

COMMUNICATION

## Electronic Supplementary Information

### High-Efficiency Perovskite Nanocrystal Light-Emitting Diodes via Decorating NiO<sub>x</sub> on Nanocrystals Surface

Weilin Zheng,<sup>‡</sup><sup>a</sup> Qun Wan,<sup>‡</sup><sup>a</sup> Qinggang Zhang,<sup>a</sup> Mingming Liu,<sup>a</sup> Congyang Zhang,<sup>a</sup> Bo Wang,<sup>a</sup> Long Kong,<sup>a</sup> Liang Li,<sup>\*,a</sup>

a. School of Environmental Science and Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China.

b. Shanghai Institute of Pollution Control and Ecological Security, Shanghai 200092, China.

E-mail addresses: liangli117@sjtu.edu.cn

<sup>‡</sup> These authors contributed equally to this work.

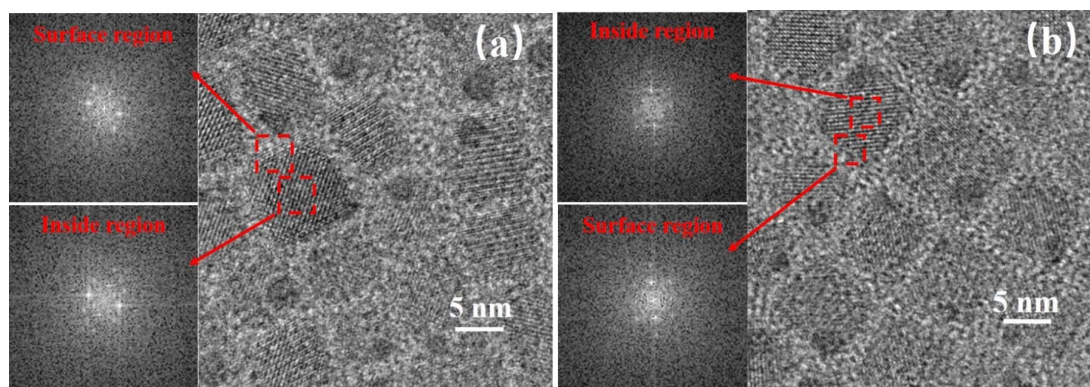


Figure S1 HRTEM images of (a) CsPbBr<sub>3</sub>-DDAB and (b) CsPbBr<sub>3</sub>-DDAB-Ni NCs.

Table S1 Interplanar spacing of CsPbBr<sub>3</sub>-DDAB and CsPbBr<sub>3</sub>-DDAB-Ni NCs

Pe-QDs		Interplanar spacing (110)	Interplanar spacing (001)
CsPbBr <sub>3</sub> -DDAB	Inside	3.94 Å	5.87 Å
	Surface	3.92 Å	5.85 Å
CsPbBr <sub>3</sub> -DDAB-Ni	Inside	3.92 Å	5.89 Å
	Surface	4.16 Å	5.91 Å

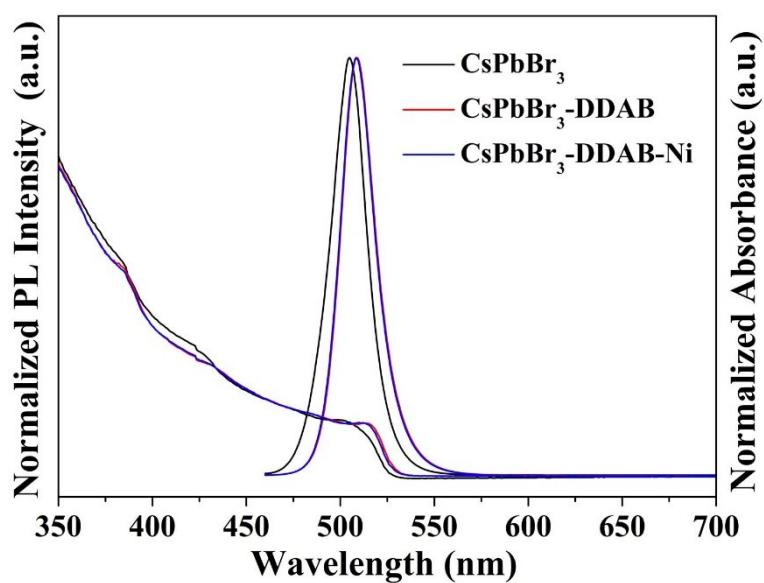


Figure S2 PL (absorbance is 0.5 at 450 nm) and UV-vis absorption spectra of CsPbBr<sub>3</sub>, CsPbBr<sub>3</sub>-DDAB, and CsPbBr<sub>3</sub>-DDAB-Ni NCs.

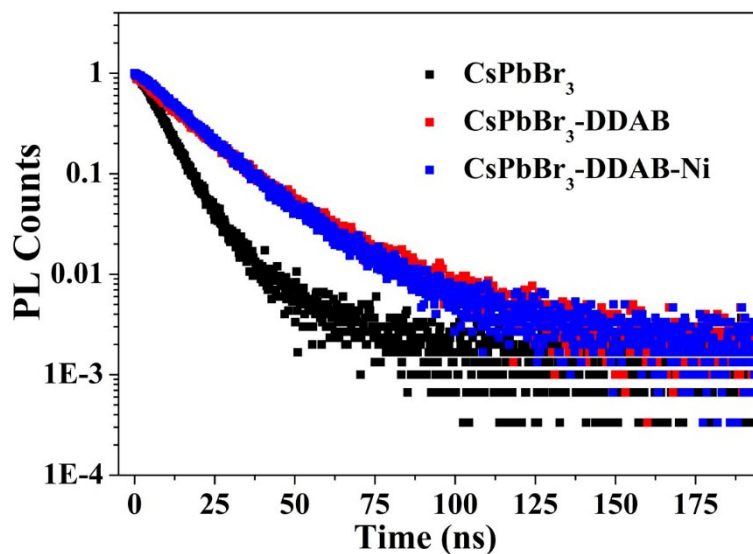


Figure S3 Time-resolved PL decays and the fitted curves for the CsPbBr<sub>3</sub>, CsPbBr<sub>3</sub>-DDAB, and CsPbBr<sub>3</sub>-DDAB-Ni NCs solutions detected with excitation of 450 nm.

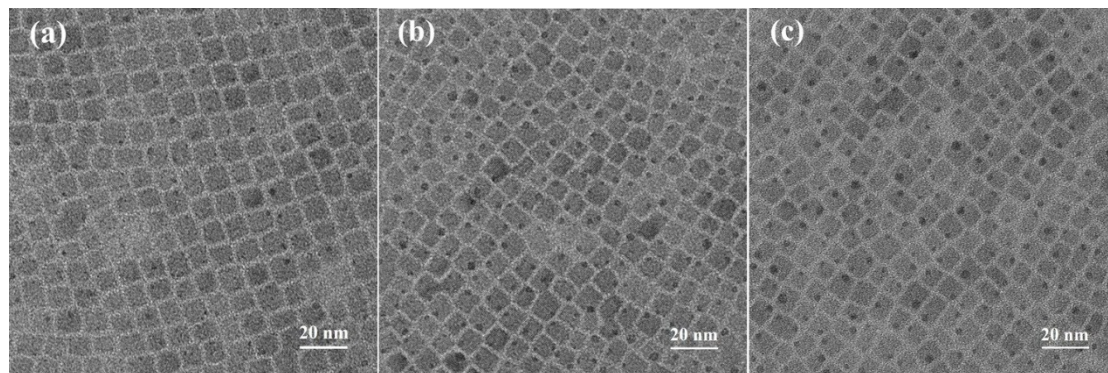


Figure S4 TEM images of (a) CsPbBr<sub>3</sub>, (b) CsPbBr<sub>3</sub>-DDAB, and (c) CsPbBr<sub>3</sub>-DDAB-Ni NCs

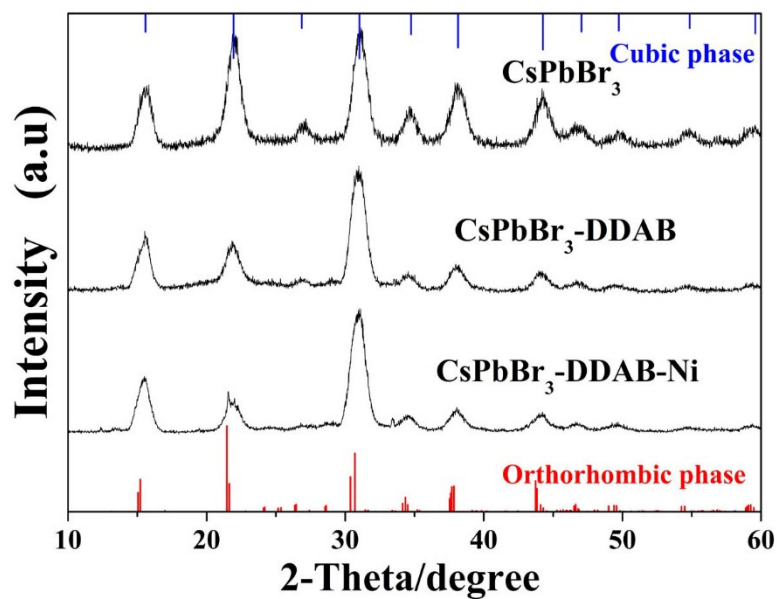


Figure S5 XRD patterns of  $\text{CsPbBr}_3$ ,  $\text{CsPbBr}_3\text{-DDAB}$ , and  $\text{CsPbBr}_3\text{-DDAB-Ni}$  NCs



Figure S6 Optical images of the  $\text{CsPbBr}_3\text{-DDAB-Ni}$  NCs under illumination with a 450 nm LED light ( $175 \text{ mW/cm}^2$ ).

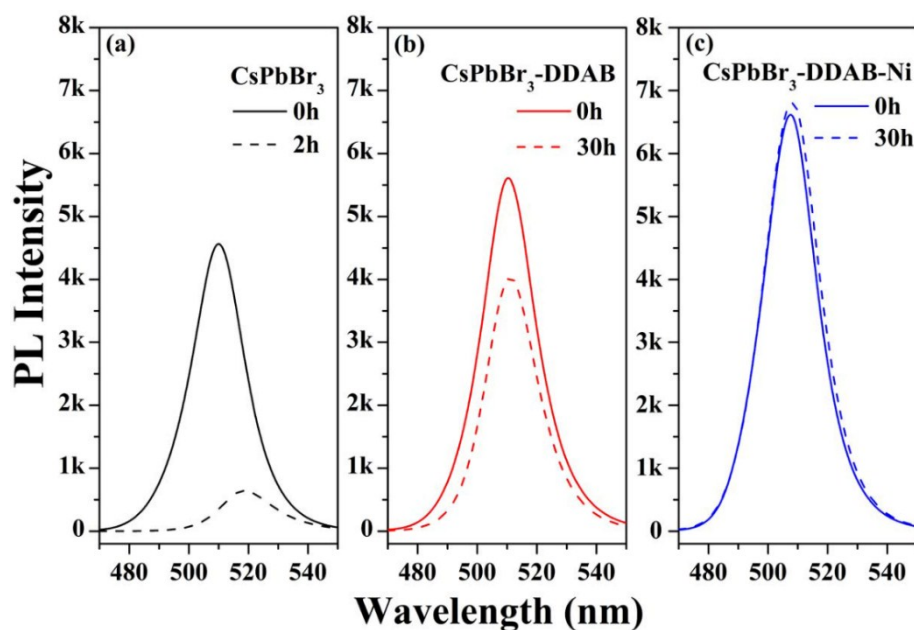


Figure S7 PL spectra of the CsPbBr<sub>3</sub>, CsPbBr<sub>3</sub>-DDAB, and CsPbBr<sub>3</sub>-DDAB-Ni NCs solution as a function of the illumination time with a 450 nm LED light (175 mW/cm<sup>2</sup>).

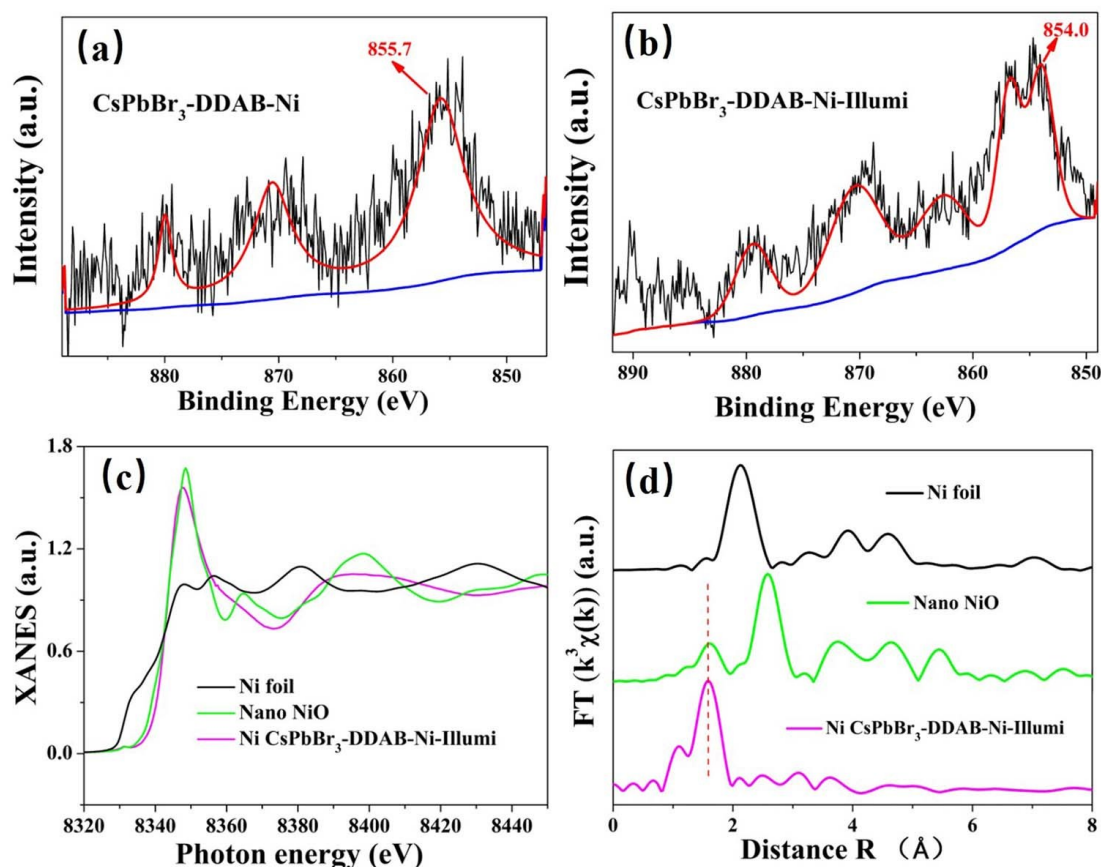


Figure S8 2p XPS spectra of the CsPbBr<sub>3</sub>-DDAB-Ni NCs (a) before and (b) after light irradiation for 30 hours; (c) Ni K-edge XANES spectra; and (d) Ni K-edge Fourier transformed EXAFS spectra in the R space.

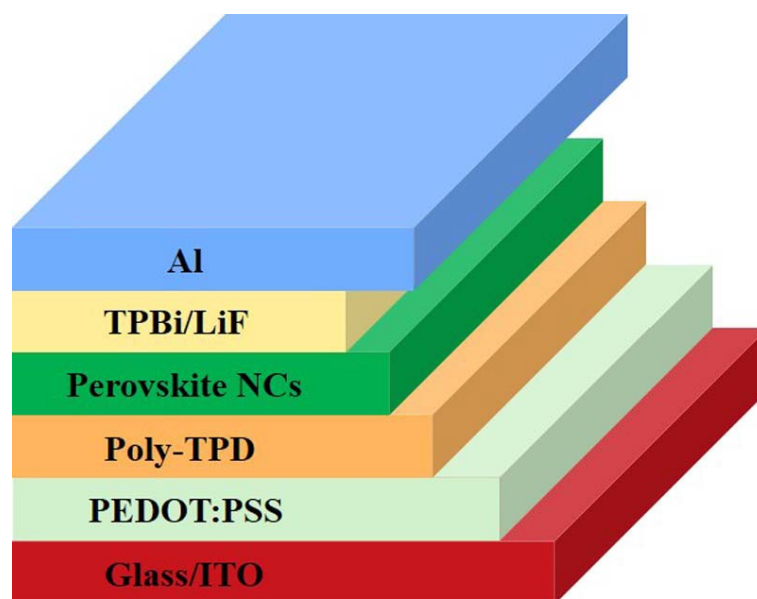


Figure S9 Illustration of the schematic perovskite LED device structure

Table S2 Characteristics of LED devices. L (Luminance), EQE (external quantum efficiency),  $V_{on}$  (turn-on voltage), CE (current efficiency)

Pe-QDs	$L_{max}$ ( $cd\ m^{-2}$ )	Peak EQE (%)	Turn-on Voltage (V) @ $1\ cd\ m^{-2}$	$CE_{max}$ ( $cd\ A^{-1}$ )
<b>CsPbBr<sub>3</sub></b>	451	0.5	5.6	0.9
<b>CsPbBr<sub>3</sub>-DDAB</b>	416	3.2	4.2	6.1
<b>CsPbBr<sub>3</sub>-DDAB-Ni</b>	553	6.5	3.0	12.6
<b>CsPbBr<sub>3</sub>-DDAB-Ni- Illumi</b>	870	9.2	3.0	17.8

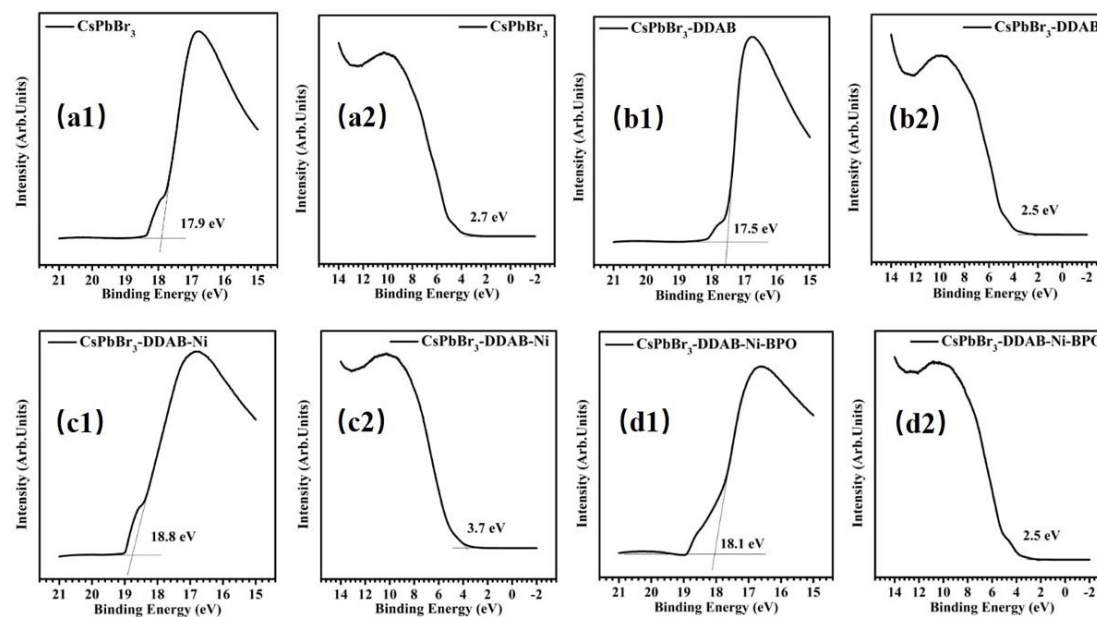


Figure S10 High-binding energy secondary-electron cutoff regions of Pe-NCs and VB-edge region of Pe-NCs.

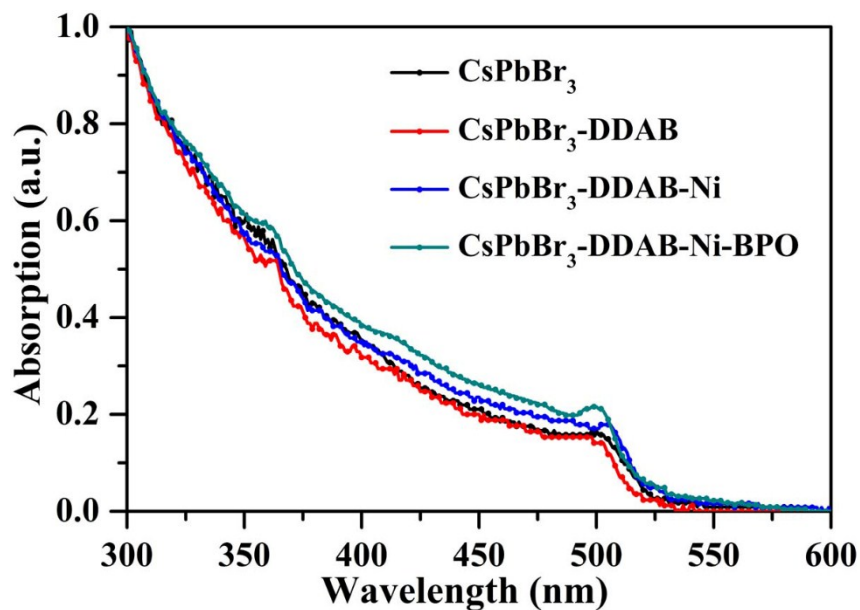


Figure S11 UV-vis absorption spectra of CsPbBr<sub>3</sub>, CsPbBr<sub>3</sub>-DDAB, CsPbBr<sub>3</sub>-DDAB-Ni, and CsPbBr<sub>3</sub>-DDAB-Ni-BPO films

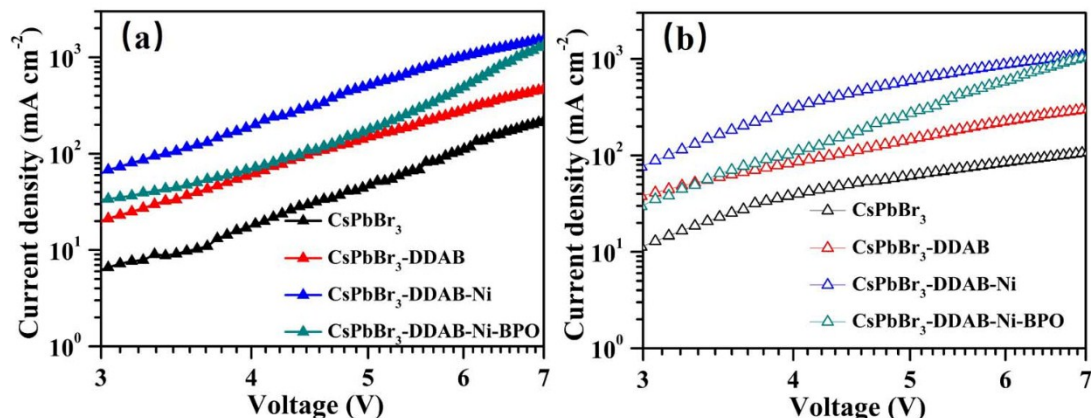


Figure S12 Current density–voltage (J–V) characteristics of (a) electron-only and (b) hole-only Pe-LED devices with CsPbBr<sub>3</sub>, CsPbBr<sub>3</sub>-DDAB, CsPbBr<sub>3</sub>-DDAB-Ni, and CsPbBr<sub>3</sub>-DDAB-Ni-BPO films.

The mobility was measured by the space charge limited current (SCLC) method by a hole-only device with a structure of ITO/PEDOT: PSS/Poly-TPD/Perovskite NCs/MoO<sub>3</sub>/Al or an electron-only device with a structure of ITO/ZnO/Perovskite NCs TPBi/LiF/Al and estimated through the Mott-Gurney equation<sup>1</sup>.

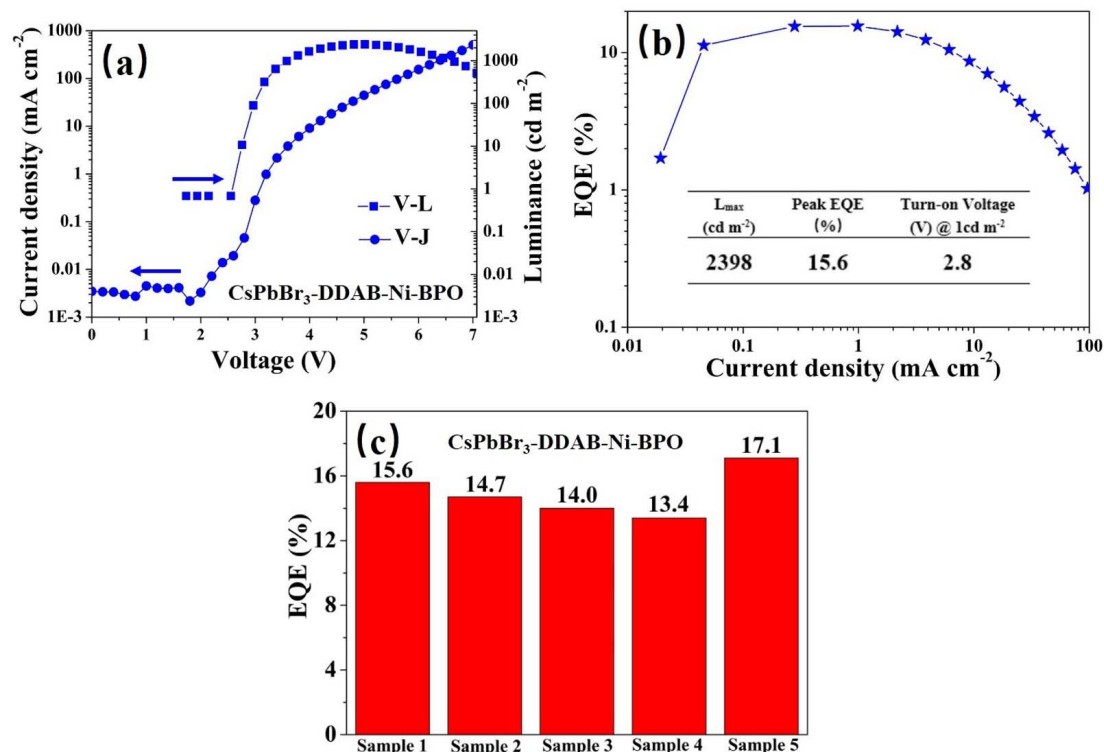


Figure S13 (a) Current density and Luminance versus driving voltage characteristics; (b) EQE versus current density characteristics with inserted table showing characteristics of LED devices; (c) EQE values of LEDs fabricated with different batches of CsPbBr<sub>3</sub>-DDAB-Ni-BPO NCs.



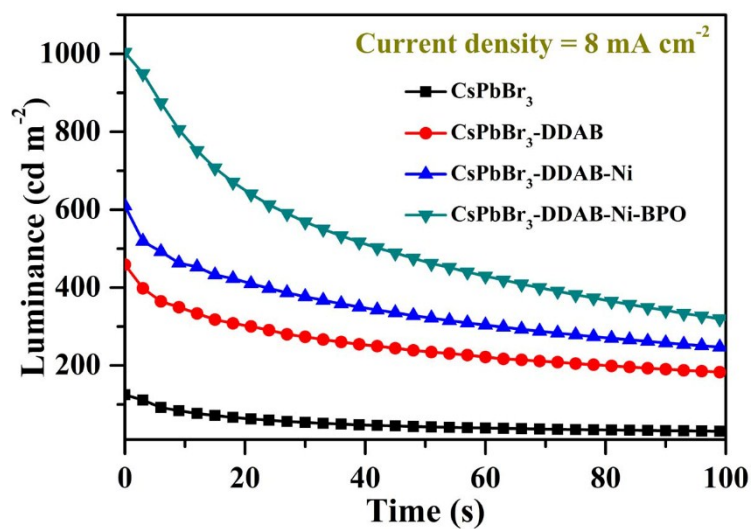


Figure S14 Lifetime measurements of the CsPbBr<sub>3</sub>-based LED devices.

Table S3. Summary of the performance of LEDs based on CsPbBr<sub>3</sub> NCs

Composition and types	V <sub>ON</sub> (V)	EL (nm)	Max. Luminance (Cd/m <sup>2</sup> )	Peak EQE (%)	Max. CE (Cd/A)	Publication Date and Ref
CsPbBr <sub>3</sub> NCs	4.2	516	946	0.12	0.43	2015 <sup>2</sup>
CsPbBr <sub>3</sub> NCs	3.5	516	1377	0.06	0.19	2016 <sup>3</sup>
CsPbBr <sub>3</sub> NCs	3.0	515	330	3	≈9	2016 <sup>4</sup>
CsPbBr <sub>3</sub> NCs	3.4	512	15185	6.27	13.3	2016 <sup>5</sup>
CsPbBr <sub>3</sub> NCs	4.6	515	12090	1.19	3.11	2017 <sup>6</sup>
CsPbBr <sub>3</sub> NCs	2.9	518	3059	1.1	3.66	2017 <sup>7</sup>
CsPbBr <sub>3</sub> NCs	2.6	512	1660	8.73	—	2017 <sup>8</sup>
CsPbBr <sub>3</sub> NCs	2.4	518	4212	0.35	1.38	2017 <sup>9</sup>
CsPbBr <sub>3</sub> NCs	2.8	516	7085	6.5	18.13	2018 <sup>10</sup>
CsPbBr <sub>3</sub> NCs	≈7	≈520	≈450	1.43	4.69	2018 <sup>11</sup>
CsPbBr <sub>3</sub> NCs	2.4	515	55800	11.6	45.5	2018 <sup>12</sup>
CsPbBr <sub>3</sub> NCs	2.7	508	≈1000	8.08	—	2018 <sup>13</sup>
CsPbBr <sub>3</sub> NCs	≈3	512	18600	15.17	≈50	2018 <sup>14</sup>
CsPbBr <sub>3</sub> NCs	2.4	518	76940	16.48	66.7	2018 <sup>15</sup>
CsPbBr <sub>3</sub> NCs	2.6	517	2270	9.7	31.7	2019 <sup>16</sup>
CsPbBr <sub>3</sub> NCs	≈3.5	520	≈500	8.2	25.7	2019 <sup>17</sup>
<b>CsPbBr<sub>3</sub> NCs</b>	<b>2.8</b>	<b>512</b>	<b>2114</b>	<b>16.8</b>	<b>32.4</b>	<b>This work</b>

As we know, the morphologies of emitting layer for perovskite light-emitting diodes (PeLEDs) could be bulk form, thin films and nanocrystals (NCs). In this paper, we focused on studying the device performances of PeLEDs based on NCs. Here, we collected the data about the device performances of CsPbBr<sub>3</sub> NCs LEDs, which is shown in the Table S2. To our knowledge, the EQE of 16.8% in our work may be the highest value for the LEDs fabricated with CsPbBr<sub>3</sub> NCs. Additionally, the highest EQE of 21.3% has been achieved by using all-inorganic CsPbBr<sub>0.6</sub>I<sub>2.4</sub> NCs as emitters<sup>18</sup>, which is the record-holder for all-inorganic NCs fabricated in LEDs.

## References

1. G. Li, J. Huang, H. Zhu, Y. Li, J.-X. Tang and Y. Jiang, *Chem. Mater.*, 2018, **30**, 6099-6107.
2. J. Song, J. Li, X. Li, L. Xu, Y. Dong and H. Zeng, *Adv. Mater.*, 2015, **27**, 7162-7167.
3. X. Zhang, H. Lin, H. Huang, C. Reckmeier, Y. Zhang, W. C. Choy and A. L. Rogach, *Nano Lett.*, 2016, **16**, 1415-1420.
4. J. Pan, L. N. Quan, Y. Zhao, W. Peng, B. Murali, S. P. Sarmah, M. Yuan, L. Sinatra, N. M. Alyami, J. Liu,

- E. Yassitepe, Z. Yang, O. Voznyy, R. Comin, M. N. Hedhili, O. F. Mohammed, Z. H. Lu, D. H. Kim, E. H. Sargent and O. M. Bakr, *Adv. Mater.*, 2016, **28**, 8718-8725.
5. J. Li, L. Xu, T. Wang, J. Song, J. Chen, J. Xue, Y. Dong, B. Cai, Q. Shan, B. Han and H. Zeng, *Adv. Mater.*, 2017, **29**.
6. P. Liu, W. Chen, W. Wang, B. Xu, D. Wu, J. Hao, W. Cao, F. Fang, Y. Li, Y. Zeng, R. Pan, S. Chen, W. Cao, X. W. Sun and K. Wang, *Chem. Mater.*, 2017, **29**, 5168-5173.
7. H. Wu, Y. Zhang, X. Zhang, M. Lu, C. Sun, T. Zhang and W. W. Yu, *Adv. Opt. Mater.*, 2017, **5**, 1700377.
8. T. Chiba, K. Hoshi, Y. J. Pu, Y. Takeda, Y. Hayashi, S. Ohisa, S. Kawata and J. Kido, *ACS Appl. Mater. Interfaces*, 2017, **9**, 18054-18060.
9. H. Wu, Y. Zhang, X. Zhang, M. Lu, C. Sun, X. Bai, T. Zhang, G. Sun and W. W. Yu, *Adv. Electron. Mater.*, 2018, **4**.
10. Y. Tan, Y. Zou, L. Wu, Q. Huang, D. Yang, M. Chen, M. Ban, C. Wu, T. Wu, S. Bai, T. Song, Q. Zhang and B. Sun, *ACS Appl. Mater. Interfaces*, 2018, **10**, 3784-3792.
11. B. Liu, L. Wang, H. Gu, H. Sun and H. V. Demir, *Adv. Opt. Mater.*, 2018, **6**.
12. J. Song, J. Li, L. Xu, J. Li, F. Zhang, B. Han, Q. Shan and H. Zeng, *Adv. Mater.*, 2018, **30**, e1800764.
13. K. Hoshi, T. Chiba, J. Sato, Y. Hayashi, Y. Takahashi, H. Ebe, S. Ohisa and J. Kido, *ACS Appl. Mater. Interfaces*, 2018, **10**, 24607-24612.
14. S. Yuan, Z. K. Wang, M. P. Zhuo, Q. S. Tian, Y. Jin and L. S. Liao, *ACS Nano*, 2018, **12**, 9541-9548.
15. J. Song, T. Fang, J. Li, L. Xu, F. Zhang, B. Han, Q. Shan and H. Zeng, *Adv. Mater.*, 2018, **30**, e1805409.
16. J. H. Park, A. Y. Lee, J. C. Yu, Y. S. Nam, Y. Choi, J. Park and M. H. Song, *ACS Appl. Mater. Interfaces*, 2019, **11**, 8428-8435.
17. D. Yang, P. Li, Y. Zou, M. Cao, H. Hu, Q. Zhong, J. Hu, B. Sun, S. Duhm, Y. Xu and Q. Zhang, *Chem. Mater.*, 2019, **31**, 1575-1583.
18. 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.