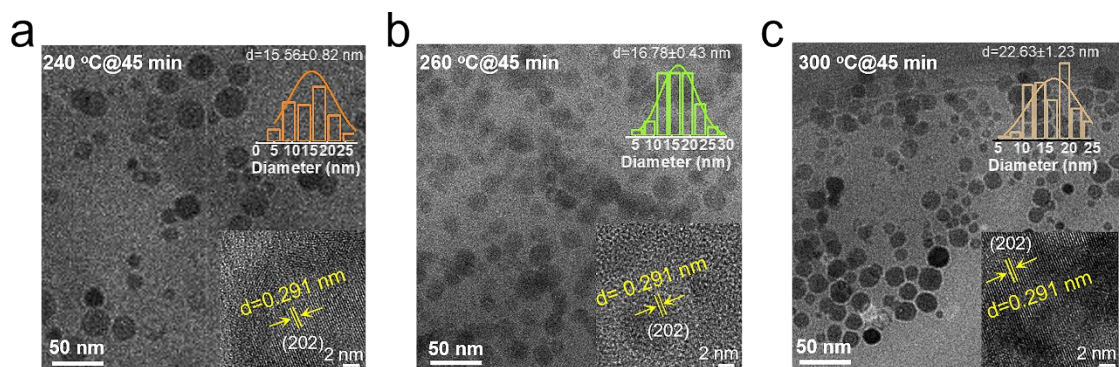
The TRPL curve was fitted using a double exponential decay curve:

$$y = A_1 \exp(-t / \tau_1) + A_2 \exp(-t / \tau_2) + I_0 \quad \backslash * \text{MERGEFORMAT (2)}$$

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

where  $\tau_1$  and  $\tau_2$  represent the fast and slow decay processes, associated with the lifetimes of de-trapping to defect states and radiative recombination, respectively.  $A_1$ ,  $A_2$ , and  $I_0$  are constants.  $\tau_{ave}$  represents the average PL lifetime.

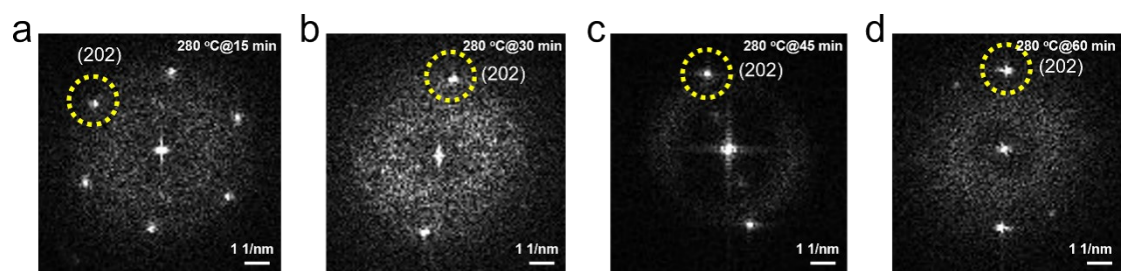
As the reaction time increases, the TRPL exhibits a trend of first increasing and then decreasing.  $\tau_{ave}$  was fitted using eq 2, and the results show that  $\tau_{ave}$  increases from 179.1 ns to 455.7 ns, indicating that CsEuBr<sub>3</sub> NCs at this reaction temperature have the lowest defect density. When the reaction time increases to 60 min, more organic ligands are replaced on the surface of NCs, resulting in the loss of a certain length of organic ligands as spacing. This promotes their fusion and defect density increase, leading to a loss of good photoelectronic performance.



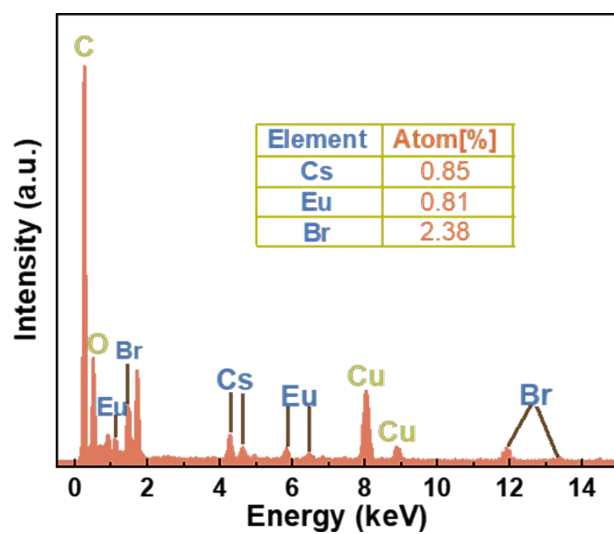
**Fig. S8** TEM images of CsEuBr<sub>3</sub> NCs synthesized by reaction at different temperatures:

(a) 240 °C; (b) 260 °C; (c) 300 °C.

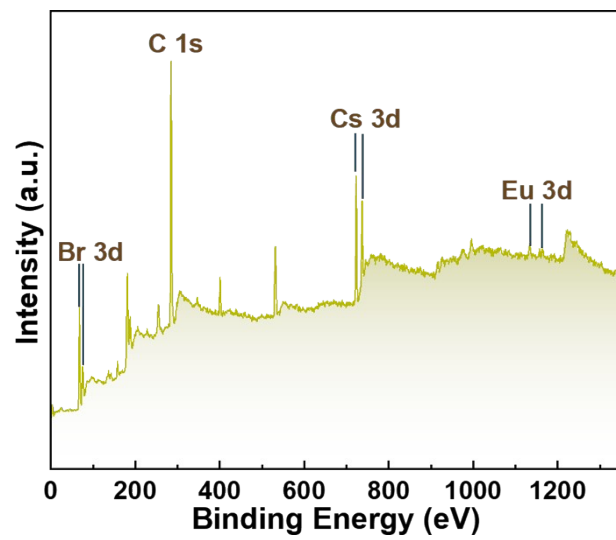




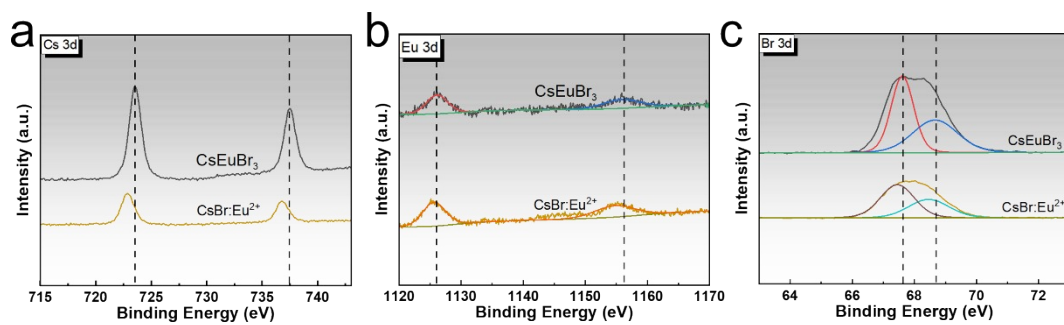
**Fig. S9** The FFT images shown correspond to the RHTM images of CsEuBr<sub>3</sub> NCs synthesized at 280 °C for different reaction time: (a) 15 min; (b) 30 min; (c) 45 min; (d) 60 min.



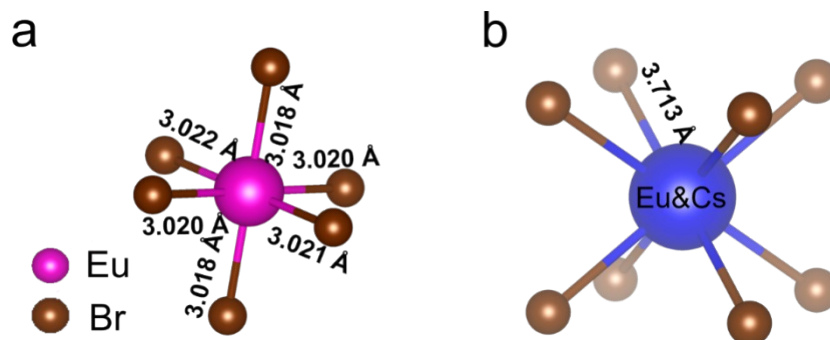
**Fig. S10** Energy dispersive spectroscopy (EDS) spectrum and the composition analysis of CsEuBr<sub>3</sub> NCs.



**Fig. S11** XPS spectrum of CsEuBr<sub>3</sub> NCs.



**Fig. S12** XPS spectra and the relevant results of different elements: (a) Cs 3d, (b) Eu 3d, (c) Br 3d of CsEuBr<sub>3</sub> NCs, and CsBr:Eu<sup>2+</sup>.

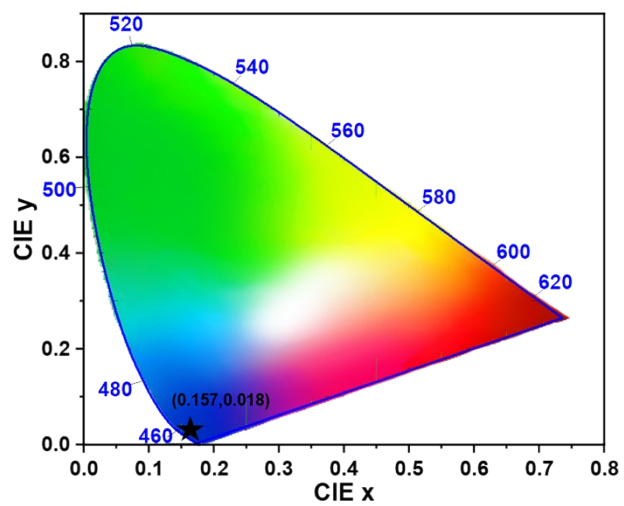


**Fig. S13** (a)  $[\text{EuBr}_6]^{4-}$  cluster octahedral structure. (b)  $[(\text{Eu}\&\text{Cs})\text{Br}_3]^{6-}$  cluster cubic structure.

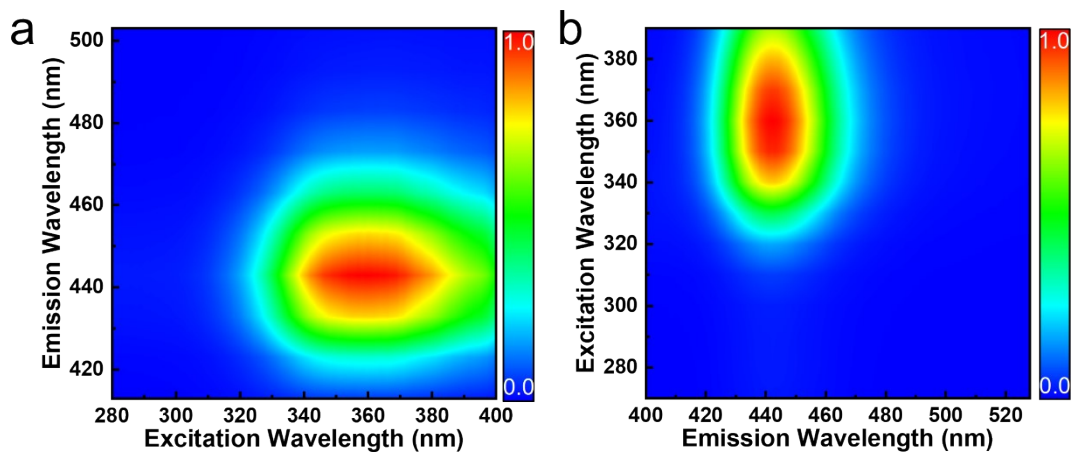
To distinguish the red-shift of the emission peaks of  $\text{CsEuBr}_3$  NCs compared to  $\text{CsBr:Eu}^{2+}$  NCs, we introduce a distorted lattice to explain the red shift of the emission spectrum of  $\text{CsEuBr}_3$ . The distortion index  $D$  can be expressed as,<sup>1</sup>

$$D = \frac{1}{n} \sum_{i=1}^n \frac{|d_i - d_{av}|}{d_{av}} \quad \backslash * \text{MERGEFORMAT (4)}$$

where  $n$  denotes the number of ligands,  $d_{av}$  denotes the average distance, and  $d_i$  denotes the distance between  $\text{Eu}^{2+}$  and the  $i$ -th ligand  $\text{Br}^-$ . The distortion index of  $\text{CsEuBr}_3$  is calculated as  $3.88 \times 10^{-4}$ , which is greater than the distortion index of  $\text{CsBr:Eu}^{2+}$ , resulting in a red shift of the emission peak of  $\text{CsEuBr}_3$  NCs.

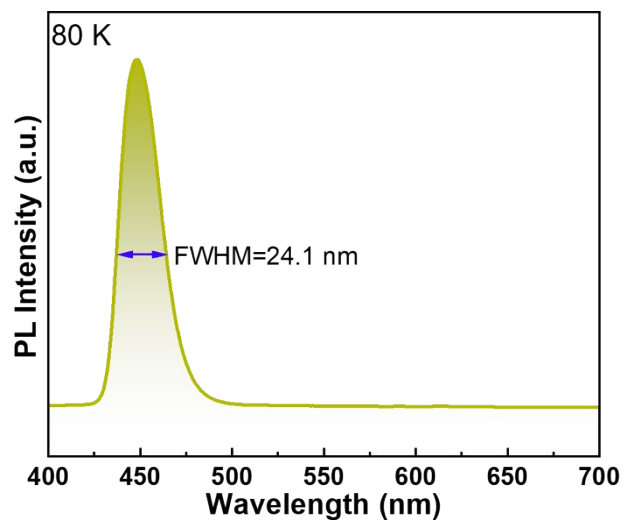


**Fig. S14** CsEuBr<sub>3</sub> NCs deep blue emission in CIE coordinates.



**Fig. S15** (a) Detection of emission spectra corresponding to different excitations. (b)

Detection of the excitation spectra corresponding to the different emissions.



**Fig. S16** FWHM of CsEuBr<sub>3</sub> NCs at 80 K.



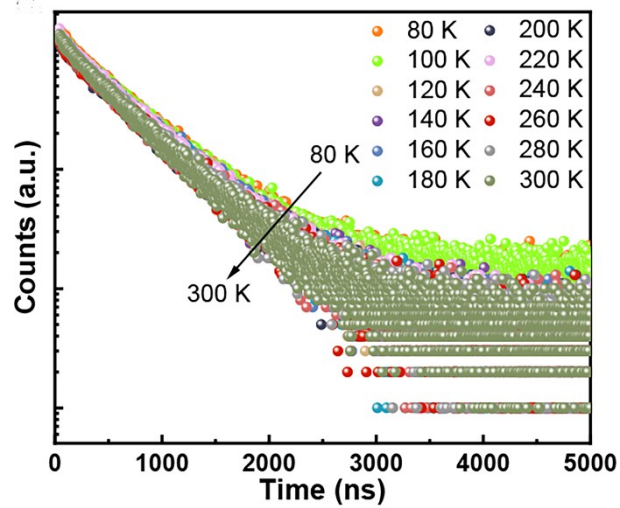
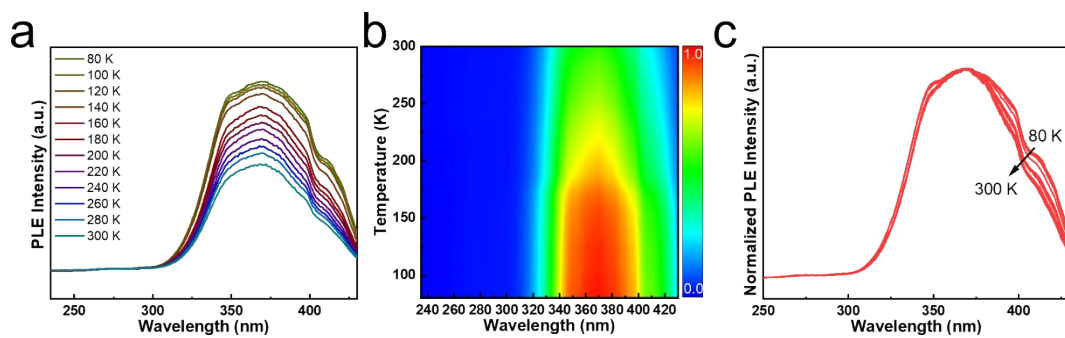
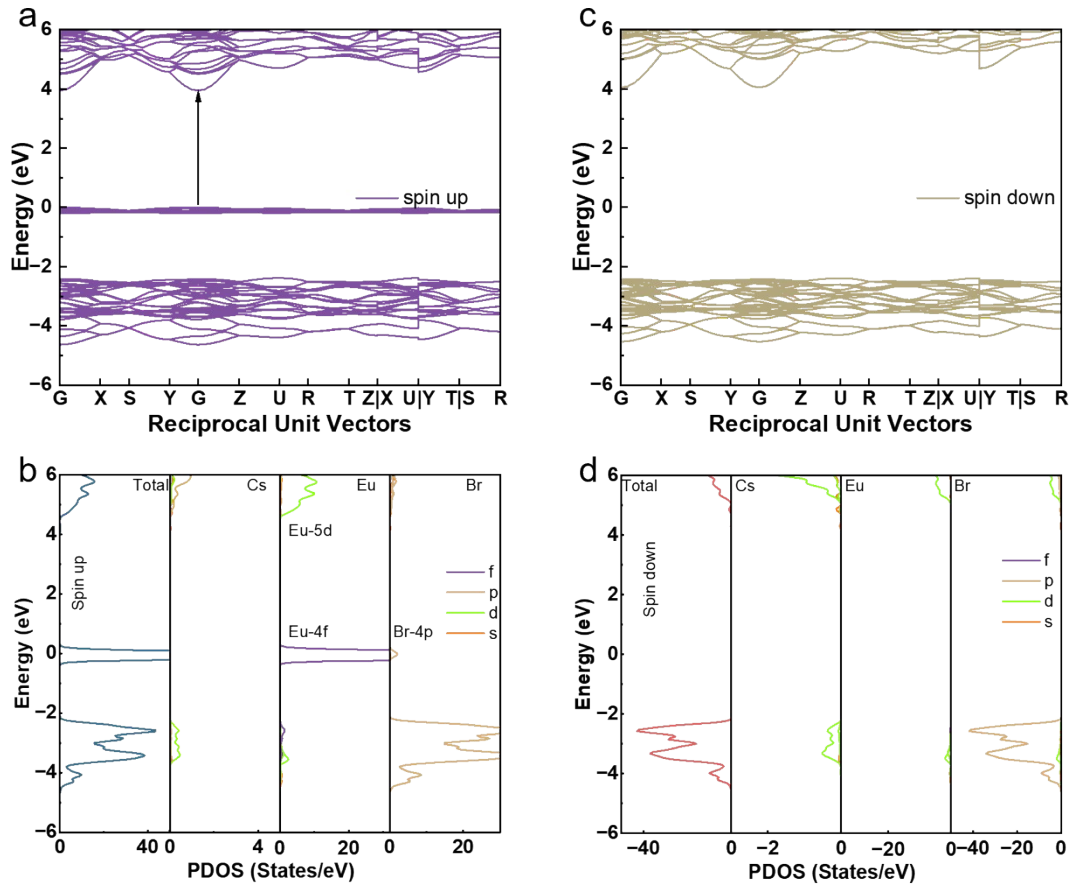


Fig. S17 TRPL decay curves of CsEuBr<sub>3</sub> NCs upon 340 nm excitation monitored at 443 nm from 80 to 300 K.

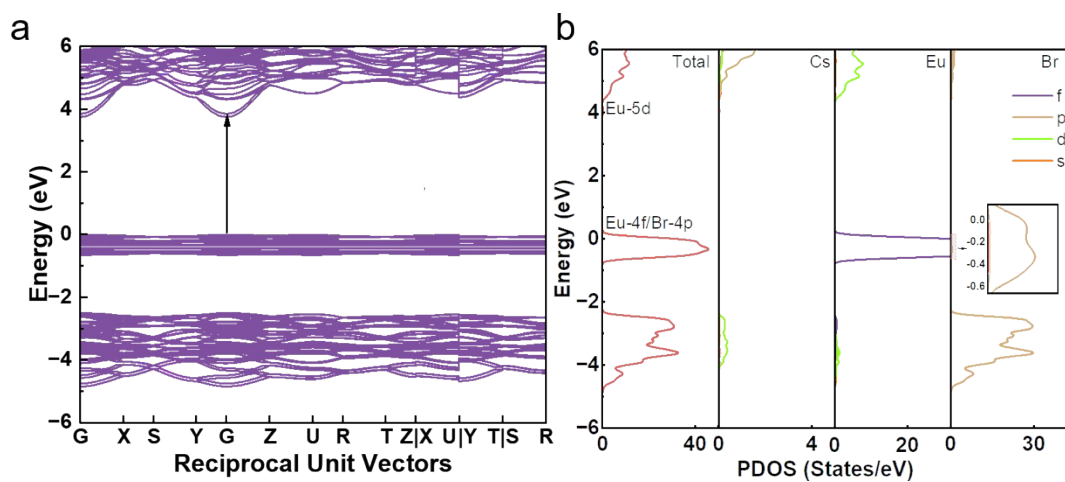
Fig. S17 shows a typical PL decay curve of CsEuBr<sub>3</sub> NCs monitored at 443 nm emission at 88-300 K. The results indicate that the PL lifetime of CsEuBr<sub>3</sub> at 80 K is longer than that at 300 K, which may be related to the thermally assisted escape route and temperature-dependent rapid non-radiative recombination.



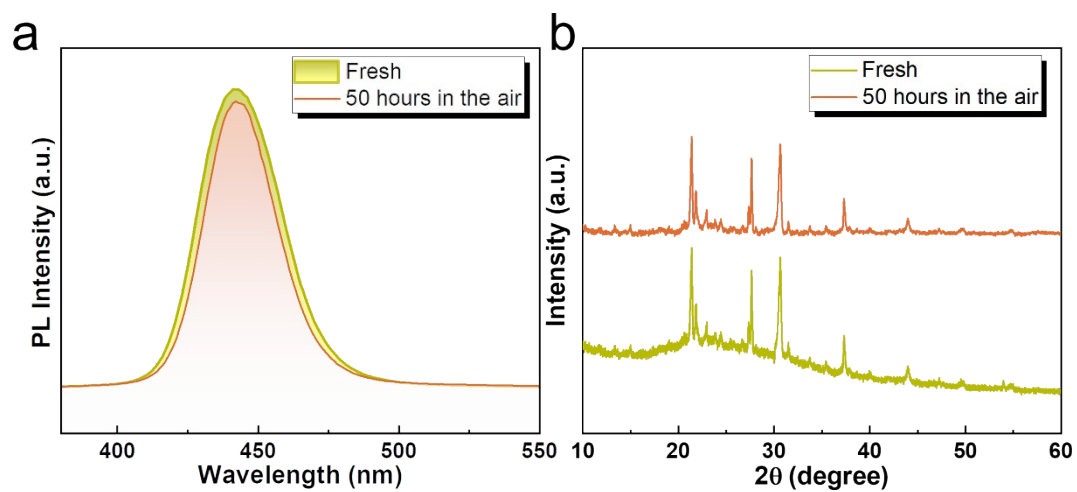
**Fig. S18** (a) Temperature-dependent PLE spectra of CsEuBr<sub>3</sub> NCs. (b) Pseudocolor map of temperature-dependent PLE spectra of the CsEuBr<sub>3</sub> NCs. (c) Normalized temperature-dependent PLE spectra of CsEuBr<sub>3</sub> NCs.



**Fig. S19** (a) The band structure and (b) PDOS of CsEuBr<sub>3</sub> hosts calculated with the PEBO functional with spin-up electrons, respectively. (c) The band structure and (d) PDOS of CsEuBr<sub>3</sub> hosts calculated with the PEBO functional with spin-down electrons, respectively.

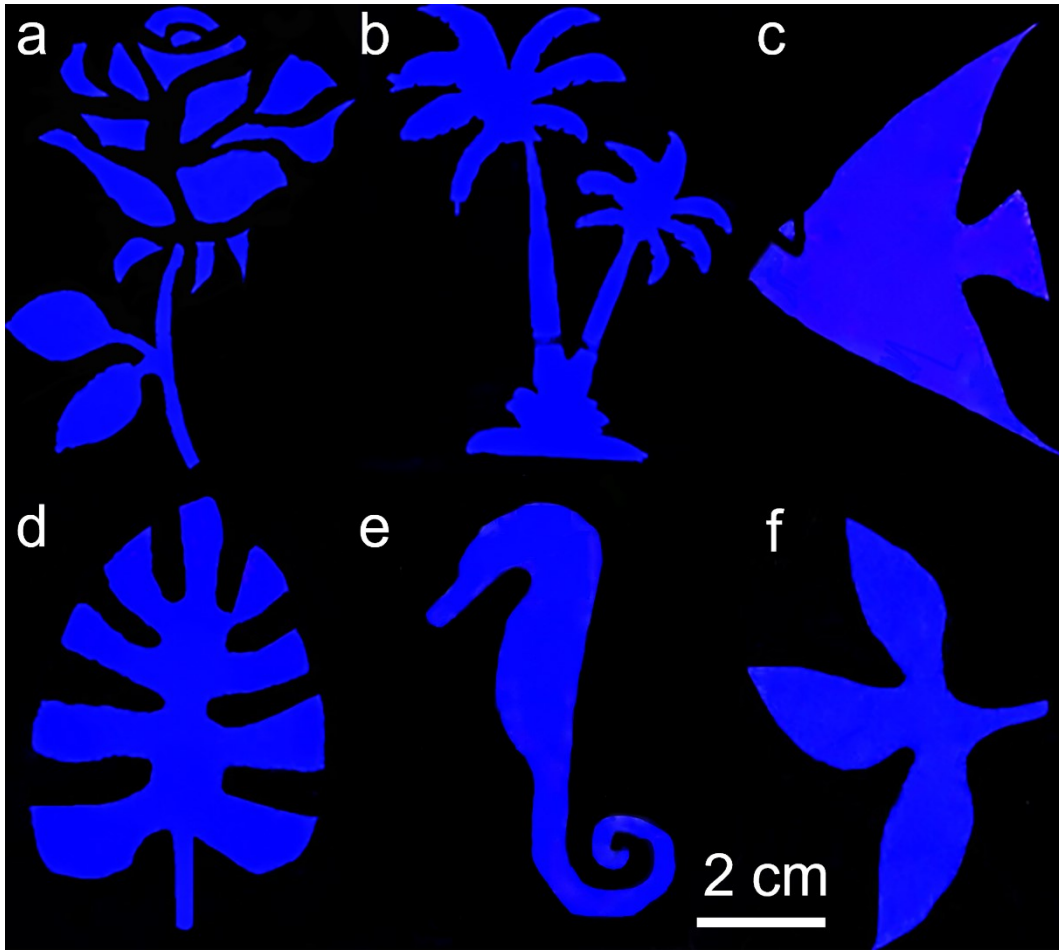


**Fig. S20** (a) The band structure and (b) PDOS of CsEuBr<sub>3</sub> hosts calculated with the PEB0+SOC functional, respectively.

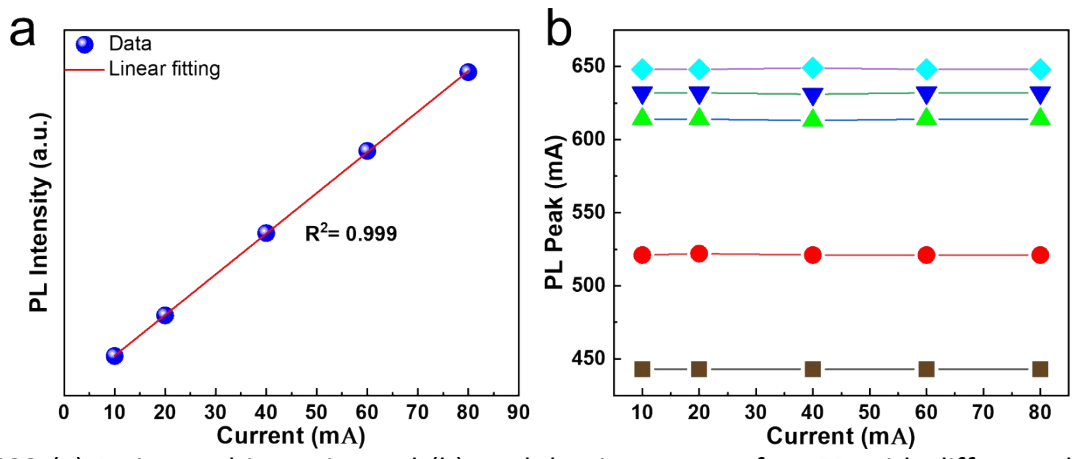


**Fig. S21** CsEuBr<sub>3</sub> NCs films placed in an air environment (25–30 °C, 20–30% humidity)

for 50 h of a) PL and b) XRD.



**Fig. S22** (a) “Rose”, (b) “coconut tree”, (c) “flounder”, (d) “turtle leaf”, (e) “seahorse”, and (f) “clover” patterns made with composite film ink print.



**Fig. S23** (a) PL integral intensity and (b) peak luminescence of WLED with different driving currents.

The PL intensity and drive current follow a linear relationship equation:

$$y = ax + b \quad \backslash * \text{MERGEFORMAT (6)}$$

$x$  is the drive current,  $a$  and  $b$  are constants.

**Table S1** Summary of different experimental conditions.

Experiment number	Reaction temperature	Reaction time	Eu to Cs molar feed ratio
1	280 °C	45 min	4:1
2	280 °C	45 min	4:2
3	280 °C	45 min	4:3
4	280 °C	45 min	4:4
5	240 °C	45 min	4:1
6	260 °C	45 min	4:1
7	280 °C	45 min	4:1
8	300 °C	45 min	4:1
9	280 °C	15 min	4:1
10	280 °C	30 min	4:1
11	280 °C	45 min	4:1
12	280 °C	60 min	4:1



**Table S2** Comparison of the properties of CsEuBr<sub>3</sub> NCs with lead-based perovskites.

Fluorescent materials	Emission peak (nm)	PLQY (%)	exciton lifetime (ns)	Huang-Rhys factor	Ref.
CsPbCl <sub>3</sub> NCs	460	80	–	–	2
CsPbBr <sub>3</sub> NCs	454	70	–	–	3
CsPb(Br <sub>x</sub> Cl <sub>1-x</sub> ) <sub>3</sub> NCs	488	82.19	32.9	–	4
CsPbBr <sub>2</sub> Cl NCs	475	37.2	13.21	–	5
CsPbBr <sub>3</sub> NCs	459	90	3.84	–	6
CsPb(Br <sub>x</sub> Cl <sub>1-x</sub> ) <sub>3</sub> NCs	488	82.19	5.27	–	7
CsPb(Br <sub>x</sub> Cl <sub>1-x</sub> ) <sub>3</sub> NCs	488	95	21.08	–	8
CsPbBr <sub>3</sub> NCs	–	–	–	0.38	10
CsPbBr <sub>3</sub> NCs	–	–	–	0.38	11
CsEuBr <sub>3</sub> NCs	443	93.51	455.8	1.54	This work

**Table S3** Comparison of the mobility and exciton activation energy of CsEuBr<sub>3</sub> NCs with lead-based perovskites.

Fluorescent materials	hole mobility (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	electron mobility (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	exciton binding energy (meV)	Ref.
CsPb(Br <sub>x</sub> /Cl <sub>1-x</sub> ) <sub>3</sub> NCs	1.06×10 <sup>-9</sup>	1.74×10 <sup>-10</sup>		8
CsPbI <sub>3</sub> NCs	2.03×10 <sup>-2</sup>	1.87×10 <sup>-2</sup>		9
FAPbBr <sub>3</sub> NCs	8.91 × 10 <sup>-9</sup>	5.67 × 10 <sup>-8</sup>		12
CsPbBr <sub>3</sub> NCs	2.43×10 <sup>-3</sup>			13
CsPbI <sub>3</sub> NCs	2.3×10 <sup>-1</sup>	5×10 <sup>-1</sup>		14
CsPbBr <sub>3</sub> NCs			47	15
CsPb(Br <sub>0.75</sub> Cl <sub>0.25</sub> ) <sub>3</sub> NCs			50.44	16
FAPbBr <sub>3</sub> NCs			57.55	17
CsPbBr <sub>3</sub> NCs			43.7	18
CsPbBr <sub>3</sub> NCs			38	19
CsPbBr <sub>3</sub> NCs			40	20
CsPbBr <sub>3</sub> NCs			40	21
CsEuBr <sub>3</sub> NCs	3×10 <sup>-1</sup>	5.0	49.69	This work

In terms of mobility parameters, Luo. et al. calculated the hole and electron mobilities of CsEuBr<sub>3</sub> to be 0.30 and 5.0 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>,<sup>22</sup> higher than those of the currently reported lead-based perovskite NCs. The exciton binding energy of CsEuBr<sub>3</sub> NCs is 49.69 meV, similar to lead-based perovskites NCs. Moderate exciton binding energy creates better conditions for carrier transport and exciton coincidence.

**Table S4** The color gamut of WLEDs.

Fluorescent materials	Color gamut (% NTSC in CIE 1931)	Ref.
CsPbX <sub>3</sub>	103	23
A <sub>2</sub> NaScF <sub>6</sub> (A = K, Rb, Cs):Mn <sup>4+</sup>	108.4	24
CsPbBr <sub>3</sub> :Sr/PbBr(OH)/molecular	124	25
CsPbX <sub>3</sub> @glass	127	26
Cs <sub>3</sub> MnBr <sub>5</sub>	104	27
Cs <sub>4</sub> PbBr <sub>6</sub>	121.3	28
CsPb(Br/I) <sub>3</sub>	126	29
h-BN@(PMA) <sub>2</sub> MA <sub>n-1</sub> PbnBr <sub>3n+1</sub>	106.1	30
CsEuBr <sub>3</sub> NCs	127.1	This work

## Notes and references

- 1 M. Liao, F. Wu, J. Wang, D. Zhu, X. Zhang, H. Dong, Z. Lin, M. Wen and Z. Mu, *ACS Appl. Mater. Interfaces*, 2022, **14**, 47892
- 2 B.-B. Zhang, S. Yuan, J.-P. Ma, Y. Zhou, J. Hou, X. Chen, W. Zheng, H. Shen, X.-C. Wang, B. Sun, O. M. Bakr, L.-S. Liao and H.-T. Sun, *J. Am. Chem. Soc.*, 2019, **141**, 15423.
- 3 Y. S. Shin, Y. J. Yoon, K. T. Lee, J. Jeong, S. Y. Park, G.-H. Kim and J. Y. Kim, *ACS Appl. Mater. Interfaces*, 2019, **11**, 23401.
- 4 S. Zhang, H. Liu, X. Li and S. Wang, *Nano Energy*, 2020, **77**, 105302.
- 5 W. H. Jeong, Z. Yu, L. Gregori, J. Yang, S. R. Ha, J. W. Jang, H. Song, J. H. Park, E. D. Jung, M. H. Song, S. H. Park, H. J. Snaith, A. Boretti, F. De Angelis, D. Meggiolaro, J. Lee, H. Choi and B. R. Lee, *J. Mater. Chem. A*, 2021, **9**, 26750.
- 6 Y. Xie, B. Peng, I. Bravić, Y. Yu, Y. Dong, R. Liang, Q. Ou, B. Monserrat and S. Zhang, *Adv. Sci.*, 2020, **7**, 2001698.
- 7 G. H. Ahmed, J. K. El-Demellawi, J. Yin, J. Pan, D. B. Velusamy, M. N. Hedhili, E. Alarousu, O. M. Bakr, H. N. Alshareef and O. F. Mohammed, *ACS Energy Lett.*, 2018, **3**, 2301.
- 8 H. Zhu, G. Tong, J. Li, E. Xu, X. Tao, Y. Sheng, J. Tang and Y. Jiang, *Adv. Mater.*, 2022, **34**, 2205092.
- 9 F. Zhao, H. Duan, S. Li, J. Pan, W. Shen, S. Li, Q. Zhang, Y. Wang and L. Liao, *Angew. Chem. Int. Ed.*, 2023, **62**, e202311089.
- 10 Lao. X, Yang. Z, Su. Z, Bao. Y, Zhang. J, Wang. X, Cui. X, Wang. M, Yao. X and Xu. S *J. Phys. Chem. C*, 2019, **123**, 5128.
- 11 C. M. Iaru, J. J. Geuchies, P. M. Koenraad, D. Vanmaekelbergh and A. Y. Silov, *ACS Nano*, 2017, **11**, 11024.
- 12 H. Chen, L. Fan, R. Zhang, C. Bao, H. Zhao, W. Xiang, W. Liu, G. Niu, R. Guo, L. Zhang and L. Wang, *Adv. Opt. Mater.*, 2020, **8**, 1901390.
- 13 Y. Gao, Y. Liu, F. Zhang, X. Bao, Z. Xu, X. Bai, M. Lu, Y. Wu, Z. Wu, Y. Zhang, Q. Wang, X. Gao, Y. Wang, Z. Shi, J. Hu, W. W. Yu and Y. Zhang, *Adv. Mater.*, 2022, **34**, 2207445.
- 14 E. M. Sanehira, A. R. Marshall, J. A. Christians, S. P. Harvey, P. N. Ciesielski, L. M. Wheeler, P. Schulz, L. Y. Lin, M. C. Beard and J. M. Luther, *Sci. Adv.*, 2017, **3**, eaao4204.
- 15 B. T. Diroll, H. Zhou and R. D. Schaller, *Adv. Funct. Mater.*, 2018, **28**, 1800945.
- 16 H. M. Ghaithan, S. M. H. Qaid, Z. A. Alahmed, M. Hezam, A. Lyras, M. Amer and A. S. Aldwayyan, *J. Phys. Chem. C*, 2021, **125**, 886.

- 17 D. Han, M. Imran, M. Zhang, S. Chang, X. Wu, X. Zhang, J. Tang, M. Wang, S. Ali, X. Li, G. Yu, J. Han, L. Wang, B. Zou and H. Zhong, *ACS Nano*, 2018, **12**, 8808.
- 18 Z. Shi, Y. Li, Y. Zhang, Y. Chen, X. Li, D. Wu, T. Xu, C. Shan and G. Du, *Nano Lett.*, 2017, **17**, 313.
- 19 Q. Zhang, R. Su, X. Liu, J. Xing, T. C. Sum and Q. Xiong, *Adv. Funct. Mater.*, 2016, **26**, 6238.
- 20 X. Li, Y. Wu, S. Zhang, B. Cai, Y. Gu, J. Song and H. Zeng, *Adv. Funct. Mater.*, 2016, **26**, 2435.
- 21 B. Ai, C. Liu, Z. Deng, J. Wang, J. Han and X. Zhao, *Phys. Chem. Chem. Phys.*, 2017, **19**, 17349.
- 22 J. Luo, L. Yang, Z. Tan, W. Xie, Q. Sun, J. Li, P. Du, Q. Xiao, L. Wang, X. Zhao, G. Niu, L. Gao, S. Jin and J. Tang, *Adv. Mater.*, 2021, **33**, 2101903.
- 23 J. Lin, Y. Lu, X. Li, F. Huang, C. Yang, M. Liu, N. Jiang and D. Chen, *ACS Energy Lett.*, 2021, **6**, 519.
- 24 Y. Y. Zhou, E. H. Song, M. G. Brik, Y. J. Wang, T. Hu, Z. G. Xia and Q. Y. Zhang, *J. Mater. Chem. C*, 2019, **7**, 9203.
- 25 T. Xuan, S. Guo, W. Bai, T. Zhou, L. Wang, R.-J. Xie, *Nano Energy*, 2022, **95**, 107003.
- 26 S. Chen, J. Lin, S. Zheng, Y. Zheng and D. Chen, *Adv. Funct. Mater.*, 2023, **33**, 2213442.
- 27 B. Su, M. S. Molokeev and Z. Xia, *J. Mater. Chem. C*, 2019, **7**, 11220.
- 28 X. Chen, F. Zhang, Y. Ge, L. Shi, S. Huang, J. Tang, Z. Lv, L. Zhang, B. Zou and H. Zhong, *Adv. Funct. Mater.*, 2018, **28**, 1706567.
- 29 Q. Wang, Y. Tong, M. Yang, H. Ye, X. Liang, X. Wang and W. Xiang, *J. Mater. Sci. Technol.*, 2022, **121**, 140.
- 30 G. Zhou, Y. Xu and Z. Xia, *ACS Appl. Mater. Interfaces*, 2020, **12**, 27386.