# Supporting Information: All-inorganic Encapsulation for Extremely Stable Cesium Lead Halide Perovskite Nanocrystals: Toward Full-color Display Application

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# MATERIAL DETAILS

Here, we list the details of all chemical materials involved in this work in Table S1

Name	Detail	
$CH_3NH_3Br$ (MABr)	99.5%, Xi'an Polymer Light Technology Corp.	
$PbCl_2$	99.99%, Xi'an Polymer Light Technology Corp.	
$PbBr_2$	99.99%, Xi'an Polymer Light Technology Corp.	
$PbI_2$	99.99%, Xi'an Polymer Light Technology Corp.	
$\operatorname{CsCl}$	99.99%, Xi'an Polymer Light Technology Corp.	
$\mathrm{CsBr}$	99.99%, Xi'an Polymer Light Technology Corp.	
CsI	99.99%, Xi'an Polymer Light Technology Corp.	
N,N-dimethylformamide (DMF)	AG, Sinopharm Chemical Reagent Co.	
Chlorobenzene	99%, Sinopharm Chemical Reagent Co.	
Polyvinylidene fluoride (PVDF)	ZZBIO Co., Ltd.	
ethylene-co-vinyl acetate (EVA)	25 wt.%, Aladdin Biochemical Technology Co., Ltd.	
Oleic acid (OA)	99%, Aladdin Biochemical Technology Co., Ltd.	
oleylamine (OAm)	80-90%, Aladdin Biochemical Technology Co., Ltd.	
Alcohol	> 99.8%, Aladdin Bio-Chem Technology Co., LTD, China	

Table S1: Details of chemical materials.

# Methods

# $\label{eq:precursor compositions of PeNCs-SiO_2.$

PeNCs-SiO2	CsI	CsBr	CsCl	$PbI_2$	$PbBr_2$	$PbCl_2$	MS	Total Mass
	USI	USDI		1 012	$1 \text{ DDI}_2$	-	MD	
$\mathrm{CsPbCl}_3$	0	0	0.581	0	0	0.959	2	3.540
$CsPbCl_2Br$	0	0.734	0	0	0	0.960	2	3.693
$CsPbCl_{1.5}Br_{1.5}$	0	0.367	0.290	0	0.633	0.480	2	3.770
$CsPbClBr_2$	0	0	0.581	0	1.266	0	2	3.847
$CsPbBr_3$	0	0.734	0	0	1.266	0	2	4
$CsPbBr_2I$	0.896	0	0	0	1.266	0	2	4.162
$CsPbBr_{1.5}I_{1.5}$	0.448	0.367	0	0.795	0.633	0	2	4.243
$CsPbBrI_2$	0	0.734	0	1.590	0	0	2	4.324
$CsPbI_3$	0.896	0	0	1.590	0	0	2	4.486

Table S2: Precursor Compositions of  $\operatorname{PeNCs-SiO}_2$  (g)

#### Synthesis Detail of MAPbBr<sub>3</sub>–PVDF

The precursor – PVDF (0.08 mmol),  $PbBr_2$  (0.1 mmol), and MABr (0.84 g) – were weighed in a glovebox with argon atmosphere protection. The precursors were then dissolved in DMF (5 mL) and vigorously stirred at 500 rpm for 5 h. Then, a thin layer of the precursor solution was obtained after spin-coating at 3400 rpm for 25 s on the surface of a glass substrate. After heating the glass substrate on a hot plate (60 °C), the solvent evaporated gradually, and we obtained a solid film attached to the glass surface ultimately. Then, we placed the substrate in a vacuum chamber at 30 °C for 24 h to further remove residual DMF. Finally, a thin film with uniformly distributed quantum dots was obtained.

#### Synthesis Detail of CsPbBr<sub>3</sub>–EVA

PbBr<sub>2</sub> (0.4 mmol) and CsBr (0.4 mmol) were dissolved in 5 mL of DMF solution while stirring, and then mixed with oleic acid (OA, 1 mL) and oleylamine (OAm, 0.5 mL) as the ligand for the precursor solution. 0.5g of ethylene-co-vinyl acetate (EVA) was dissolved in chlorobenzene (5 mL). Subsequently, 300  $\mu$ L of the precursor solution was quickly added dropwise to the magnetically stirred EVA–chlorobenzene system. Finally, chlorobenzene gradually volatilized at room temperature, yielding CsPbBr<sub>3</sub>–EVA composite films.

#### Synthesis Detail of CsPbBrI<sub>2</sub>–EVA

(a) Preparation of Cs-oleate Precursor. 0.407 g of  $Cs_2CO_3$ , 1.25 mL of oleic acid, and 20 mL of 1-octadecene (ODE) were mixed in a three-necked flask, and heated to 120 °C under vacuum for 1 h. Subsequently, the temperature was increased to 150 °C in a nitrogen environment for 10 min until the  $Cs_2CO_3$  was completely dissolved.

(b) Synthesis of PeNCs CsPbBrI<sub>2</sub>. 0.0918 g of PbBr<sub>2</sub>, 0.2305 g of PbI<sub>2</sub>, 20 mL of ODE, 2.6 mL of oleic acid, and 2.6 mL of OAm were also mixed in the three-necked flask. Afterwards, the flask filled with nitrogen was heated to 160 °C for 10 minutes, then injected the 1.6 mL

of Cs-oleate precursor rapidly. After 5 s of reaction, quickly placed the mixed solution into ice bath, and finally collected the CsPbBrI<sub>2</sub>.

(c) Synthesis of CsPbBrI<sub>2</sub>–EVA. 0.5g of ethylene-co-vinyl acetate (EVA) was dissolved in chlorobenzene (5 mL). Subsequently, 300  $\mu$ L of the pre-prepared CsPbBrI<sub>2</sub> solution was quickly added dropwise to the magnetically stirred EVA–chlorobenzene system. Finally, chlorobenzene gradually volatilized at room temperature, yielding CsPbBrI<sub>2</sub>–EVA composite films.

#### Fabrication of PeNCs-Photoresist and Photolithography Process

The entire process was performed under dust-free conditions (25 °C, 45% RH environment). (a) Preparation of PeNCs-Photoresist (PeNCs-PR). 0.2 g of PeNCs–SiO<sub>2</sub> powder was added to 10 mL of negative photoresist SU-8 2015, and the mixed solution was magnetically stirred under dust-free conditions for 3 h until the PeNCs–SiO<sub>2</sub> powders were fully dispersed, obtaining a PeNCs-photoresist (PeNCs-PR) suspension. The concentrations of the red (CsPbBrI<sub>2</sub>– SiO<sub>2</sub>), green (CsPbBr<sub>3</sub>–SiO<sub>2</sub>), and blue (CsPbBr<sub>1.5</sub>Cl<sub>1.5</sub>–SiO<sub>2</sub>) PeNCs-PR solutions were no more than 30 wt.%.

(b) Pretreatment of substrate. The 2-inch glass substrates were cleaned via ultrasonication and then boiled at 523 K for 15 min. The substrates were cleaned with a piranha wet etch (using 90 mL  $H_2SO_4$  and 360 ml  $H_2O_2$ ) followed by a de-ionized water rinse. Subsequently, the glass substrates were dried with nitrogen.

(c) Photolithographic process. 1 mL PeNCs-PR solution was dispensed on the pretreated substrate. Each type of PeNCs-PR was spin-coated at 500 rpm for 10 s and then at 3000 rpm for 25 s. After the spin coating process, the substrates were baked at 368 K for 3 min. Hereafter, the substrates were exposed under a customized mask via i-line ( $120 \text{ mJ/cm}^2$ ) for 10 s and immediately baked at 368 K for the second time for 4 min. Afterward, the substrates were developed for 5 min and rinsed with isopropanol solution and de-ionized water successively. The substrates were finally dried using nitrogen gas. The aforementioned

process was repeated for each R, G, and B pattern.

### EXPERIMENTAL DETAILS

**Photoluminescence and Absorption Tests** The PL was measured using a F-7000 spectrometer (HITACHI, Japan) with excitation from a 365-nm UV light source. The absorption spectra was measured using a FLS-980 (Edinburgh Instruments, USA).

**X-Ray Diffraction** The XRD spectra were obtained using a SmartLab SE (Rigaku, Japan).

**Brunner–Emmet–Teller measurements** The BET measurements were operated by using a ASAP–2460 (Micromeritics).

**TEM and EDS** The TEM was measured using a Talos F200X (Thermo Fisher, USA), and the samples were prepared using a focused ion beam from a Helios 660(Thermo Fisher, USA). The EDS elementary mapping was carried out using the built-in camera of a Talos F200X.

Photoluminescence Quantum Yield The PLQY was tested using a Spectro 320 (Instrument System, Germany) with a 150-mm integrating sphere (ISP-150, Instrument System, Germany). The excitation source was a 365-nm UVA LED.

Aging Test The ambient storage was carried out indoors at 25 °C, with approximately 70% relative humidity (RH), without direct light illumination. The water soaking was carried out by submerging 1 g of PeNCs–SiO<sub>2</sub> in a homemade aluminum tank filled with purified water. In the UV illumination test, 365-nm UVA-LEDs, placed on the aging stages and powered by 100 mA DC current, were employed as the UV sources. 1 gram of each sample was placed in a tank, covered by a glass plate, and placed up-side-down against one UVA-LED for illumination. The average distance between the UVA-LED chip and the sample was 1 cm, the power density of the UVA illumination was 6.136 mW/cm<sup>2</sup>, and the temperature was RT. For all the aging tests, except for the ambient storage, samples were taken out for

PL measurements at regular intervals using a Spectro 320 (Instrument System, Germany) with excitation from a 365-nm UVA-LED.

Thermal Cycling Test The samples were heated using a temperature-controlled heat sink (LED-850, Instrument System, Germany), and the excitation source was a 405-nm laser (Changchun New Industries Optoelectronics Tech Co.,Ltd, China). The PL spectra were captured via fiber using a spectrometer (QE-65, Ocean optics, USA). As illustrated in Figure S2, After several heating–cooling cycles, CsPbBr<sub>3</sub>–EVA and CsPbBrI<sub>2</sub>–EVA suffered severe PL losses, the final PL intensities were 51 % and 67 % of the initial one, respectively.

Thermal Treatment Test The samples were heated to 100 °C and 200°C in ambient air in a tube furnace. After the temperature of samples recovered to RT, we used a Spectro 320 (Instrument System, Germany) with a 150-mm integrating sphere (ISP-150, Instrument System, Germany) to measure PL intensity. The excitation source was a 365-nm UVA LED. The reason we chose 200 °C as the highest temperature is that it lies beyond the highest possible working temperature of our sample and below the phase transition or melting temperatures of all perovskite QDs.



Figure S1: High-angle annular dark-field imaging (HAADF) and elementary mappings of CsPbBr\_{1.5}Cl\_{1.5}--SiO\_2 sample



Figure S2: a) Thermal cycling test of a) CsPbBr<sub>3</sub>–EVA and b) CsPbBrI<sub>2</sub>–EVA

## SUPPORTING DATA

#### **Time-Resolved Photoluminescence**

The time-resolved photoluminescence values of all nine  $PeNCs-SiO_2$  samples are illustrated in **Figure S3**, with the averaged time constants listed in Table S3, calculated via the Eq. **S1**.

$$\tau_{ave} = \frac{A_1 t_1^2 + A_2 t_2^2}{A_1 t_1 + A_2 t_2} \tag{S1}$$



Figure S3: Time-resolved photoluminescence (TRPL) of PeNC–SiO<sub>2</sub>: (A) CsPbCl<sub>3</sub>; (B) CsPbCl<sub>2</sub>Br; (C) CsPbCl<sub>1.5</sub>Br<sub>1.5</sub>; (D) CsPbClBr<sub>2</sub>; (E) CsPbBr<sub>3</sub>; (F) CsPbBr<sub>2</sub>I; (G) CsPbBr<sub>1.5</sub>I<sub>1.5</sub>; (H) CsPbBr<sub>2</sub>I; (I) CsPbI<sub>3</sub>.

Samples	$A_1$	$\tau_1 (ns)$	$A_2$	$\tau_2 (\mathrm{ns})$	$\tau_{ave} (ns)$
CsPbCl <sub>3</sub> –SiO <sub>2</sub>	1.90	0.97	0.094	33.13	21.17
$CsPbCl_2Br-SiO_2$	13.68	1.99	0.20	15.48	3.37
$CsPbCl_{1.5}Br_{1.5}-SiO_2$	9.75	3.56	0.23	25.86	6.82
$CsPbClBr_2-SiO_2$	8.79	3.87	0.29	20.83	6.43
$CsPbBr_3-SiO_2$	2.51	7.39	0.35	45.3	24.86
$CsPbBr_2I-SiO_2$	9.19	8.13	0.41	45.77	15.69
CsPbBr <sub>1.5</sub> I <sub>1.5</sub> –SiO <sub>2</sub>	35.22	5.36	0.67	24.46	6.89
$CsPbBrI_2-SiO_2$	44.79	5.25	0.29	27.9	6.00
$CsPbI_3$ - $SiO_2$	4.05	11.94	0.38	68.69	31.98

Table S3: Time Constants of TRPLs

## Chromaticity



Figure S4: Gamuts of (a) CsPbCl\_{1.5}Br\_{1.5}-CsPbBr\_3-CsPbBrI\_2 and (b) LED-CsPbBr\_3-CsPbBrI\_2

PeNCs	(x, y)	FWHM (nm)	Peak wavelength (nm)	Color purity
$CsPbCl_3$	(0.1700, 0.0064)	18.1	412.7	1.00
$CsPbCl_2Br$	(0.1544, 0.0222)	27.9	449.6	0.99
$CsPbCl_{1.5}Br_{1.5}$	(0.1378, 0.0557)	27.7	464.1	0.97
$CsPbClBr_2$	(0.0518, 0.5209)	22.3	501.9	0.86
$CsPbBr_3$	(0.1174, 0.7629)	25.0	519.6	0.86
$CsPbBr_2I$	(0.4912, 0.5055)	47.6	578.5	0.99
$CsPbBr_{1.5}I_{1.5}$	(0.6168, 0.3824)	47.5	621.7	1.00
$CsPbBrI_2$	(0.6837, 0.3158)	39.4	660.3	1.00
$CsPbI_3$	(0.7179, 0.2802)	55.9	687.5	1.00

Table S4: Chromatic Parameters of the  $\mathrm{PeNCs}\mathrm{-\!SiO}_2$  samples

Table S5: Gamuts of the Two Scenarios

Pixel System (B-G-R)	NTSC	Rec. 2020
$CsPbCl_{1.5}Br_{1.5}-CsPbBr_3-CsPbBrI_2$	127.34%	95.09%
$LED-CsPbBr_3-CsPbBrI_2$	126.17%	94.21%



Figure S5: Blue LED spectrum



Figure S6: (a) Relative PL intensities changes of white light LED fabricated by PeNCs–SiO<sub>2</sub> ;(b) Photochromatic stability of white light LED



Figure S7: (a) Organic solvent soaking test of SiO<sub>2</sub>-coating PeNCs and (b) unshelled PeNCs



Figure S8: Relative PL intensities of a)  $CsPbBr_{1.5}Cl_{1.5}-SiO_2$  b)  $CsPbBr_3-SiO_2$  and c)  $CsPb-BrI_2-SiO_2$  after undergoing thermal treatment test and cooling to RT

Table S6: Chromatic parameters of the blue LED in Fig. S5

Chromatic parameters	Values
(x, y)	(0.1408, 0.0395)
Peak Wavelength (nm)	459.92
Dominant Wavelength (nm)	464.06
FWHM (nm)	14.01
Color Purity	1.00

Table S7: Properties and identification information of several samples with MS

Samples	BET surface area, $m^2/g$	Average pore size,nm
Original MS	1014	3.58
Sintered MS at $500^{\circ}$ C	1016	3.61
Sintered MS at $600^{\circ}$ C	1019	3.53
Sintered MS at $700^{\circ}C$	1013	3.59
$PeNCs-SiO_2$	3.735	15.48

Composites	Material	Test condition	Relative PL	Test duration
CsPbX <sub>3</sub> -SiO <sub>2</sub>	MS encapsulation	Illuminated with 365 nm LED light	> 100%	4000 h (This work)
CsPbBr <sub>3</sub> –PM	Polystyrene microspheres	Ambient conditions	50%	$1400 \ h^1$
$CsPbBr_3-MS$	MS encapsulation	Illuminated with 450 nm LED light	${>}100\%$	$1000 \ h^2$
$CsPbBr_3-PS$	Polystyrene	Water soaking	70%	$192 h^{3}$
CsPbX <sub>3</sub> –PMMA	Polymethyl methacrylate	RT with $70\%$ humidity	75%	$72 \ h^4$
MAPbBr <sub>3</sub> –TMOS	Tetramethyl orthosilicate	Illuminated with 450 nm LED light	61%	$49 \ h^5$
$CsPbX_3$ – $CaF_2$	Hot-injection, $CaF_2$	air with $100\%$ humidity	60%	$48 h^6$
CsPbBr <sub>3</sub> –TMOS	Tetramethyl orthosilicate	100% RH at room temperature	55%	$48 h^7$
CsPbBr <sub>3</sub> –AlOx	Atomic layer deposition	$100 \text{ mW/cm}^2 \text{ solar irradiation}$	50%	$8 h^8$
CsPbBr <sub>3</sub> –TDPA	Alkyl phosphate	Water soaking	80%	$5 h^9$
$CsPbX_3$ -TEOS	Tetraethyl orthosilicate	Water soaking	40%	$4 h^{10}$
CdSe QD	Core/shell QDs	Sealed on the LED chip	50%	$200 h^{11}$
CdSe QD–SAM	$QD-SiO_2/Al_2O_3$ monolith	Sealed on the LED chip	85%	$400 \ h^{11}$
CdSe QD-AS	Alloyed thick shell QDs	$85^\circ\mathrm{C},85\%$ relative humidity	85%	$400 \ h^{12}$

Table S8: Datasheet of stability of various types of QDs/NCs.

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