

Supplementary Information

for

Broadband photodetectors from silane-passivated CsPbBr₃ nanocrystals by ultrasound-mediated synthesis

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1. Sonication time effect on reaction temperature

The standard condition reported in our manuscript was determined based on preliminary experiment using solely isoparaffin and setting the ultrasound amplitude at 40%. Above 40% amplitude the internal temperature increases well above boiling point of the solvent isoparaffin (bP: 138°C) leading to evaporation of the solvent which in turns change the concentration of the reaction. The time-temperature profile obtained at 160W (40% amplitude) is presented in Fig. S1 bellow.

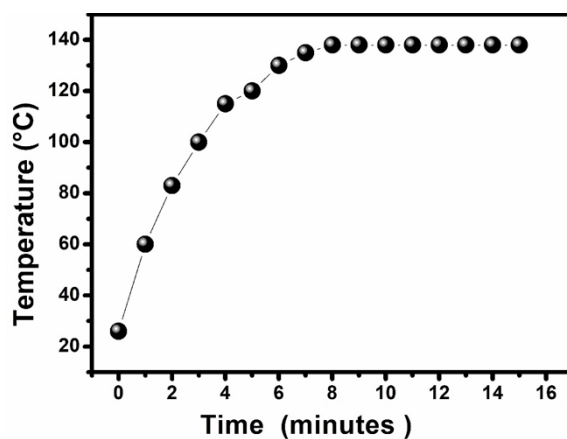


Fig. S1. Temperature as a function of time using 160W (40 % amplitude).

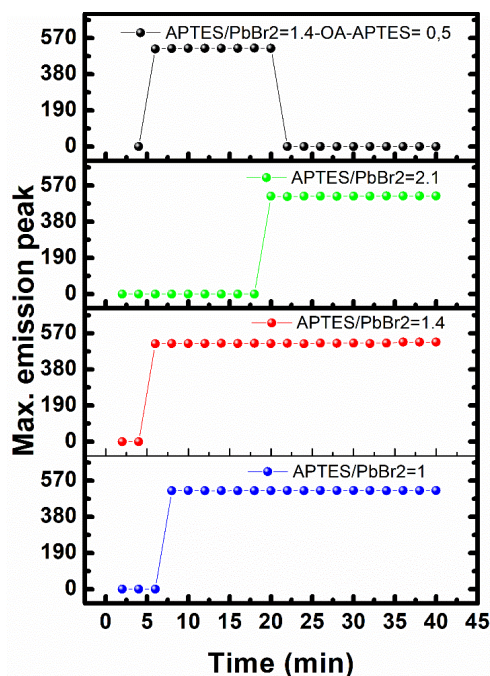


Fig. S2. Graph of the maximum emission of PL spectra per time of aliquots of CsPbBr₃-OA-APTS in toluene collected at different times of synthesis. APTS/PbBr₂=1.4 (red dots), APTS/PbBr₂=1.4-OA:APTS =0.5 (black dots), APTS/PbBr₂=2.1 (green dots) and APTS/ PbBr₂=1(blue dots).

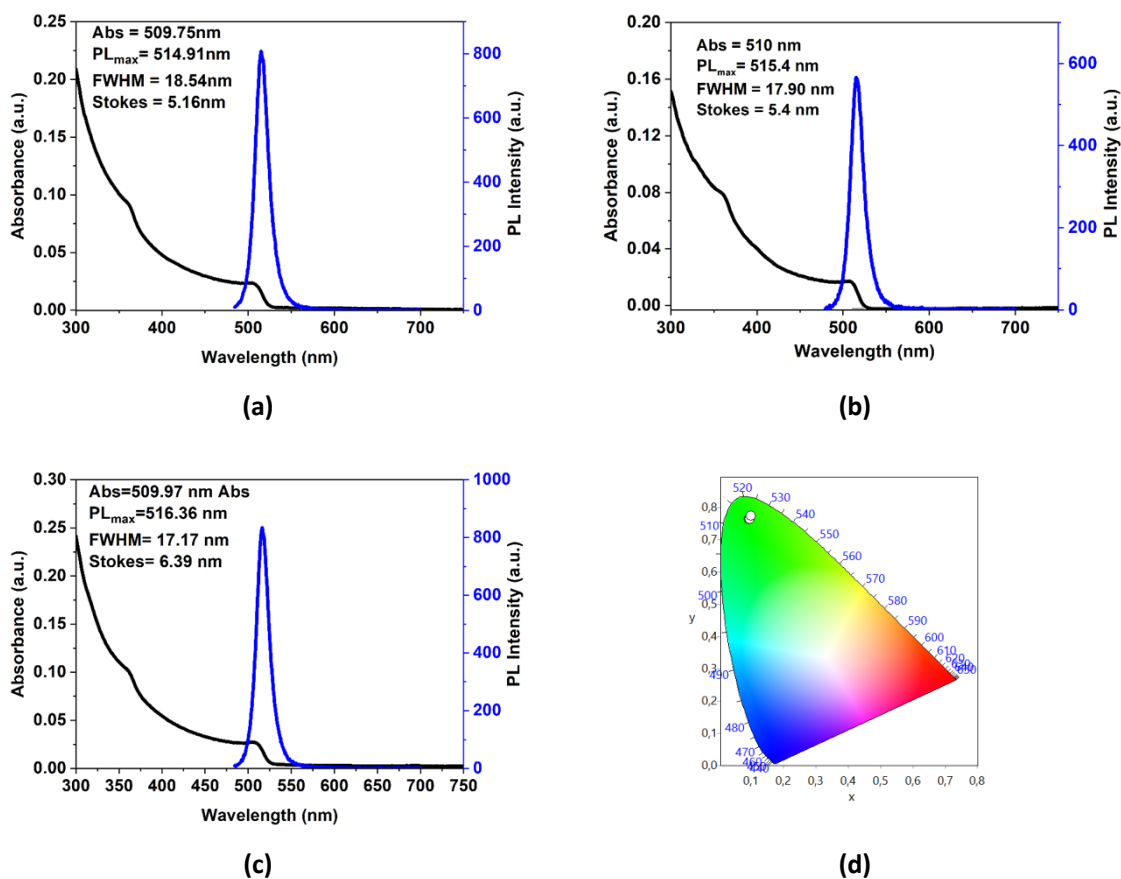


Fig. S3. UV-vis absorption spectrum (black line) and PL emission spectrum (blue line) a) APTS/PbBr₂=1.4, b) APTS/PbBr₂=1.4-OA:APTS=0.5, and c) APTS/PbBr₂ =2.1.

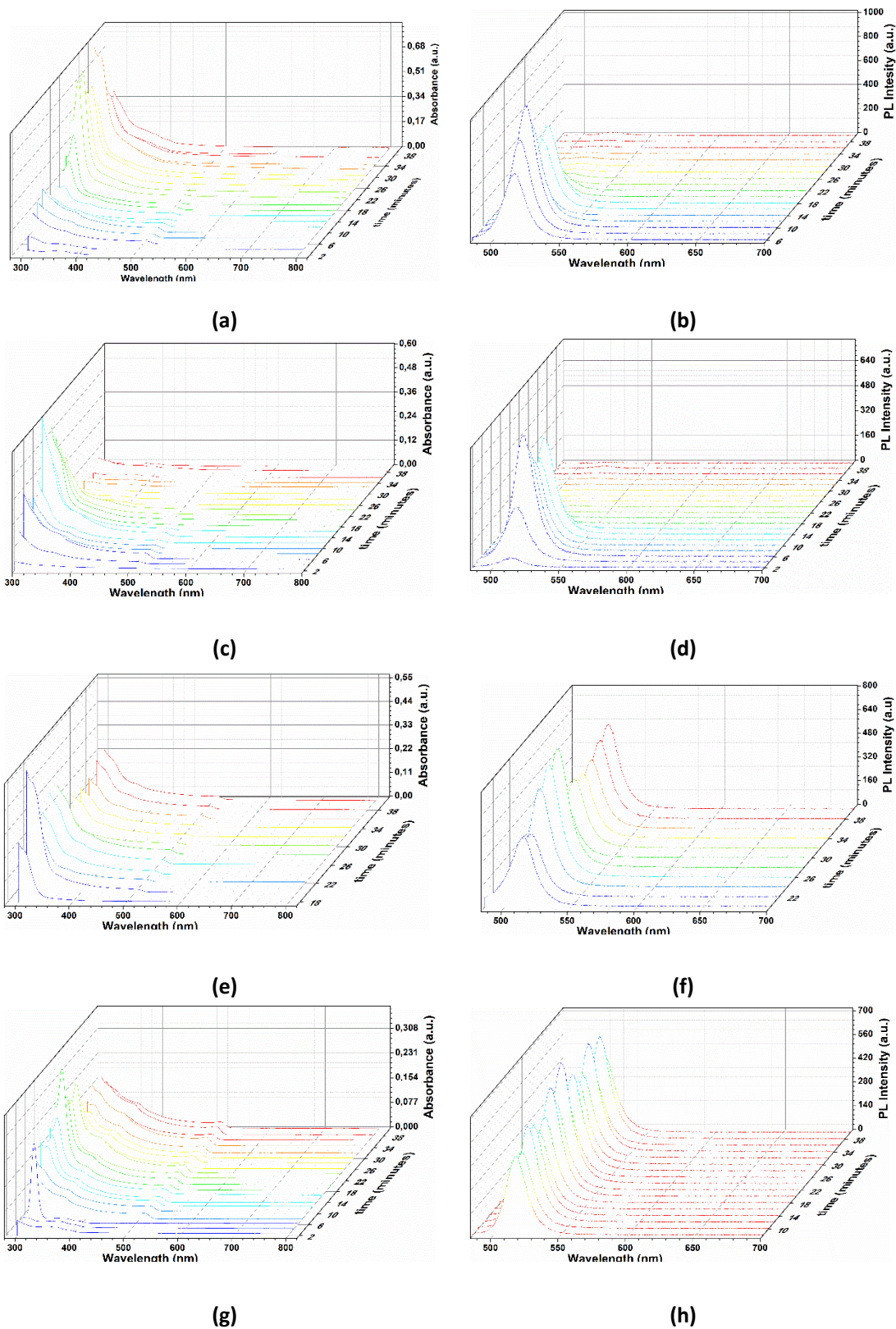


Fig. S4. Absorption spectra (left) PL spectra (right) of aliquots of CsPbBr₃-OA-APTS in toluene collected at different times of synthesis. a) and b) APTS/PbBr₂=1.4, c) and d) APTS/PbBr₂=1.4-OA:APTS= 0.5, e) and f) APTS/PbBr₂=2.1 and g) and h) APTS/ PbBr₂=1.

2. Photoluminescence quantum yield (PLQY)

The PLQY was calculated using the comparative method using the dye with known absolute quantum yield and absorption in a region with a wavelength like the sample by equation 1:

$$\Phi_{f,x} = \Phi_{f,st} * \frac{F_x}{F_{st}} * \frac{f_{st}}{f_x} * \frac{n^2_x}{n^2_{st}} \quad \text{equation (1)}$$

In the equation 1 the x denotes the samples and st denotes the standard, Φ is the PLQY, F is the integral photon flux, f is the absorption factor, n is the refractive index of the solvent. The relative integral photon fluxes F of the spectrally corrected and blank corrected spectra of the samples were calculated using the equation 2

$$F = \int_{\lambda_{em}} I_c * \lambda_{em} d\lambda_{em} \quad \text{equation (2)}$$

The index I_c denotes the corrected spectra. The limits of the integration of the emission spectra cover the complete emission band of the samples and standard. The absorption factors were calculated using the equation 3:

$$f = 1 - 10^{-A(\lambda_{ex})} \quad \text{equation (3)}$$

The index A is the value of the absorbance at the excitation wavelength. For the determination of relative PLQY of CsPbBr₃ NCs was used sodium fluorescein that has $\Phi = 0.89$ in a 0.1M NaOH solution. The solution of fluorescein and the dispersion of the sample (CsPbBr₃ NCs) were prepared, and the measurements of the emission and absorption spectrums was done with identical instrument configurations (excitation wavelength, excitation and emission monochromator slit widths, speed, time integration). The spectra of the solvents used for the samples and standard were also measured under the same conditions to obtain the corrected spectra. The concentrations of the sample and standard solutions were adjusted for the A values corresponding at the excitation wavelength are close as possible and the absorbance spectra must be less than 0.1 (Figure S2).

After preparing the solutions absorption and emission spectrum of the CsPbBr₃ NCs were recorded and again after 5 minutes to certify that the absorption and emission remained constant (Figure S3 (a) and (b)). The dispersions of CsPbBr₃ NCs were diluted by a factor of 5 to assess whether the absorbance values and the maximum emission decreased by the same factor and whether the shape of the spectrum remains the same (Figure S3 (c) and (d)).

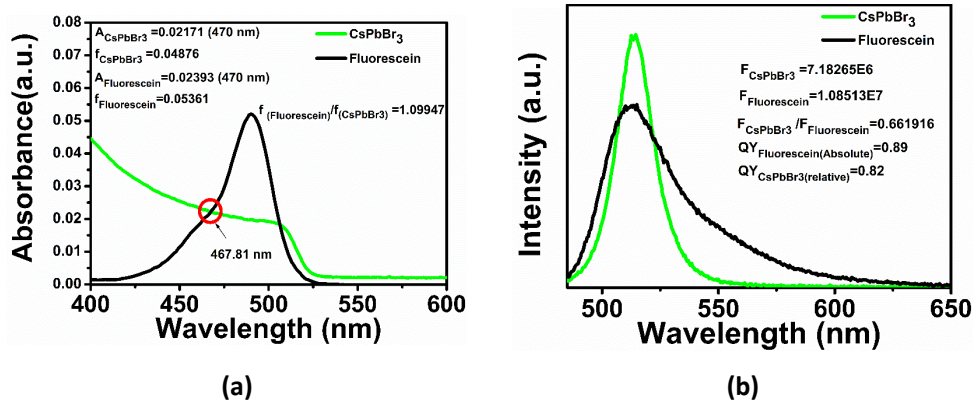
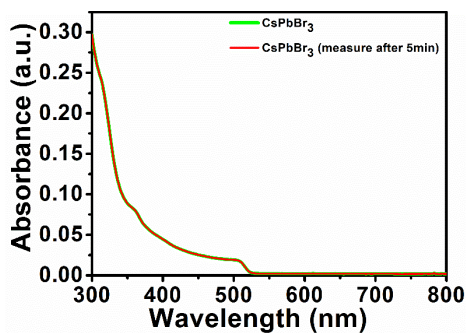
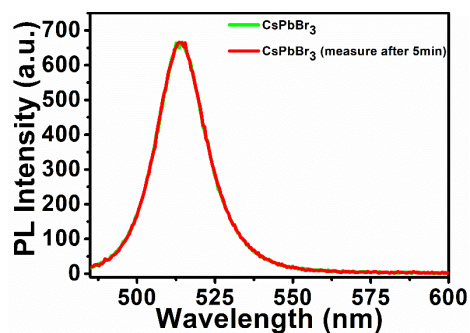


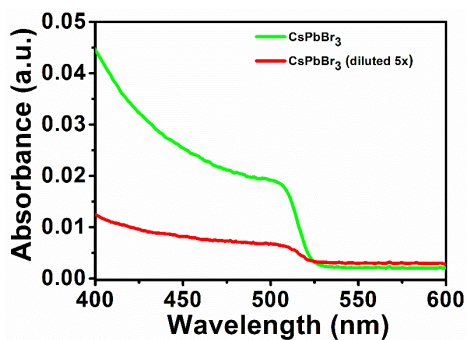
Fig. S5. Sodium fluorescein in 0.1M NaOH solution and CsPbBr₃ NCs in toluene (a) absorption spectra and (b) emission spectra.



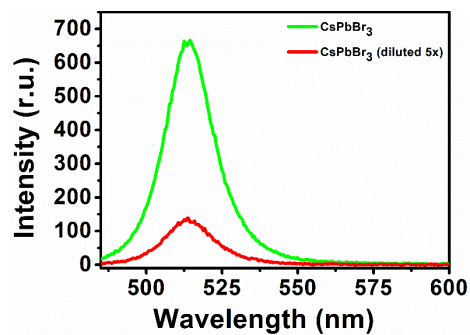
(a)



(b)

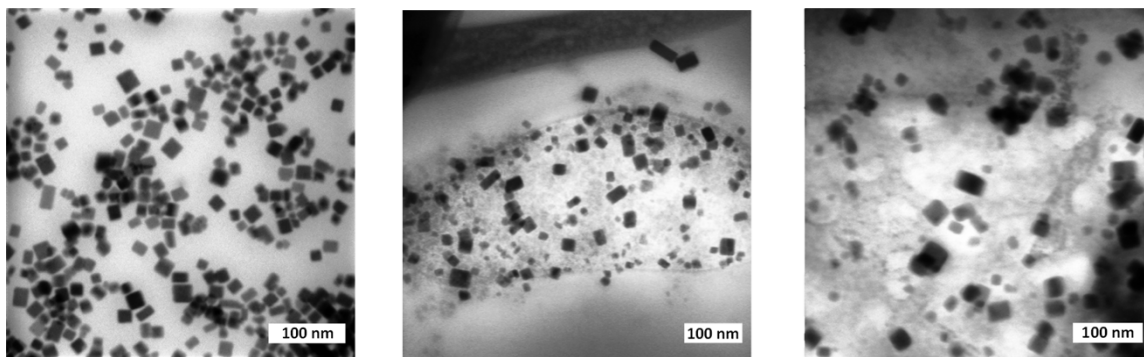


(c)



(d)

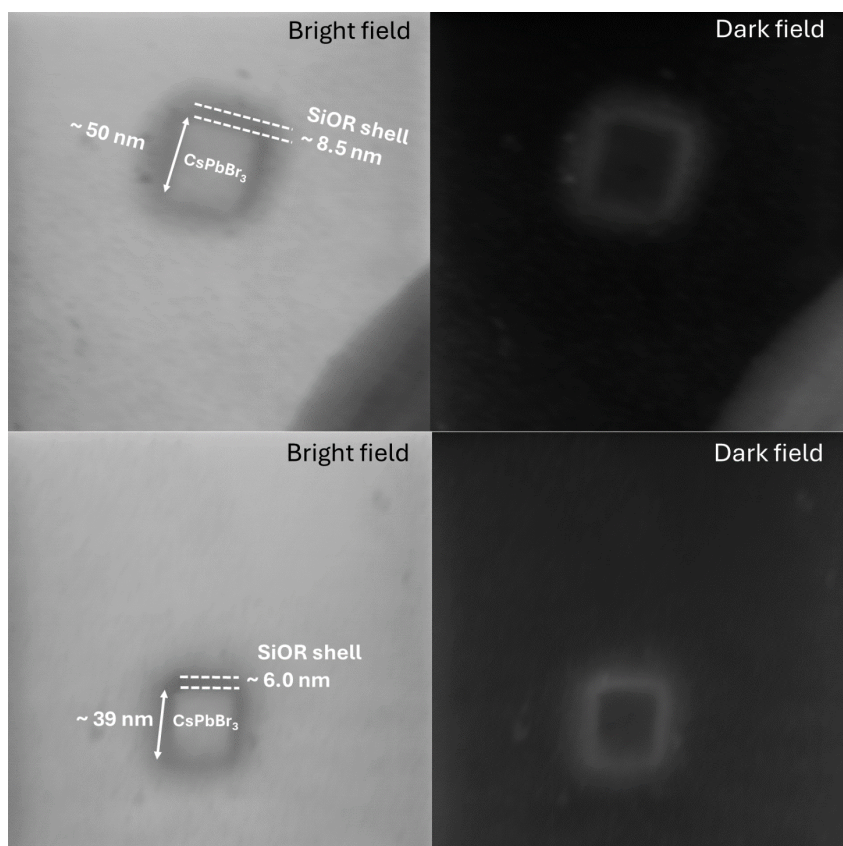
Fig. S6. Spectrums a) absorption and b) emission of CsPbBr₃ NCs in toluene and spectrums measure after 5 minutes. Spectrums c) absorption and d) emission of CsPbBr₃ NCs in toluene diluted by a factor roughly 5.



(a)

(b)

(c)



(d)

Fig. S7. STEM image of CsPbBr₃ ensemble with a) PbBr₂:APTS=1:1.4, b) PbBr₂:APTS=2.1 molar ratio and c) PbBr₂:APTS =1:1.0. (d) STEM bright and dark field images for isolated CsPbBr₃ NCs prepared under optimized PbBr₂:APTS =1:1.0. This sample was isolated as a powder and aged over 2 years under ordinary conditions.

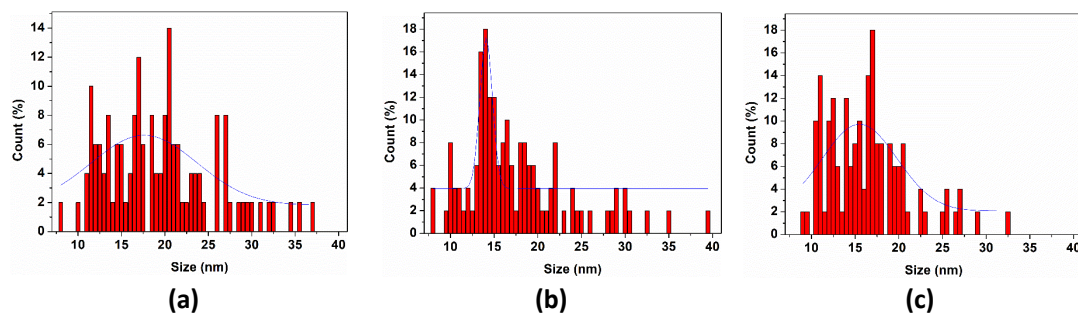


Fig. S8. Lateral size distribution calculated by STEM of CsPbBr₃ NCs with OA and APTS like ligand surface. a) PbBr₂:APTS =1:2.1 1:1.4, b) PbBr₂:APTS =1:1.4 and c) PbBr₂:APTS =1:1.0.

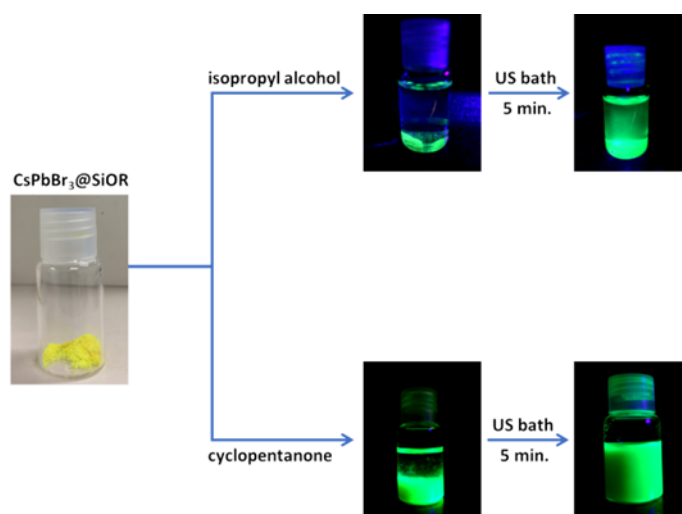


Fig. S9. Photographs of CsPbBr₃@SiOR dispersed in polar solvents under UV-light.

3. CsPbBr₃@SiOR stability evaluation under moisture

For this experiment, we used a two-years-old CsPbBr₃@SiOR powder sample. During this period, this sample was storage under ordinary laboratory condition without any special care. Visually, it presents intense bright green emission under UV light just like the fresh sample. The powder was dispersed from toluene, and it deposited on glass substrate by spin-coating (1000 rpm, 60s, annealing at 100°C). The process was repeated 5 times to render a 320 nm thick film. Then, the sample was transferred to a chamber with controlled RH = $69.7 \pm 2\%$ and T $\approx 25^\circ\text{C}$. PL signal was collected using a fiber- spectrometer exciting the sample with a 405 nm laser (P = 80 mW) as shown in Fig. S9. The PL spectra were collected every 15 minutes for 5 hours. The adjustment of humidity was done by using a potassium iodide (KI) aqueous saturated solution prepared by mixing 192g of KI in 100 mL of water. The mixture was heated to completely dissolve the KI and then cooled to form a precipitate (approximately 25% of the total volume). The KI Saturated solution was placed in the chamber 24 hours before starting the experiment and monitored real-time by a humidity and temperature sensor.

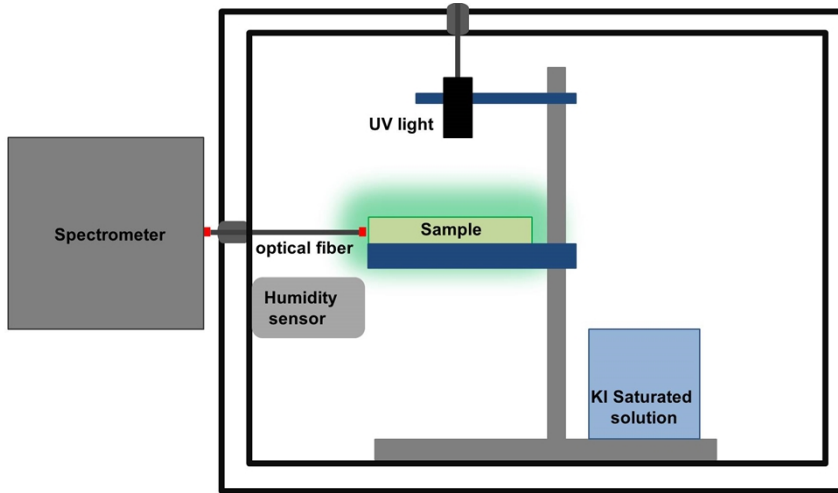


Fig. S10 Schematic representation for the setup for stability evaluation under moisture.

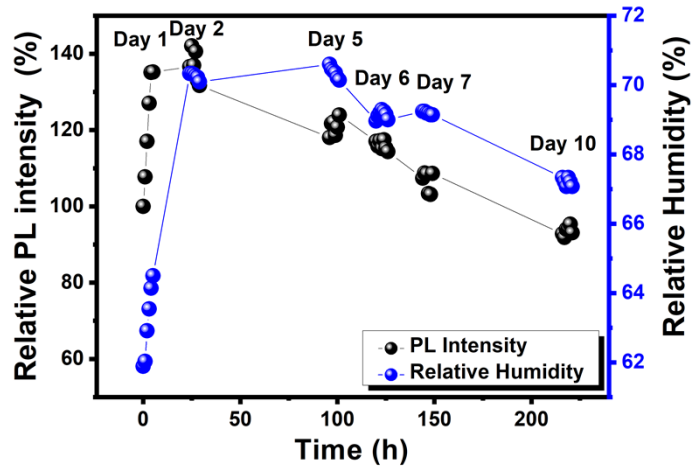


Fig. S11. Excitation-normalized PL spectra collect under high humidity for CsPbBr₃@SiOR film n glass.

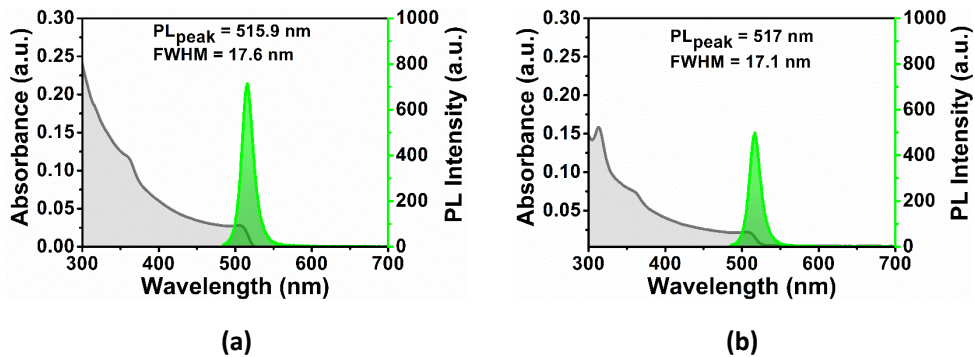


Fig. S12. UV-vis and PL spectra for CsPbBr₃@SiOR prepared with (a) PbBr₂/APTS = 1:1.4 and (b) 1:2.1.

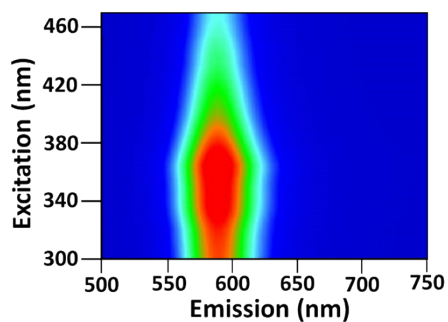


Fig. S13. Two-dimensional photoluminescence excitation (2D-PL) spectra measured for a purified sample prepared with PbBr_2 :APTS =1 molar ratio (red color indicates higher PL).

Table S1. Parameters obtained of the lateral size distribution of CsPbBr_3 NCs with OA and APTS ligands.

PbBr_2 /APTS molar ratio	Minimum size [nm]	Maximum size [nm]	Diameter [nm]	Standard deviation
1:1	9.42	32.72	16.66	± 4.60
1:1.4	8.14	39.87	17.44	± 5.78
1:2.1	8.49	37.23	19.67	± 6.21

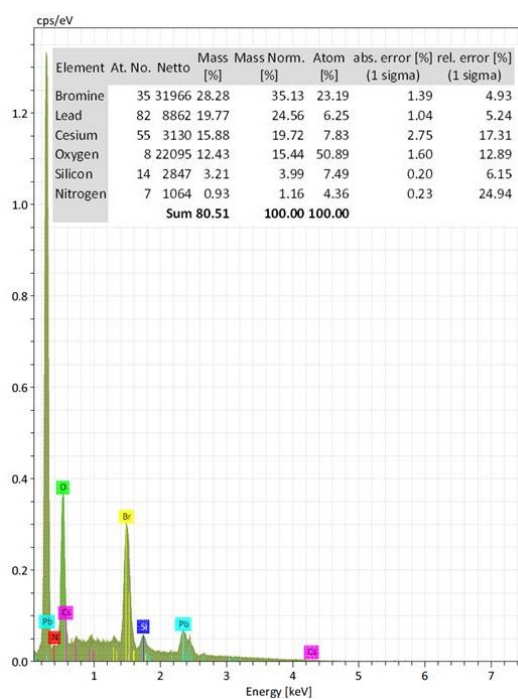
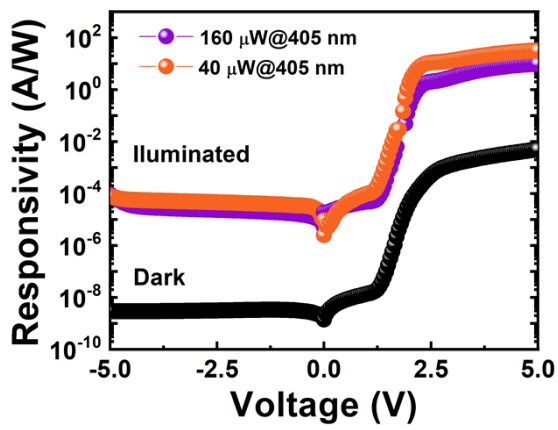
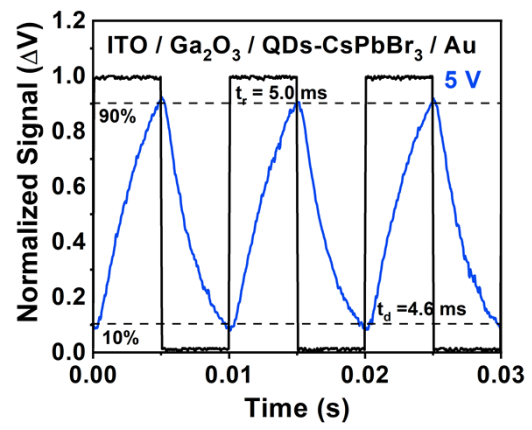


Fig. S14. EDS spectrum of CsPbBr_3 @SiOR (PbBr_2 /APTS =1:1).



(a)



(b)

Fig. S15. Responsivity of the photodiode PD upon different excitation power at 405 nm.