

# **Insight to Ligand Passivation Strategies for Multiple-Type Surface Defects in High Performance Perovskite Quantum Dots Light-Emitting Diodes**

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## **Supporting Information**

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## Captions

**Fig. S1** (a) Pristine, (b) D-QDs, (c) N-QDs, (d) single-step post-processing PeQDs.

**Fig. S2** EDS element mapping results of N-QDs film on Si substrate.

**Fig. S3** Structural image of the three potential binding modes of 3-NDS ligand on the PeQD surface, including (a) binding with surface  $\text{Pb}^{2+}$  ions through the  $\text{SO}_3^-$  group, (b) electrostatic interaction with surface  $\text{Br}^-$  ions through the  $(\text{CH}_2)_2\text{N}(\text{CH}_3)^+$  group, and (c) dual-site anchoring involving both anionic and cationic groups of 3-NDS calculated by DFT.

**Fig. S4** Calculated results of binding energy of binding energy of three potential binding modes of 3-NDS ligand on the PeQD surface calculated by DFT.

**Fig. S5** Structural image of OA molecule combined with PeQDs surface calculated by DFT.

**Fig. S6** Structural image of OAm molecule combined with PeQDs surface calculated by DFT.

**Fig. S7** Structural image of DDeAB molecule combined with PeQDs surface calculated by DFT.

**Fig. S8** Structural image of perovskite with/without  $V_{\text{Br}}$  vacancy defect with 3-NDS molecule calculated by DFT.

**Fig. S9** PDOS of the Br/Pb element of perovskite (with  $V_{\text{Br}}$  vacancy defect) without/with 3-NDS molecule calculated by DFT.

**Fig. S10** Images of (a) Pristine, (b) D-QDs, (c) N-QDs films under the fluorescence microscope.

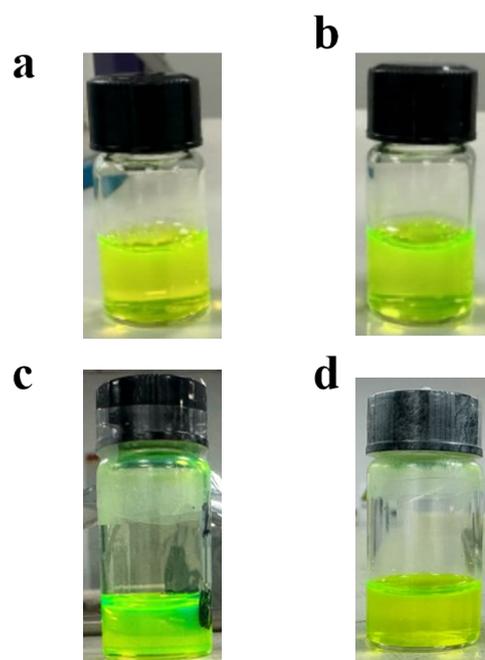
**Fig. S11** (a) Normalized EL, (b) EQE-voltage, (c) current density-current efficiency, (d) voltage-current density, (e) luminance-EQE, (f) luminance-voltage curves of PeLEDs.

**Table S1** Summary of device performance.

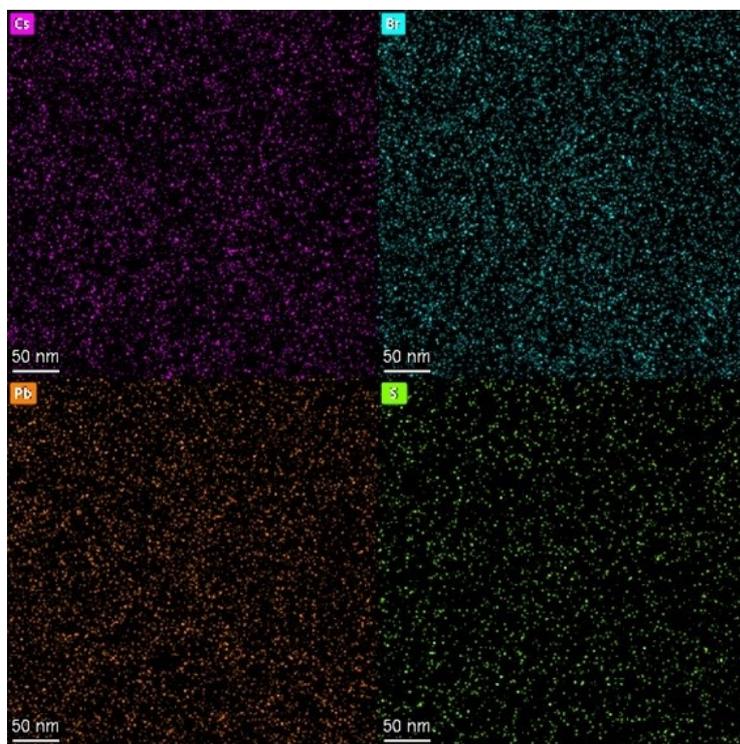
**Fig. S12** Normalized EL and PL peaks of the N-QDs.

**Table S2** Summary of our work with other PeLEDs.

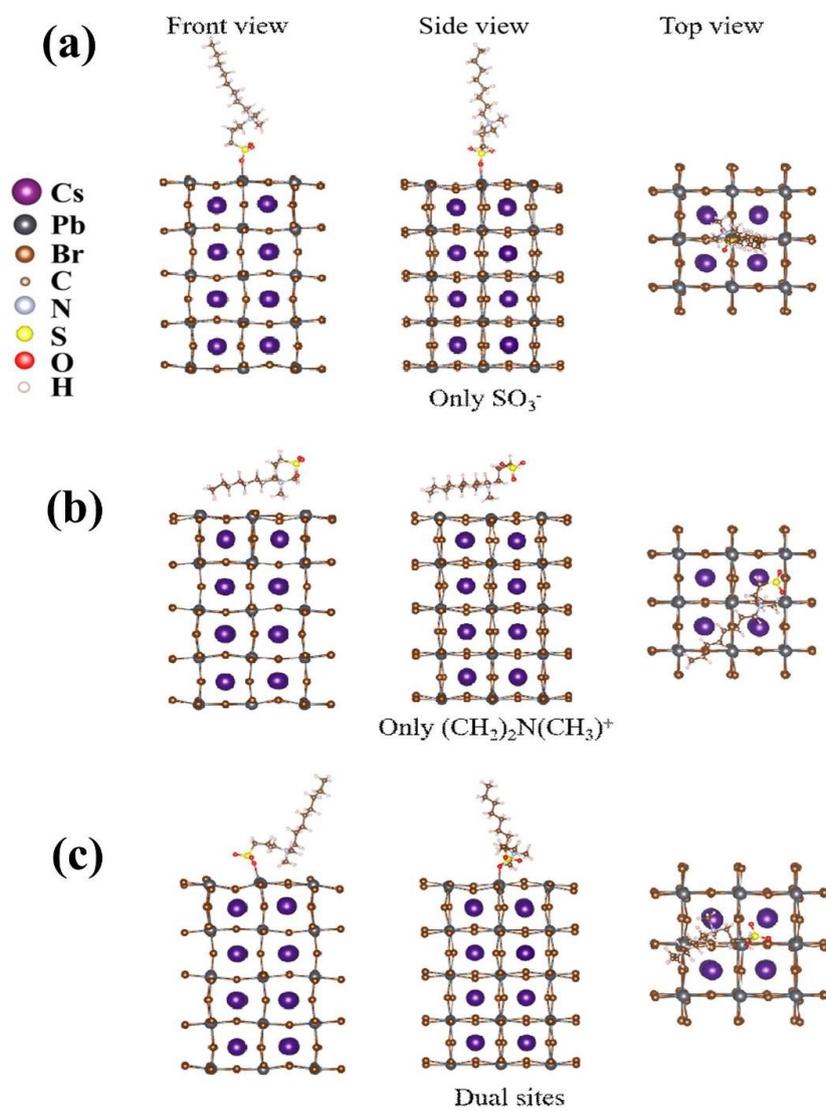
**Fig. S13** Operational stability results of the Pristine and N-QDs PeLEDs. The devices were measured under a constant voltage of 6 V at ambient conditions.



**Fig. S1**



**Fig. S2**



**Fig. S3**

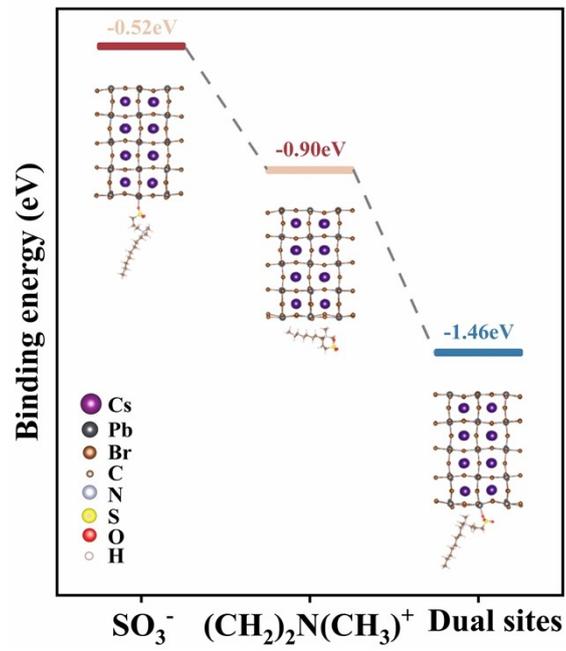


Fig. S4

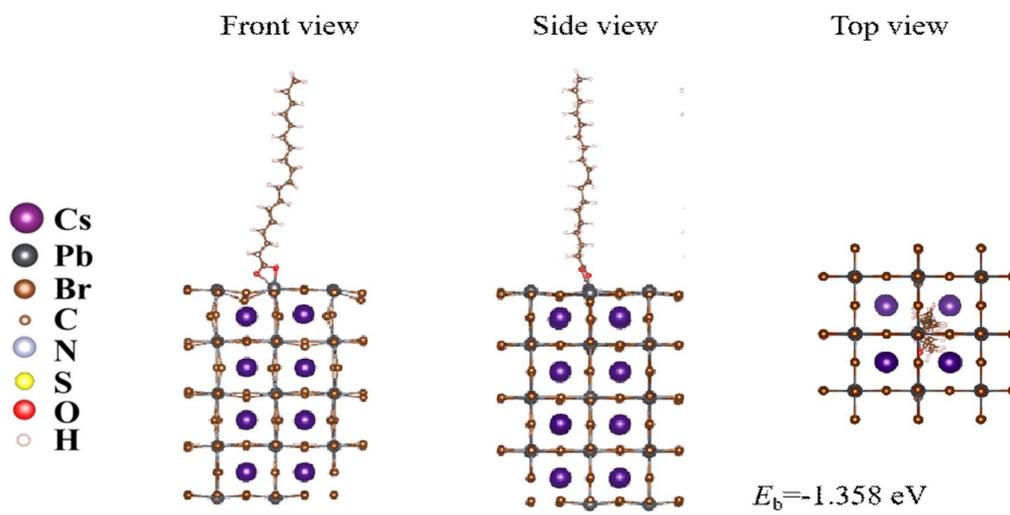


Fig. S5

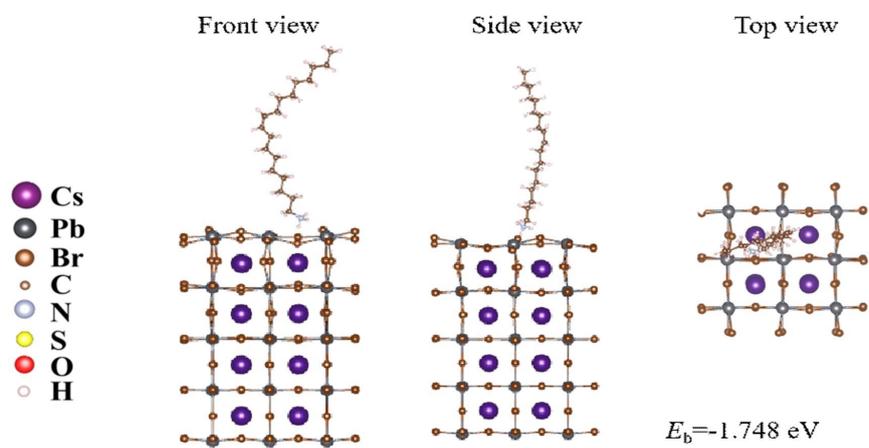


Fig. S6

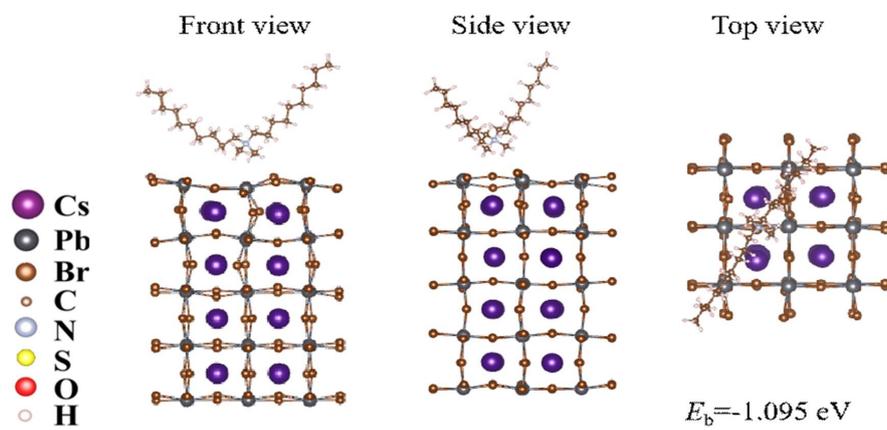


Fig. S7

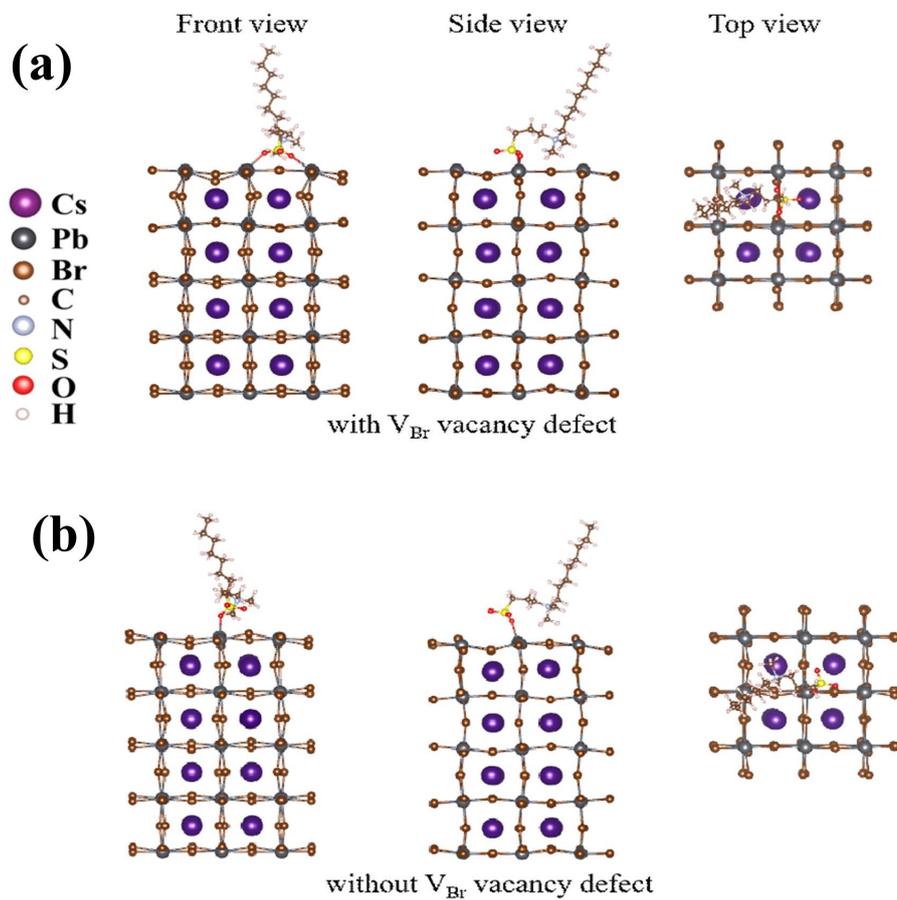
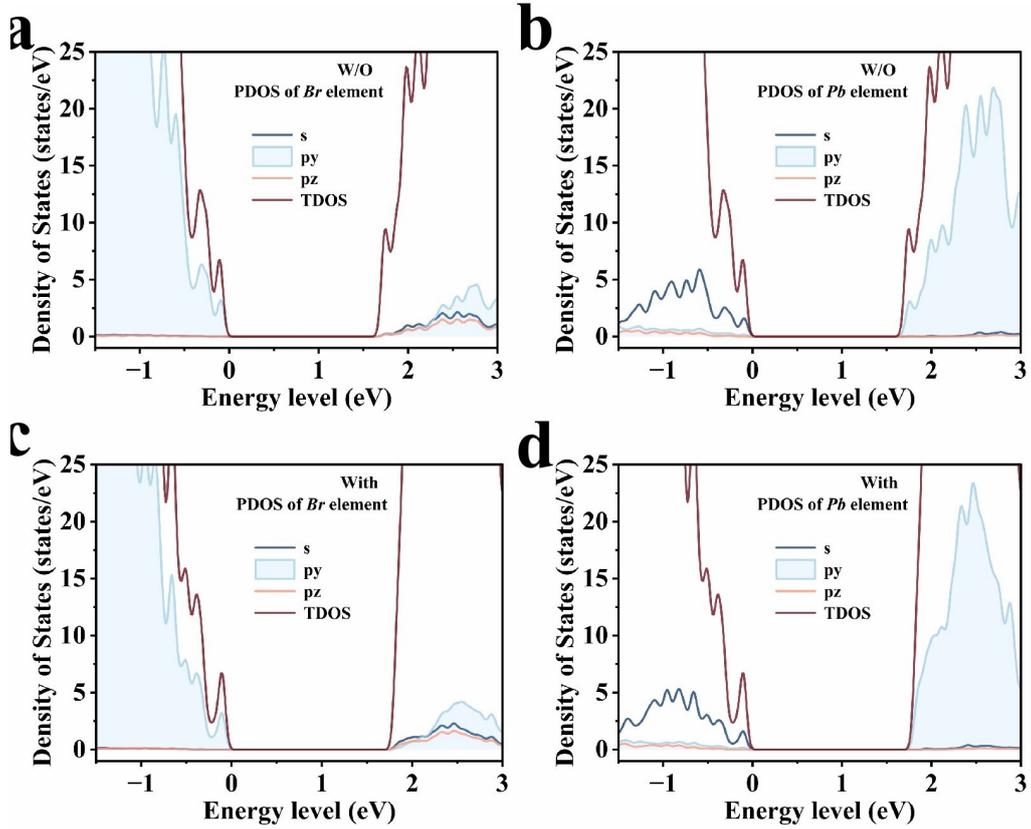
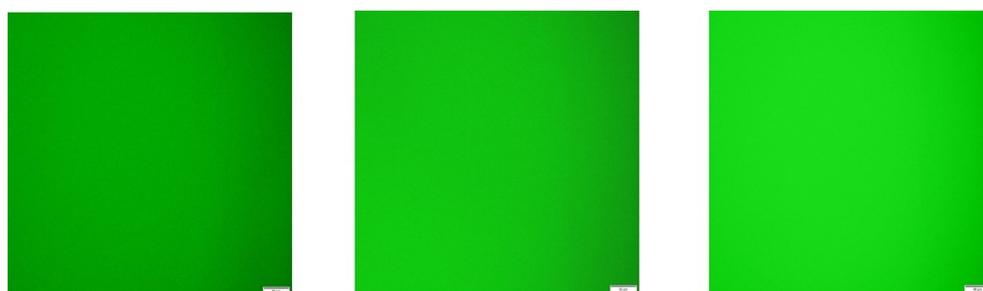


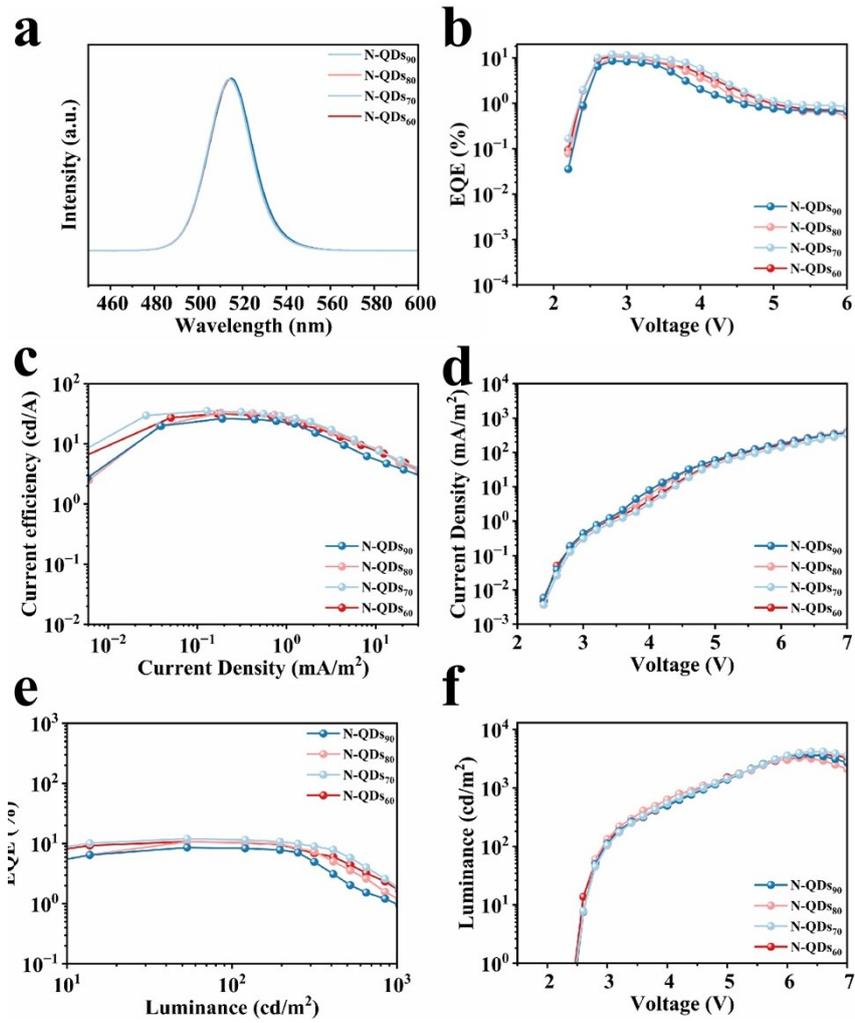
Fig. S8



**Fig. S9**



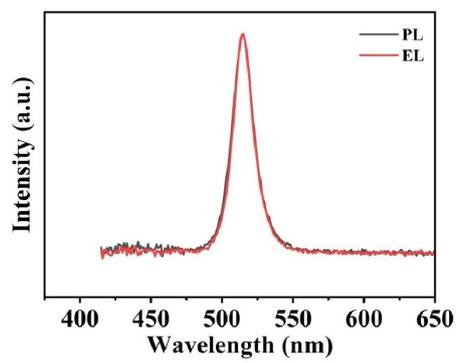
**Fig. S10**



**Fig. S11**

**Table S1**

Sample	V <sub>on</sub> (V)	CE (cd/A)	PE (I <sub>m</sub> /W)	EQE (%)	Luminance (cd/m <sup>2</sup> )
Pristine	3.3	3.64	2.22	0.72	2093
D-QDs	2.9	10.06	9.03	3.79	1806
N-QDs <sub>60</sub>	2.5	31.61	35.47	10.80	3735
N-QDs <sub>70</sub>	2.5	35.25	39.55	12.05	4177
N-QDs <sub>80</sub>	2.5	32.70	36.69	10.71	3278
N-QDs <sub>90</sub>	2.5	26.30	29.51	8.62	3716



**Fig. S12**

**Table S2**

Perovskite	Device structure	V <sub>on</sub> (V)	Peak EQE (%)	Max CE (cd/A)	Peak Brightness (cd/m <sup>2</sup> )	Ref
CsPbI <sub>3</sub>	ITO/TFTFG/Perovskite/TPBi/LiF/Al	2.6	9.67	NA	1741	[1]
DPPA-CsPbI <sub>3</sub>	ITO/PEDOT:PSS/TFB/IL/Perovskite /TPBi/LiF/Al	3	5.04	NA	2037	[2]
PbBr <sub>2</sub> -DC <sub>8</sub> AB- CsPbBr <sub>3</sub>	ITO/PEDOT:PSS/Poly-TPD/PVK/ Perovskite/B3PyMP/TPBi/LiF/Al	2.7	9.41	3.33	9770	[3]
CsPbBr <sub>3</sub> -OABr	ITO/PEDOT:PSS/ PVK/ Perovskite/ TPBi/LiF/Al	4	6.6	7.3	280.8	[4]
12-SBE-CsPbBr <sub>3</sub>	ITO/PEDOT:PSS/TFB/PVK/ Perovskite/ TPBi/LiF/Al	2.8	6.7	22.8	1723	[5]
DDAB-Ni-CsPbBr <sub>3</sub>	ITO/PEDOT:PSS/Poly-TPD/ Perovskite/ TPBi/LiF/Al	2.8	10.7	20.6	1583	[6]
Ag-TOP-CsPbBr <sub>3</sub>	ITO/Nafion-PEDOT:PSS/Poly- TPD/Perovskite/ TPBi/LiF/Al	2.88	9.3	27.35	3820	[7]
3-BAS-CsPbBr <sub>3</sub>	ITO/PVK/PVP/Perovskite/TPBi/LiF/ Al	3.1	9.25	NA	1806	[8]
CsPbI <sub>3</sub>	ITO/PEDOT:PSS/Composite HTL/Perovskite/TPBi/LiF/Al	2.7	15.3	NA	1790	[9]
CsPbCl <sub>3-x</sub> Br <sub>x</sub>	ITO/PEDOT:PSS/T- HTL/Perovskite/TPBi/LiF/Al	2.4	11.0	7.05	<1000	[10]
TDA-CsPbBr <sub>3</sub>	ITO/PVK/PVP/Perovskite/TPBi/LiF/ Al	2.8	13.6	NA	1268	[11]
LSH-CsPbI <sub>3</sub>	ITO/PEDOT:PSS/Poly-TPD/ Perovskite/ TPBi/LiF/Al	2.4	18.3	NA	3552	[12]
MeO-PEABr-CsPbBr <sub>3</sub>	ITO/m-PEDOT:PSS/ Perovskite/ PO-T <sub>2</sub> T/LiF/Al	2.4	10.85	13.48	958	[13]
<b>3-NDS-CsPbBr<sub>3</sub></b>	<b>ITO/PEDOT:PSS/Poly-TPD/ Perovskite/ TPBi/LiF/Al</b>	<b>2.5</b>	<b>12.05</b>	<b>35.25</b>	<b>4177</b>	<b>Our work</b>

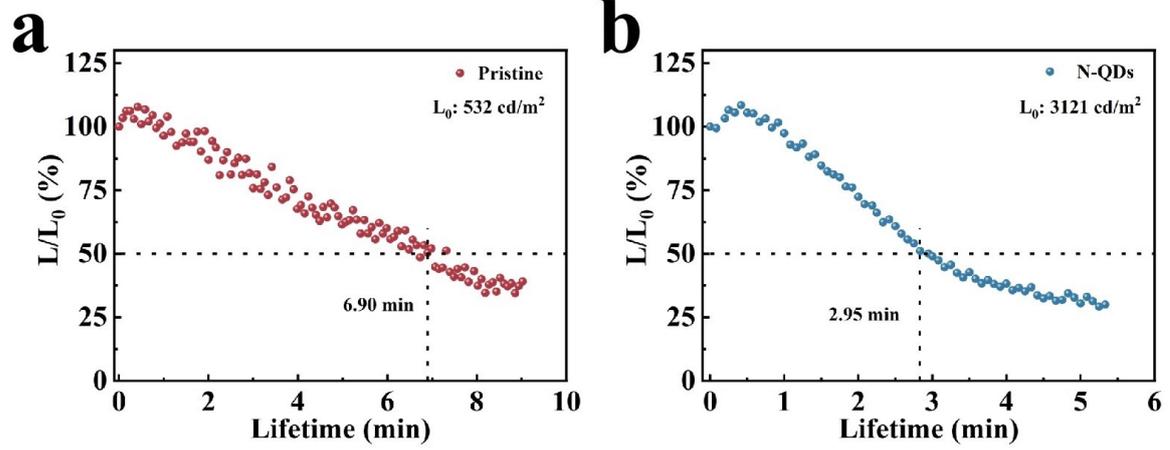


Fig. S13

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