Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Short-branched alkyl sulfobetaine passivated $CsPbBr_3$ nanocrystals for efficient green light emitting diodes

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Materials and Chemicals. The materials and reagents used were: lead bromide ($PbBr_2$, Xi'an Polymer Light Technology Corp., 99.999%), cesium carbonate (Cs_2CO_3, Energy Chemical, 99.9%), 1,3-propane sultone ($C_3H_6O_3S$, Energy Chemical, 98%), 1,4-butane sultone （$C_4H_8O_3S$，Energy Chemical, 98%), tri-n-octylamine ($C_{24}H_{51}N$, Sigma-Aldrich, 97%), trioctylphosphine oxide (TOPO, Strem Chemicals, 90%), diisooctylphosphinic acid (DOPA, Sigma-Aldrich, 90%), lecithin ($C_{42}H_{80}NO_8P$, Sigma-Aldrich, 97%), deuterated chloroform ($CDCl_3$, Sigma-Aldrich, 99.8 atom % D), acetone (C_3H_6O, SCRC, AR), n-octane (C_8H_{18}, Alfa Aesar, anhydrous 99%), n-hexane (C_6H_{14}, SCRC, AR), ethanol (EtOH, SCRC, 99.7% anhydrous), Methyl acetate (MeOAc, Alfa Aesar, 99.8% anhydrous), poly(bis(4-phenyl)(2,4,6-trimethylphenyl) amine) (PTAA, Xi'an 20 Polymer Light Technology Corp.), molybdenum trioxide (MoO_3, Fuzhou Invention Photoelectrical 8 Technology, 99.99%), aluminum (Al, Fuzhou Invention Photoelectrical Technology, 5N), lithium fluoride (LiF, Luminescence Technology Corp.), 4,6-bis(3,5-di(pyridin-3-yl)phenyl)-2-10methylpyrimidine (B3PymPm, Luminescence technology corp.), 2,4,6-tris[3-11 (diphenylphosphinyl)phenyl]-1,3,5-triazine (PO-T2T, Nichem). All reagents were used as received without further purification.

Preparation of $PbBr_2$ stock solution. 1 mmol of $PbBr_2$ and 5 mmol of TOPO was added to octane (5 mL), sonicated until dissolved, and then diluted with 20 mL hexane.

Preparation of Cs-DOPA stock solution. 100 mg of Cs_2CO_3 was added to the mixed solvent of DOPA (1 mL) and octane (2 mL), sonicated until dissolved, and then diluted with 27 mL hexane.

Preparation of lecithin stock solution. 0.5 g of lecithin was added to10 mL hexane, sonicated until dissolved.

Synthesis of TOAB. 3-Propanesultone (5 mmol) and trimethylamine (5 mmol) were dissolved in acetone and heated to 60 °C and kept under reflux for 24 hours. After completion of the reaction, the acetone is then removed under reduced pressure and a yellow oily liquid is obtained. The mixture was washed three times with ethyl acetate, and the ethyl acetate was removed under reduced pressure. After vacuum drying, it was obtained as a white powder. Yield after purification: 80 %.

Synthesis of SB-n-3. N,N-Dimethylalkylamine (10 mmol) with different carbon chain length (n) was dissolved in 15 mL acetone. Subsequently, 1,3-propane sultone (10 mmol) was slowly added and the mixture was heated to 60 °C and kept under reflux for 24 hours. After completion of the reaction, the acetone is then removed under reduced pressure and a yellow oily liquid is obtained. The mixture was washed three times with acetone, and the acetone was removed under reduced pressure. After vacuum drying, it was obtained as a white powder. Yield after purification:90 %.

Determination of charge carrier mobility and trap state density from SCLC measurement. In the space charge limited current (SCLC) method, the electron-only or hole-only devices will first exhibit an ohmic behavior, in which current is linearly at low voltage. When the voltage increases to an inflection point, the devices exhibit the filling process of trap, in which current exhibits a no-linear rise, and the voltage at the intersection point between the linear and non-linear region is defined as the trap-filled limit voltage (V_{TFL}). The trap state densities (N_{trap}) is determined by using the equation:

$$N_{trap} = \frac{2\varepsilon\varepsilon_0}{eL^2}V_{TFL}$$

where ε_0 is the vacuum permittivity, ε is the relative permittivity of perovskite (around 22 for $CsPbBr_3$), V_{TFL} is the trap-filled-limit voltage, e is the elementary charge, and L is the thickness of perovskite film. The values of carrier mobility (μ) are calculated from the Child region (after the trap-filled limit region) according to Mott-Gurney's equation:

$$\mu = \frac{8J_D L^3}{9\varepsilon\varepsilon_0 V^2}$$

where J_D is the current density and V is the applied voltage.

Tables and Figures

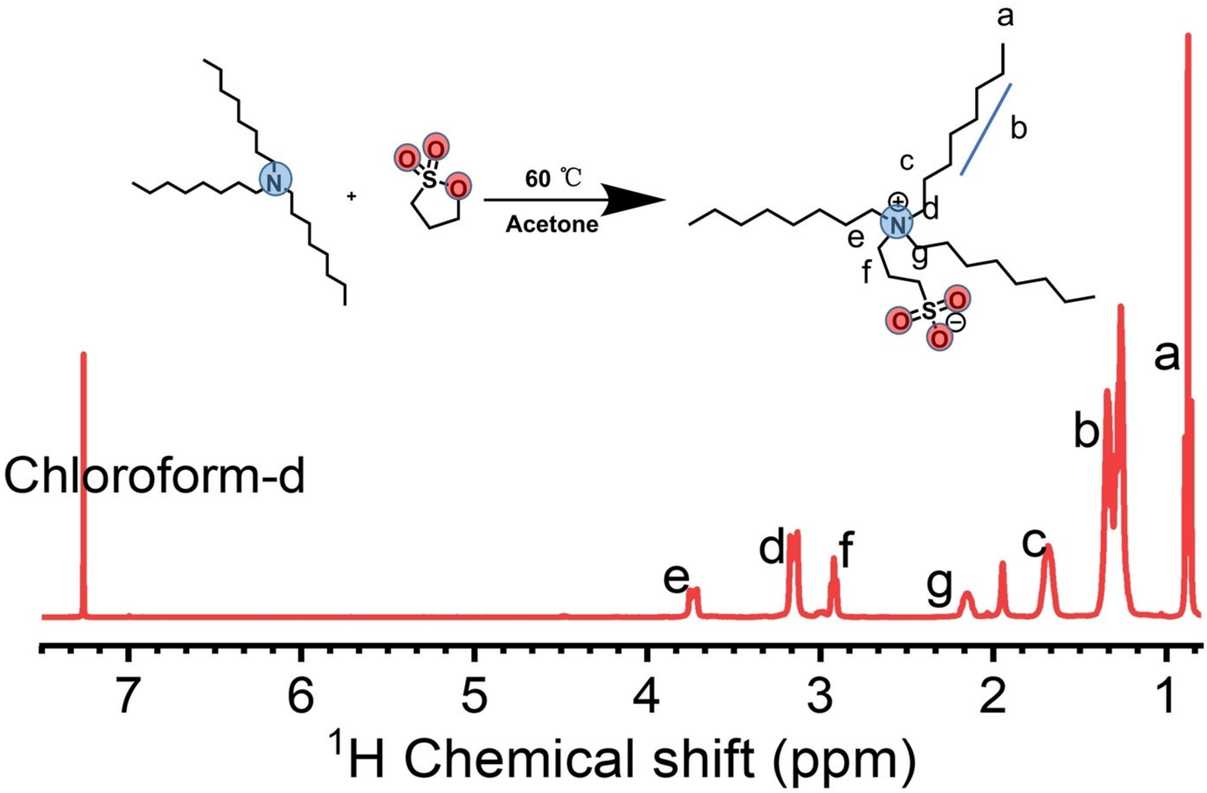

Figure S1. ^{1}H liquid-state NMR spectrum of TOAB dispersed in deuterated chloroform ($CDCl_3$). The inset shows the corresponding synthetic scheme.

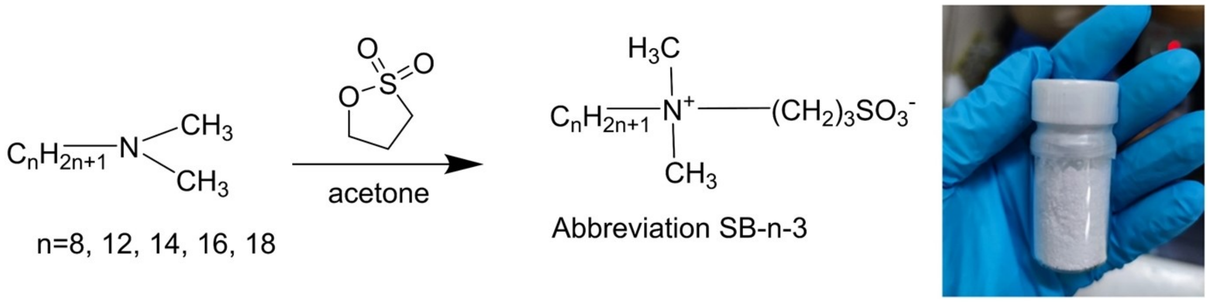

Figure S2. Summary of the synthesis of a series of long-chain sulfobetaine ligand.

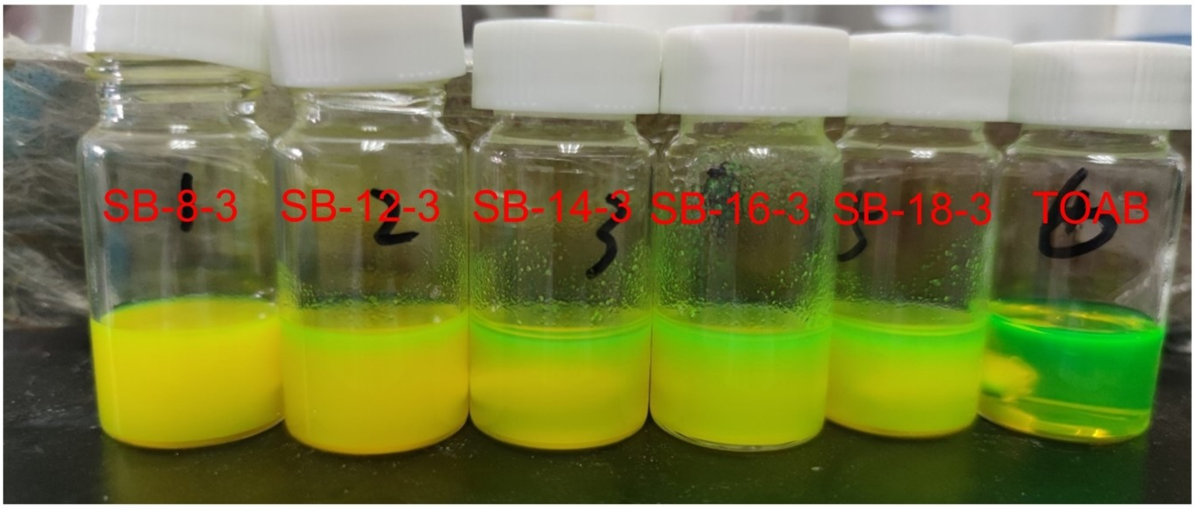

Figure S3. A photo of $CsPbBr_3$ NCs obtained by employing a variety of sulfobetaine-based ligands.

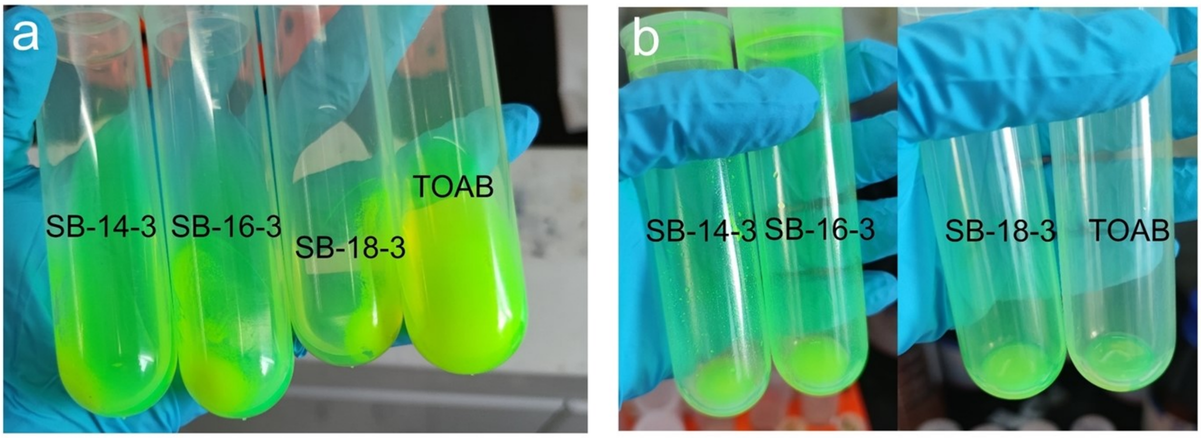

Figure S4. Photographs of $CsPbBr_3$ NCs synthesized by using several representative sulfobetaine-type ligands that were purified and post-treated with the polar solvent methyl acetate. (a) Addition of three times the volume of methyl acetate of the stock solution followed by high-speed centrifugation (10000 rpm for 5 min). (b) Upon adding 400 μL of n-octane dispersion, only $CsPbBr_3$ NCs passivated by TOAB can be dispersed.

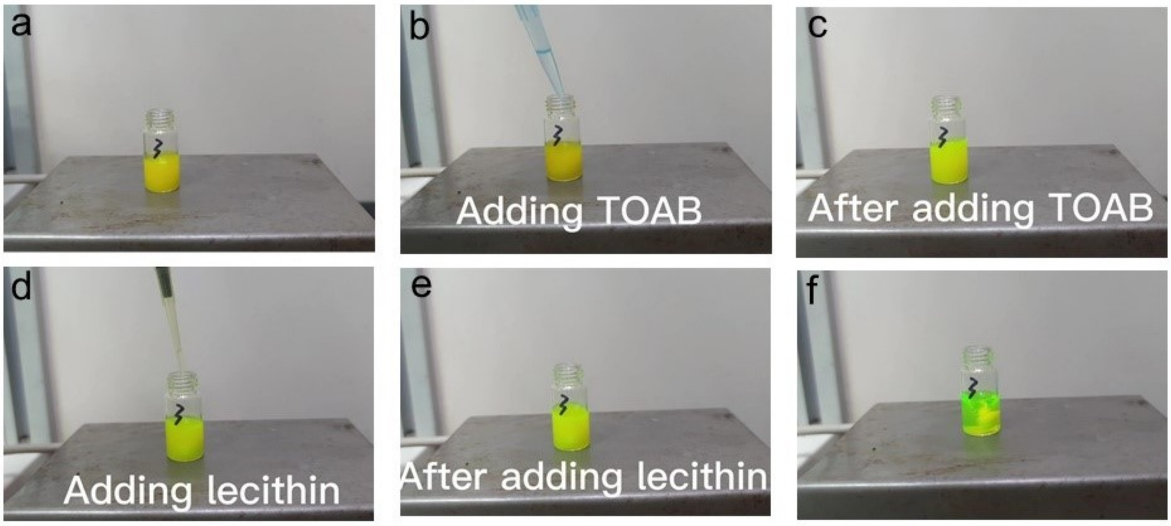

Figure S5. Photographs of several key steps of the ligand exchange process for $CsPbBr_3$ NCs. (a) After the formation of $CsPbBr_3$ NCs, (b) the addition of TOAB, (c) after the addition of TOAB, (d) the addition of lecithin, (e) after the addition of lecithin, and (f) the resulting clear and transparent NCs solution after ligand exchange.

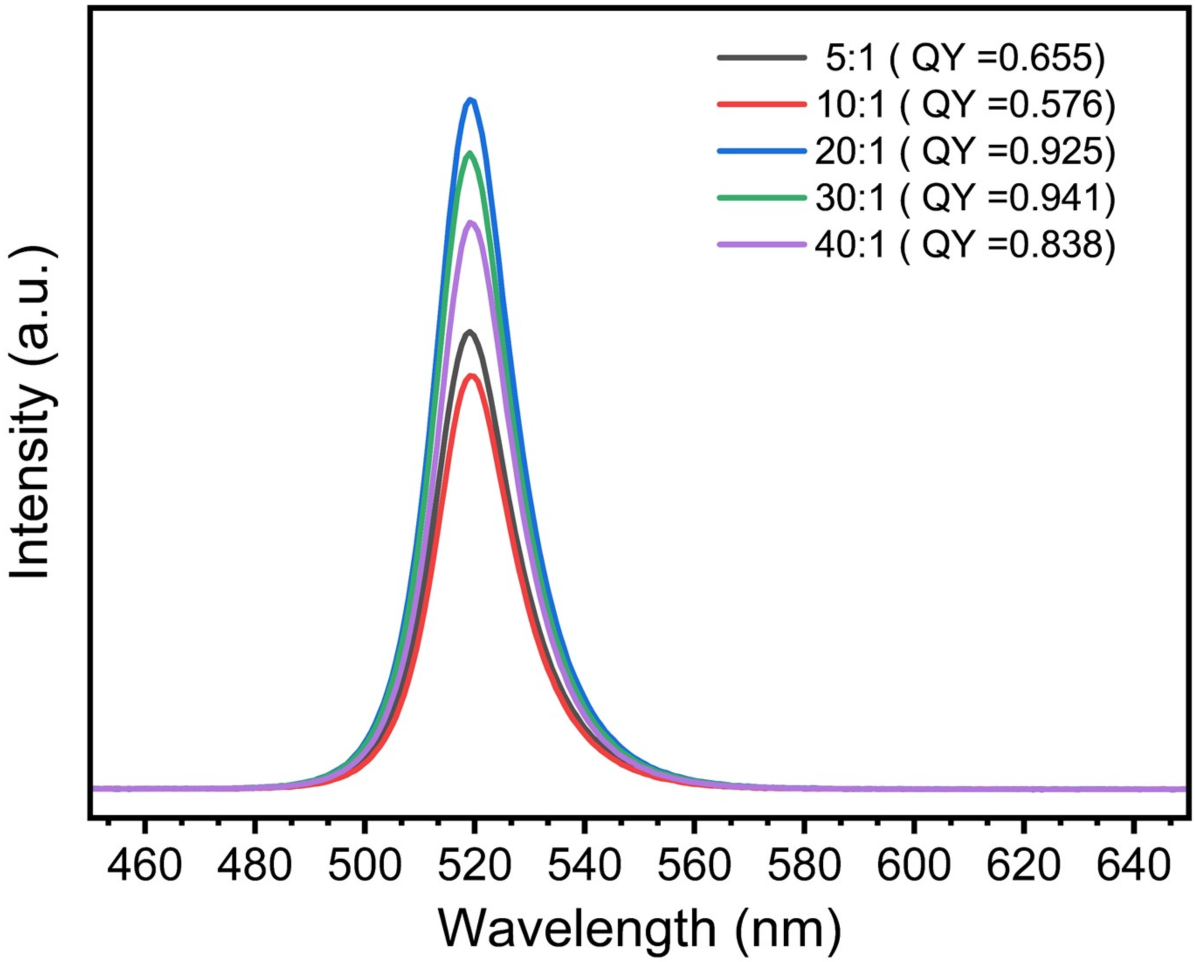

Figure S6. PL spectra of TOAB passivated NCs with different TOAB:lecithin ratios during ligand exchange (excitation wavelength 365 nm).

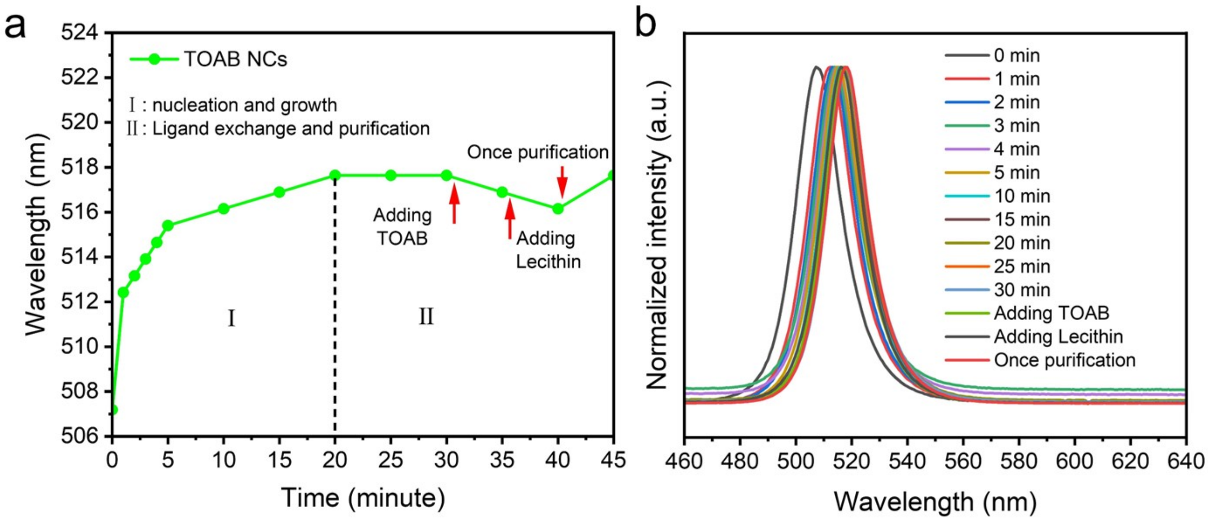

Figure S7. Nucleation and growth stage and ligand exchange stage in TOAB passivated NCs. (a) Changes in PL peak positions during nucleation and growth and ligand exchange in $CsPbBr_3$ NCs. (b) Normalized PL spectra of $CsPbBr_3$ NCs obtained at different times during nucleation and growth stage and ligand exchange stage.

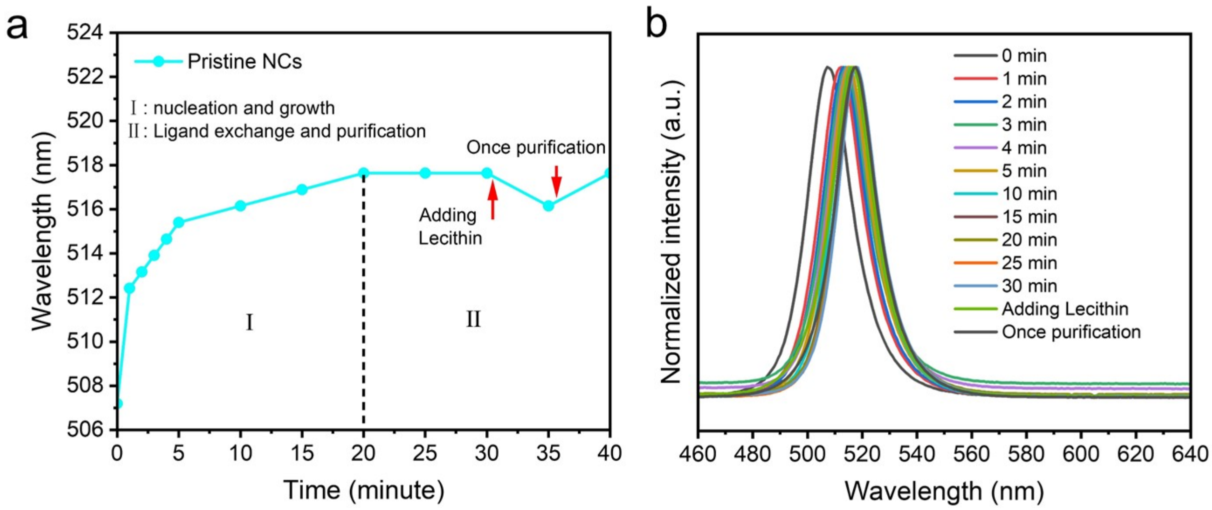

Figure S8. Nucleation and growth stage and ligand exchange stage in pristine NCs. (a) Changes in PL peak positions of $CsPbBr_3$ NCs. (b) Normalized PL spectra of $CsPbBr_3$ NCs obtained at different times.

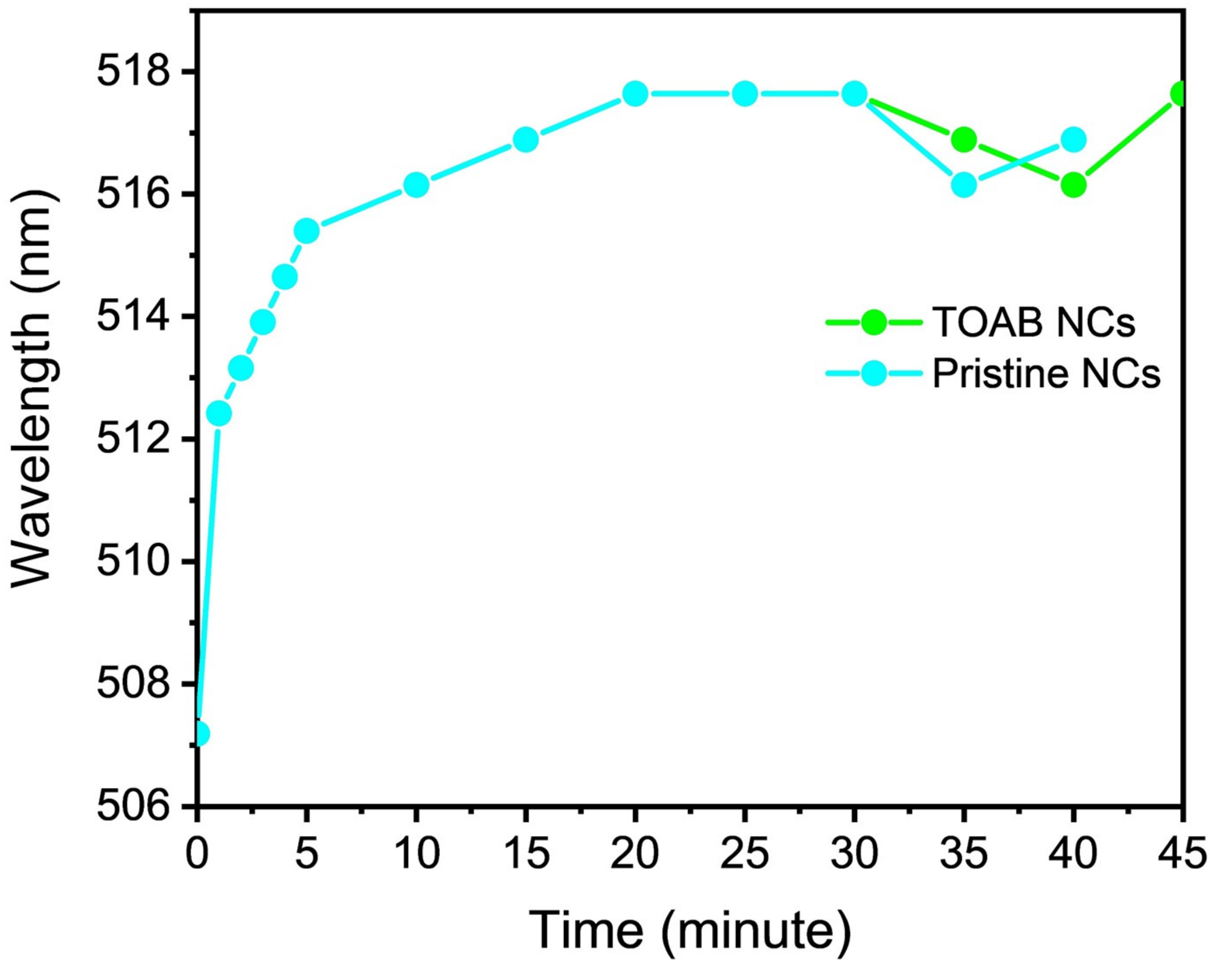

Figure S9. Changes in PL peak positions of pristine and TOAB passivated NCs during nucleation and growth stage and ligand exchange stage.

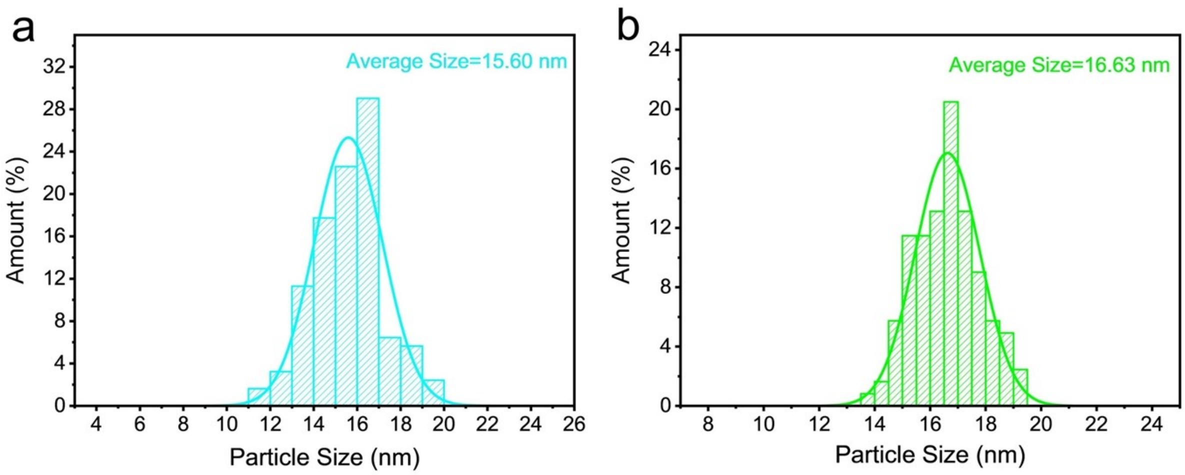

Figure S10. Particle size distribution histograms of the different $CsPbBr_3$ NCs. (a) Pristine $CsPbBr_3$ and (b) TOAB $CsPbBr_3$ NCs.

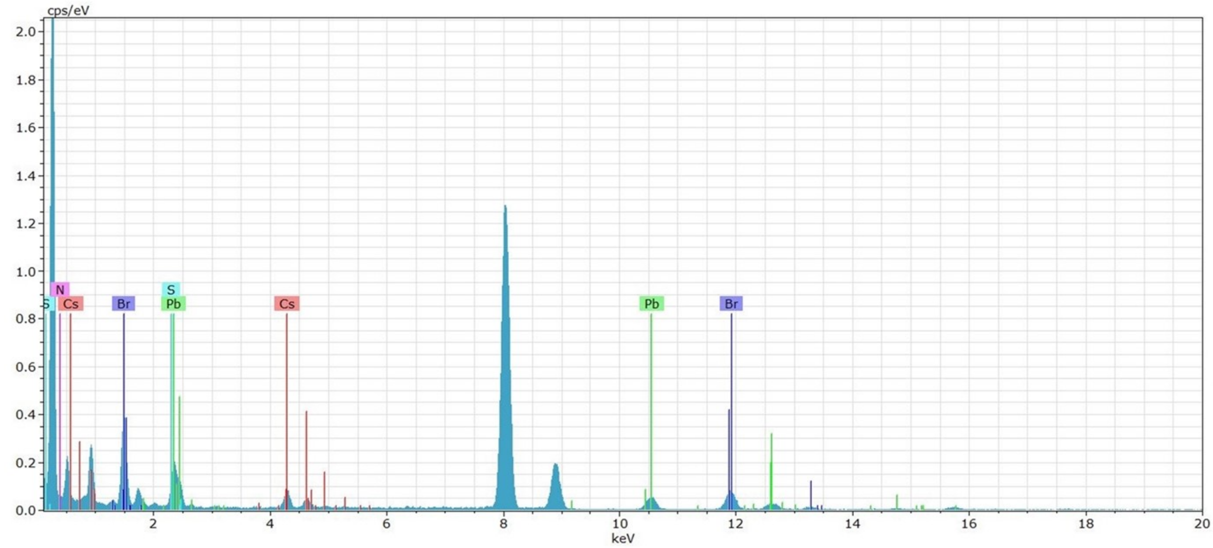

Figure S11. Energy dispersive X-ray spectroscopy of TOAB passivated $CsPbBr_3$ NCs.

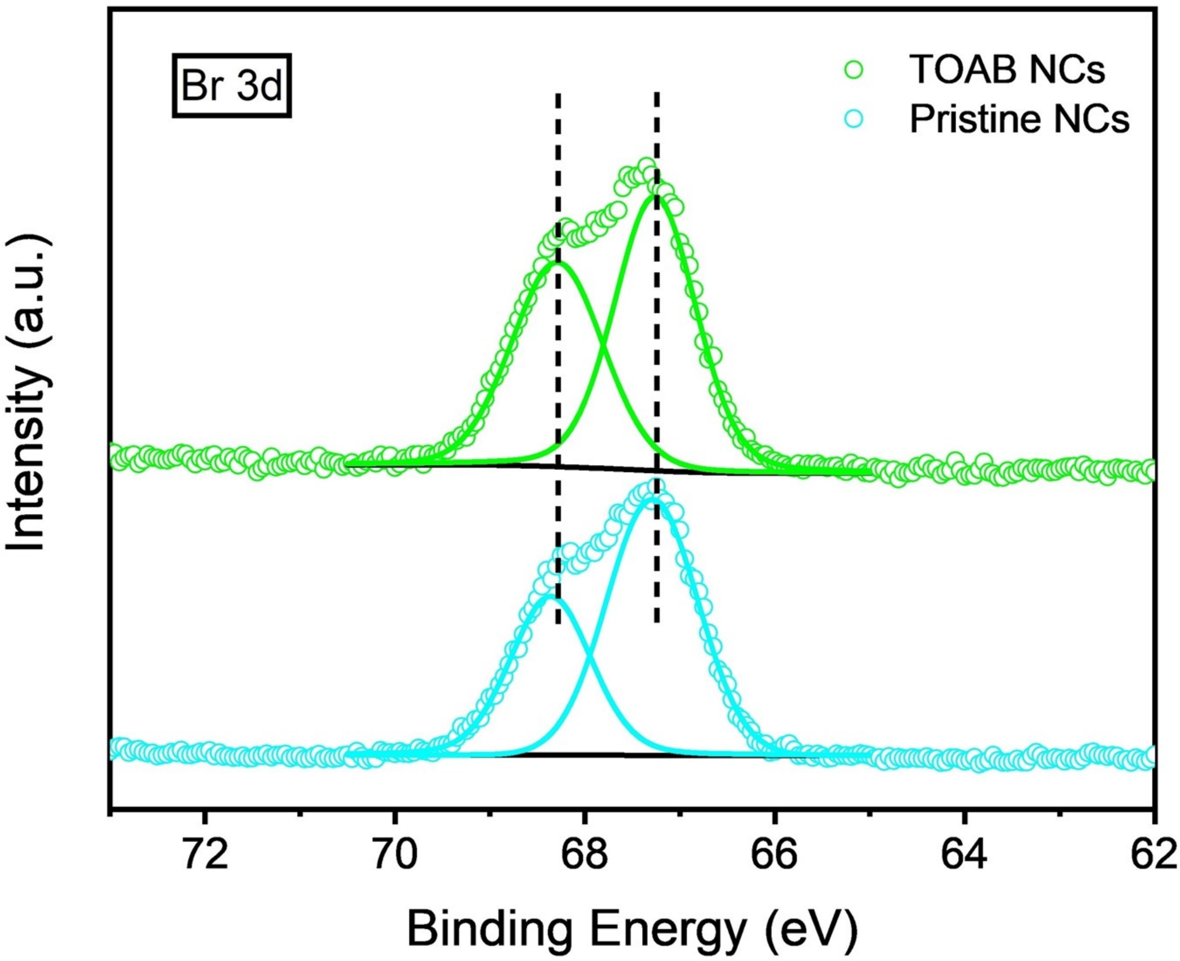

Figure S12. The high-resolution XPS analysis of pristine and TOAB passivated $CsPbBr_3$ NCs for Br 3d.

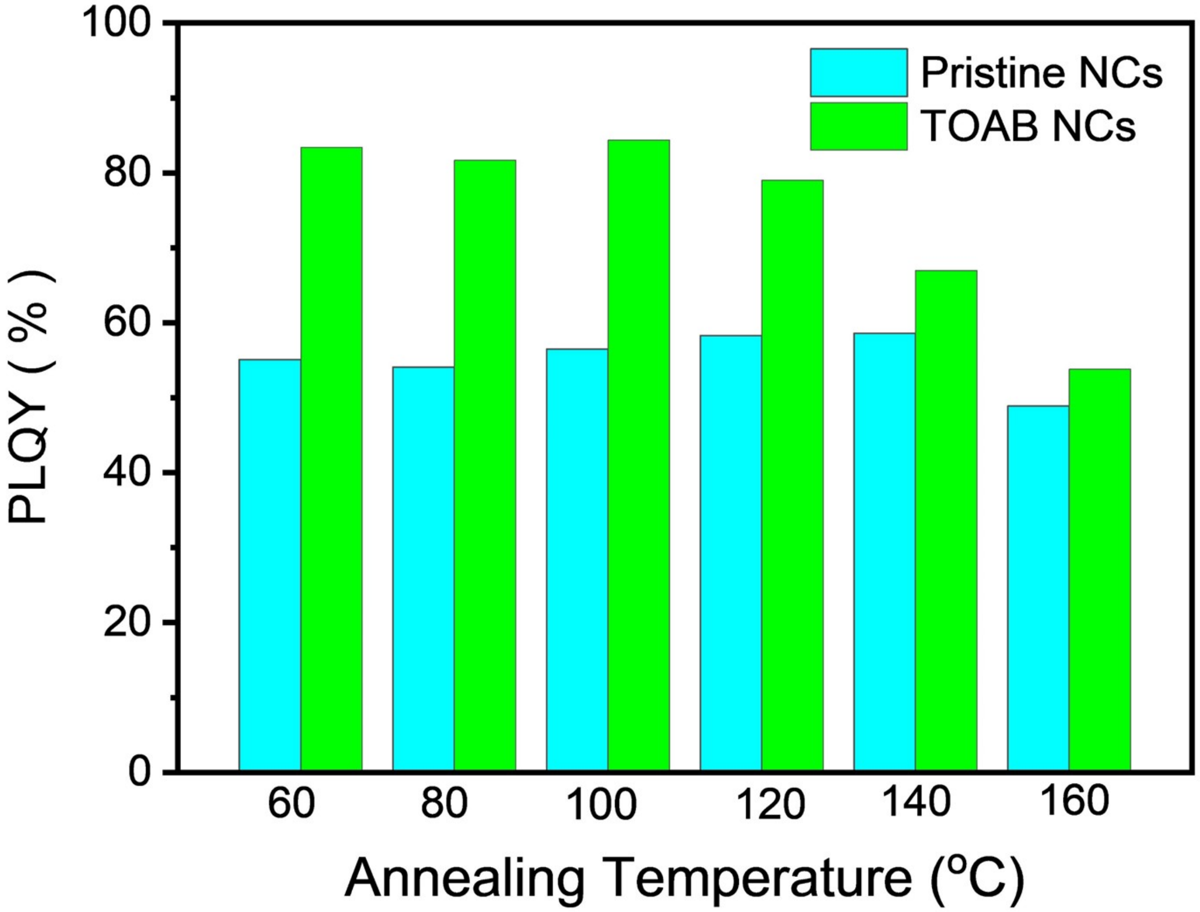

Figure S13. PLQY as a function of annealing temperature for pristine and TOAB passivated $CsPbBr_3$ NC films.

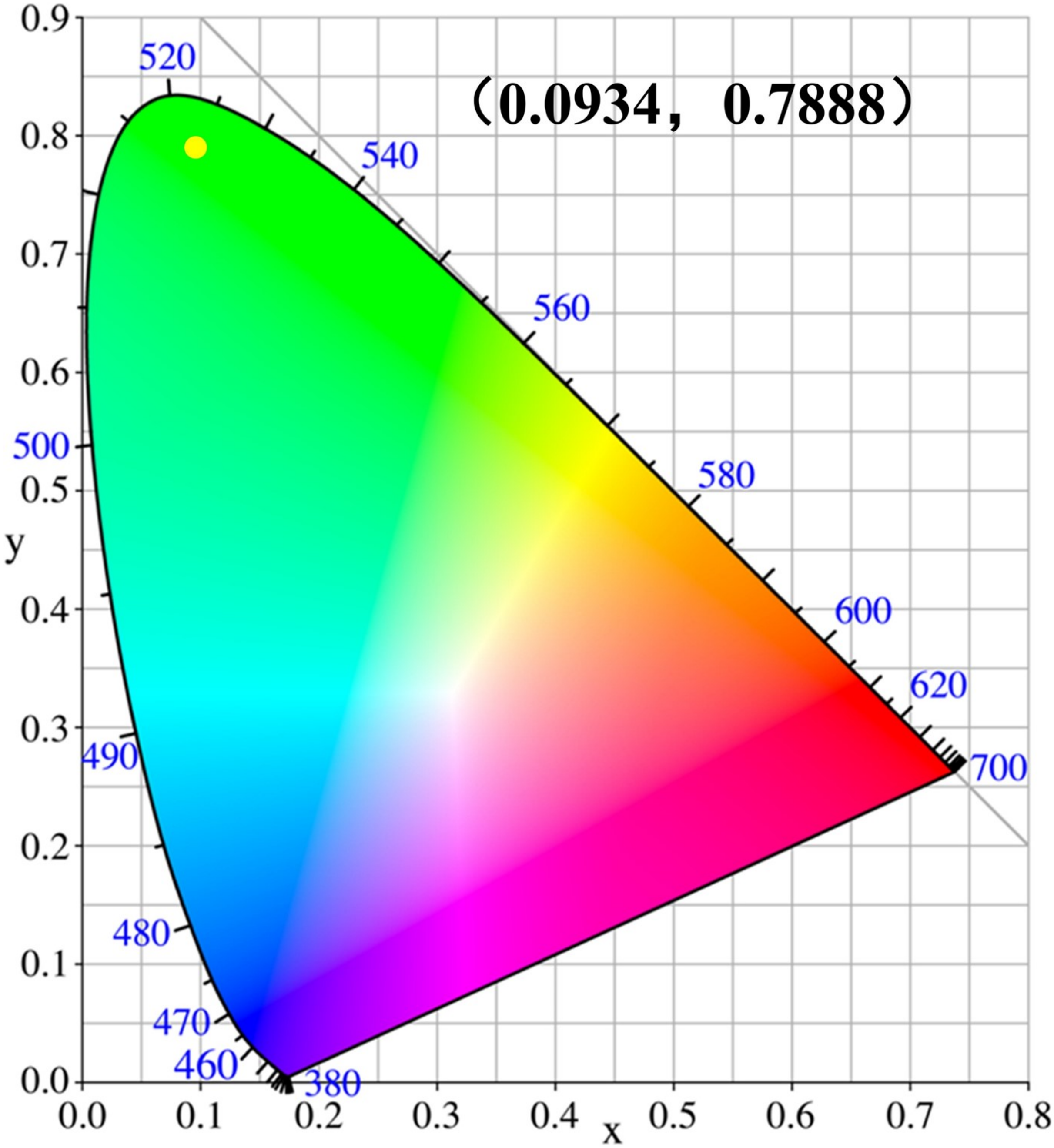

Figure S14. The corresponding Commission Internationale de l'Eclairage (CIE) coordinate of the fabricated TOAB passivated $CsPbBr_3$ NCs based LED.

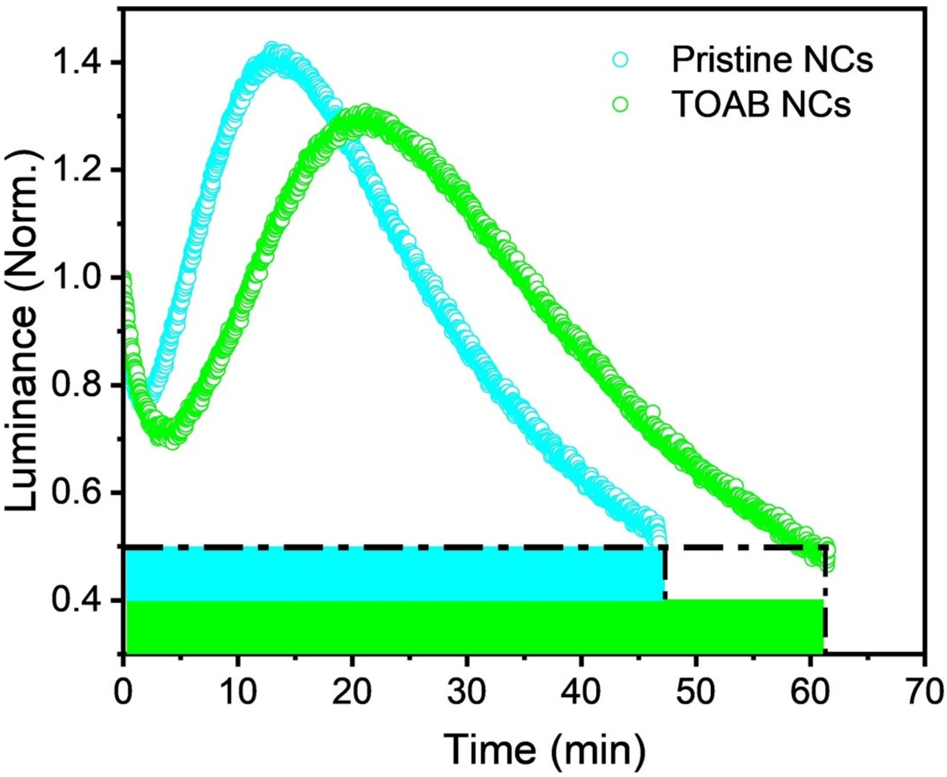

Figure S15. Operation lifetime for the NC LED at constant voltage of 4.5 V.

Table S1. The fitting of the PL decay lifetime for pristine and TOAB passivated $CsPbBr_3$ NC films. The PL was excited at 365 nm and monitored at the maximum emission peak. The average PL decay lifetimes (τ_{avg}) were obtained as:

$$\tau_{avg} = A+B_1 * \exp(-i/\tau_1)+B_2 * \exp(-i/\tau_2)+B_3 * \exp(-i/\tau_3)$$

where B_1, B_2 and B_3 stand for the statistical weights of the corresponding lifetime components

Sample	τ_1/ns	τ_2/ns	τ_3/ns	τ_{avg}/ns
Pristine NCs	6.01719 ± 0.467118	12.5094 ± 0.400032	1.35633 ± 0.0997193	5.57018 ± 0.623032
Statistical weights	62.33 %	30.7 %	6.97 %	/
TOAB NCs	4.24276± 0.235211	10.0799 ± 0.186382	43.601 ± 1.68038	7.2837 ± 1.70696
Statistical weights	33.15 %	57.4 %	9.38 %	/

Table S2. The calculation results of the radiative and non-radiative recombination rates for different NC films. The radiative recombination rates (k_r) and non-radiative recombination rates (k_{nr}) of different samples are calculated by the formula:

$$\mathrm{PLQY} = \frac{k_r}{k_r + k_{nr}}$$

Sample	k_r (ns^{-1})	k_{nr} (ns^{-1})
Pristine NCs	**3.37×10^{-2}**	**8.43×10^{-3}**
TOAB NCs	**4.43×10^{-2}**	**1.37×10^{-3}**

Table S3. V_{TFL} and trap state densities (N_{trap}) obtained from SCLC measurements for pristine and TOAB passivated $CsPbBr_3$ NC thin film.

Sample	$V_{TFL(h)}$ (V)	$V_{TFL(e)}$ (V)	$N_{trap(h)}$ (cm^{-3})	$N_{trap(e)}$ (cm^{-3})
Pristine NCs	**0.41**	**1.04**	**2.0×10^{14}**	**6.2×10^{13}**
TOAB NCs	**0.33**	**0.77**	**1.5×10^{14}**	**5.0×10^{13}**

Table S4. Carrier mobility obtained from SCLC measurement for pristine and TOAB passivated $CsPbBr_3$ NC film.

Sample	Hole mobility ($cm^2\ V^{-1}\ s^{-1}$)	Electron mobility ($cm^2\ V^{-1}\ s^{-1}$)
Pristine NCs	5.37×10^{-11}	1.92×10^{-13}
TOAB NCs	3.05×10^{-9}	1.28×10^{-11}