Supplementary Information

Bright and Stable $CsPbBr_3$ Nanoplatelets via Dual-functional Short-Chain Ligand Passivation for Deep-Blue Light-Emitting Diodes

Zhirui Liu,[a] Zhijun Liu,[a] Dian Jin,[a] Tongge Li,[a] Qian Miao,*[a] Lanlan Zhai,[a] He Huang,[a] Yun Yang,[a] Lijie Zhang,[a] Jun Zou*[b c] and Chao Zou*[a]
[a]College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325035, China
[b]Institute of New Materials & Industrial Technology, Wenzhou University, Wenzhou 325024, China
[c]School of Science, Shanghai Institute of Technology, Shanghai 201418, China

Corresponding Author*
Correspondence and phone calls about the manuscript should be directed to Qian Miao, Jun Zou, Chao Zou at the following address, phone and fax number, and e-mail address:

Prof. Qian Miao, E-mail: miaoqian@wzu.edu.cn
College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, 325035, China

Prof. Jun Zou, E-mail: zoujun@sit.edu.cn
Institute of New Materials & Industrial Technology, Wenzhou University, Wenzhou, 325024, China
School of Science, Shanghai Institute of Technology, Shanghai, 201418, China

Prof. Chao Zou, E-mail: zouchao@wzu.edu.cn
College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, 325035, China

Experimental Section

Materials:

Lead bromide ($PbBr_2$, 99.9%), Cesium carbonate (Cs_2CO_3, 99.9%), 1-Octadecene (ODE, 90%), Toluene (AR), Oleylamine (OAm, 80%), Oleic acid (OA, 90%), Methyl acetate (98%), 2-Propanol (IPA, anhydrous, 99.5%) were purchased from Meryer. Ethanesulfonic acid (EtSA, 99%), 2-Bromoethanesulfonic acid (BrEtSA, 99%), and1,2-Dibromoethane (EDB, 99%) were purchased from Adamas. Octane (anhydrous, 99%) were purchased from Aladdin. Lithium fluoride (LiF, 99%) were purchased from Alfa Aesar. Poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT: PSS, 4083), poly[bis(4-phenyl) (4-butyl-phnyl)amine] (poly-TPD, Mw≥20000), poly(N-vinylcarbazole) (PVK, Mn<50000), and 1,3,5-Tris(1-phenyl-benzimidaz ol-2-yl) benzene (TPBi, 99.9%) were purchased from Xi'an Polymer Light Technology Co. Ltd.

Preparation of $CsPbBr_3$ NPL:

First, a cesium oleate (Cs-OA) solution was obtained by dissolving 0.162 g of Cs_2CO_3 in 5 mL OA at 120 °C with continuous stirring. For preparing BrEtSA-NPL, 0.072 g of $PbBr_2$, and 0.02 g BrEtSA were dissolved in 4 mL of ODE in a vial together with 0.5 mL of OAm and 0.5 mL of OA and heated to 120 °C. Subsequently, 0.5 mL of Cs-OA was blended with $PbBr_2$ solution in ambient conditions, followed by the addition of 0.5 mL of IPA while stirring for 60 s. After 10 min of stirring and heating at 70 °C, the solution was cooled in a cold-water bath. Then the precipitate was obtained with the centrifugation of the solution at 8000 rpm for 3 min. The precipitate was redispersed in the solution (1 mL of toluene and 1 mL of methyl acetate) for further purification. The precipitates were collected and redispersed in 1 mL of octane. For Control-NPL, all the other procedures were identical except for without the presence of BrEtSA in the reaction solution. The fabrication was carried out in ambient air.

Device fabrication:

Patterned ITO-coated glass substrates were washed with deionized water, ethanol, acetone, iso-propanol and ethanol for 20 min, and dried with a nitrogen blow gun. Then the ITO was cleaned with ultraviolet ozone for 15 min. PEDOT: PSS was spin-coated onto the substrates at 5000 rpm for 40 s followed by annealing at 120 °C for 20 min in ambient air. After cooling, the substrates were then transferred into a N_2 filled glovebox (O_2 <0.1 ppm, H_2O <0.1 ppm). Next, poly-TPD (5 mg mL^{-1}) and PVK (5 mg mL^{-1}) 1:1 mixed solution was spin-coated at 2500 rpm for 30 s and followed by baking at 150 °C for 20 min. The perovskite films were obtained by spin-coating the precursor solution in glove box at 2500 rpm for 40s. Finally, TPBi (35 nm), LiF (1 nm), and Al (100 nm) were deposited under a pressure of $\sim 5\times10^{-4}$ Pa. The active area of the devices was 8 mm^2 as defined by the overlapping area of the ITO and Al electrode. All devices were tested in atmospheric environments.

Characterization:

UV-vis absorption spectra were obtained through the Shimadzu UV-1800 spectrophotometer. The steady-state photo-luminescence (PL), PL quantum yield (PLQY), and time-resolved PL (TRPL) were measured employing an FLS980 spectrofluorometer (Edinburgh Instruments Ltd). The excitation source is 365 nm from a Xe lamp for PL and the time-resolved luminescence decay was analyzed through time-correlated single-photon counting with a 375 nm laser. X-ray diffraction (XRD) analysis was performed utilizing a Bruker D8 advance X-ray diffractometer with graphite monochromatized Cu $K\alpha$ (λ=1.5405 Å) radiation, operating with a step of 0.02° and a scan speed of 4° min^{-1} in a 2θ scale from 3° to 40°. X-ray photoelectron spectroscopy (XPS) was executed using a Bruker instrument. Additionally, Transmission electron microscopy (TEM) was carried out using a JEM-2010F. ^{1}H nuclear magnetic resonance (NMR) measurements were performed with a Quantum-I Plus-400 NMR spectrometer (FT, 400 MHz for ^{1}H) by using deuterated DMSO-*d*6 as the solvent. The Fourier Transform Infrared (FTIR) spectra were recorded with a Thermo Fisher iS50 FTIR. The characterization of current density-luminance-voltage, electroluminescence (EL), external quantum efficiency (EQE) and operating lifetime of the PeLED were conducted simultaneously by using a commercialized system (Shenzhen Spectrum Research Connected Technology Co., Ltd) equipped with Keithley 2400, a fiber integrating sphere and Ocean Optics QE65 Pro spectrometer.

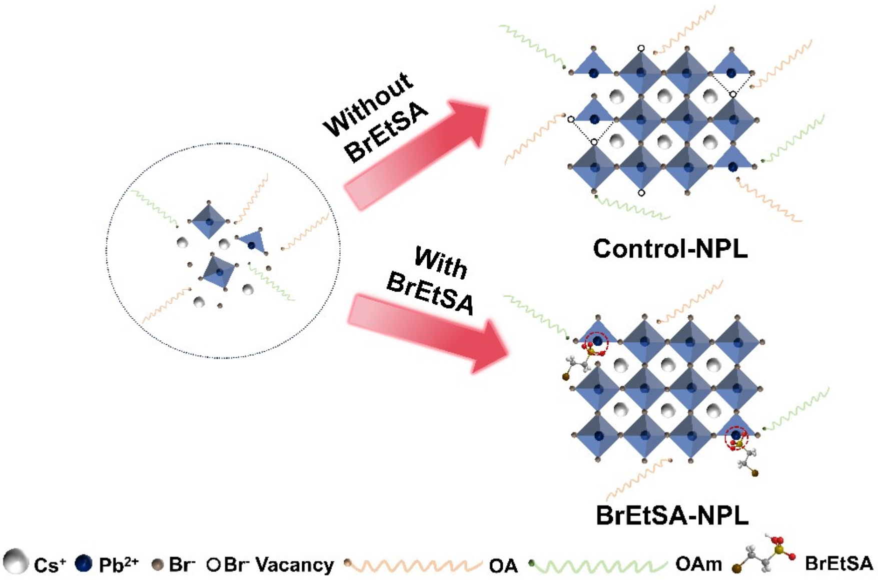

Figure S1. Schematic illustration of surface passivation of $CsPbBr_3$ NPL.

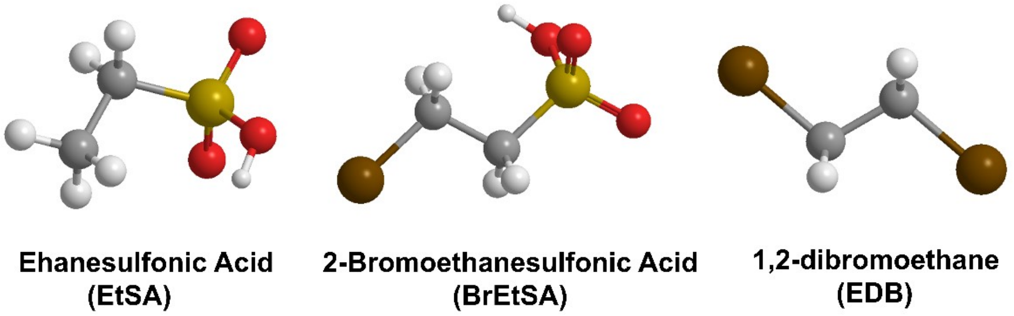

Figure S2. The molecular structures of ethanesulfonic acid, 2-bromoethanesulfonic acid, and 1,2-dibromoethane.

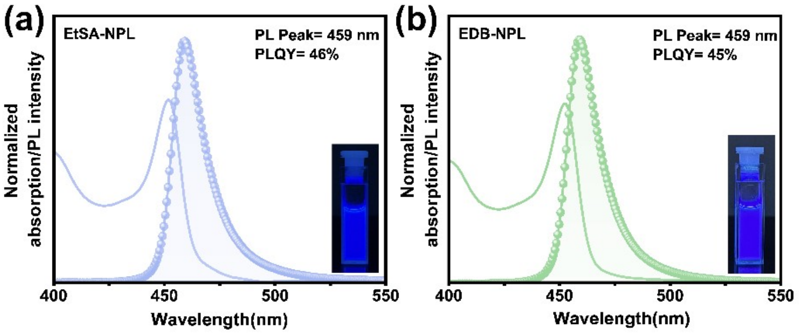

Figure S3. UV−vis absorption and PL spectra of $CsPbBr_3$. (a) EtSA-NPL, (b) EDB-NPL. The insets show photos of NPL solutions under 365 nm UV light irradiation.

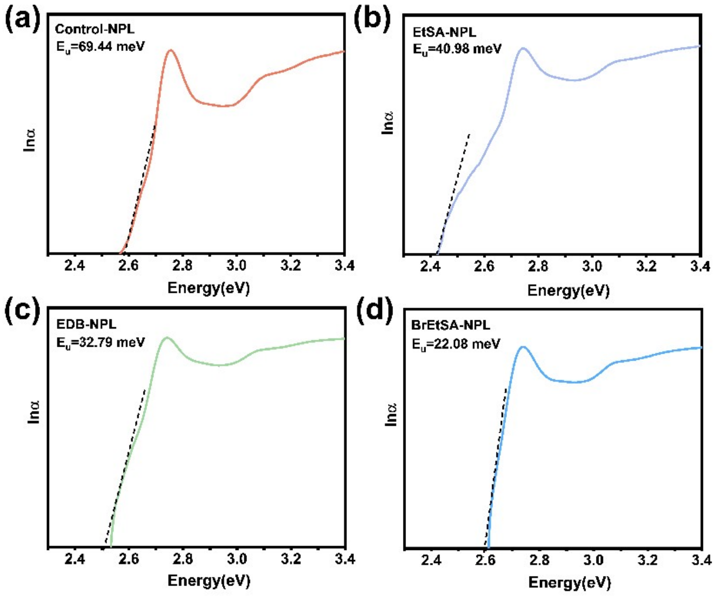

Figure S4. Ulbach energy spectra for (a) Control-NPL, (b) EtSA-NPL, (c) EDB-NPL, and (d) BrEtSA-NPL.

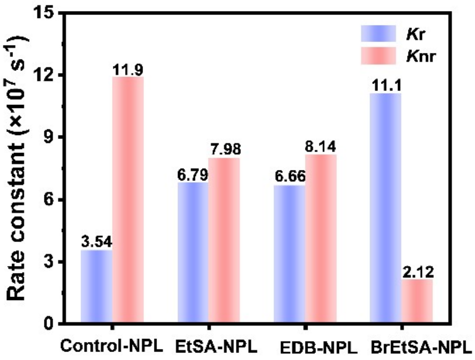

Figure S5. Calculated recombination rate constants of Control-NPL, EtSA-NPL, EDB-NPL, and BrEtSA-NPL.

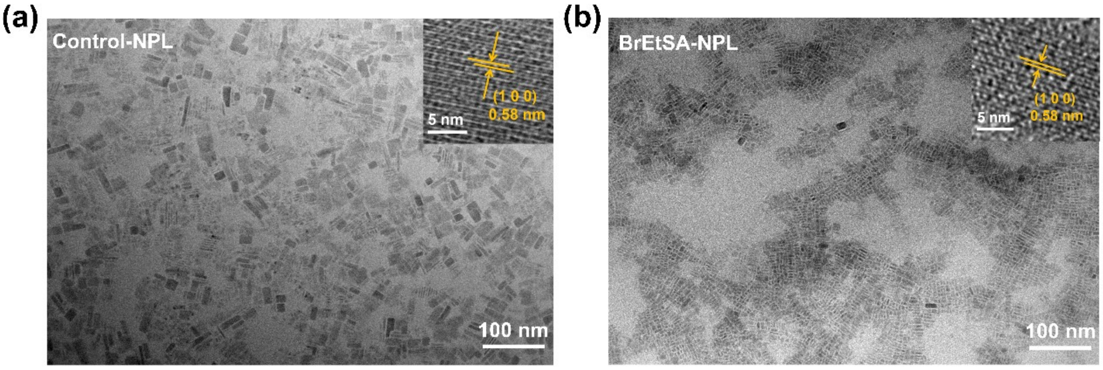

Figure S6. TEM images of (a) Control-NPL, (b) BrEtSA-NPL. The insets are HRTEM images.

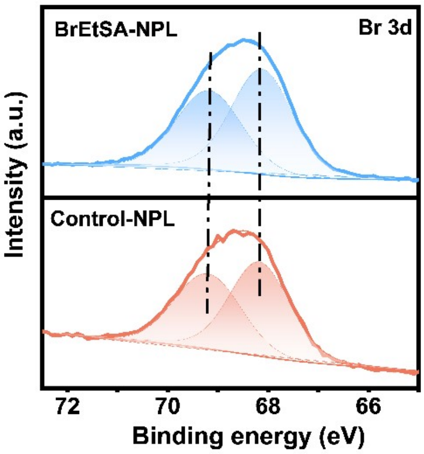

Figure S7. XPS spectra of Br 3d of Control-NPL, and BrEtSA-NPL.

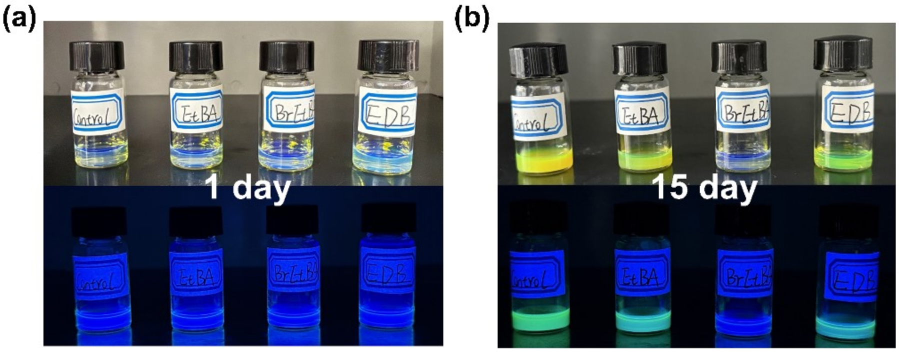

Figure S8. Photographs of sample solutions after the same storage period under daylight (top) and 365 nm UV light (bottom): (a) 1 day, (b) 15 days.

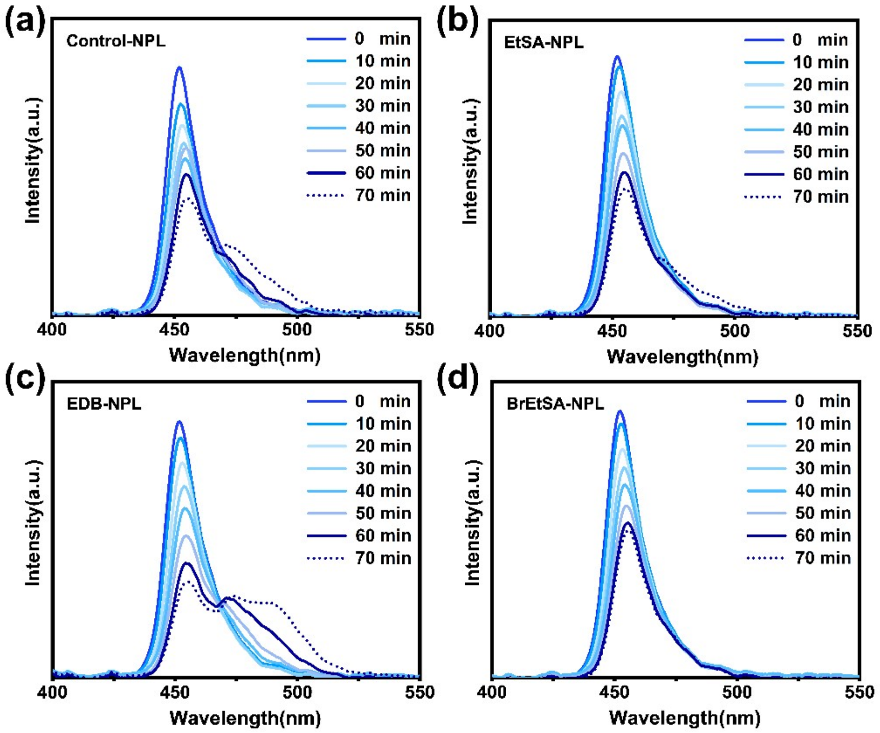

Figure S9. (a) Control-NPL, (b) EtSA-NPL, (c) EDB-NPL, and (d) BrEtSA-NPL films PL spectra under ambient conditions (room temperature, 25 ± 2 °C) with continuous UV light irradiation (365 nm, 6 mW/cm^2).

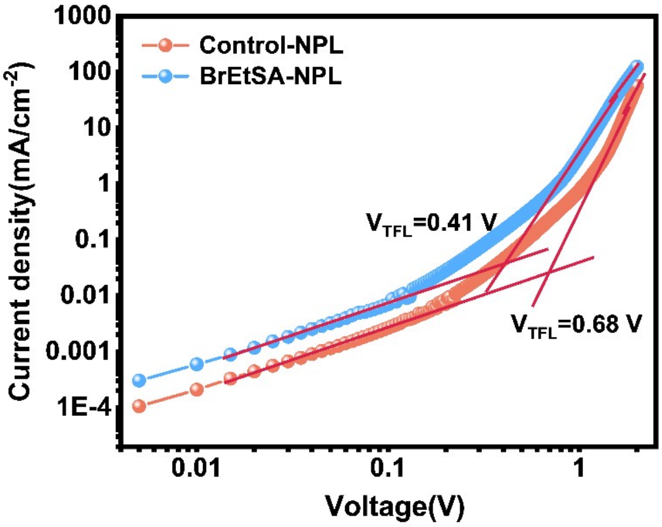

Figure S10. J-V curves of the hole-only devices.

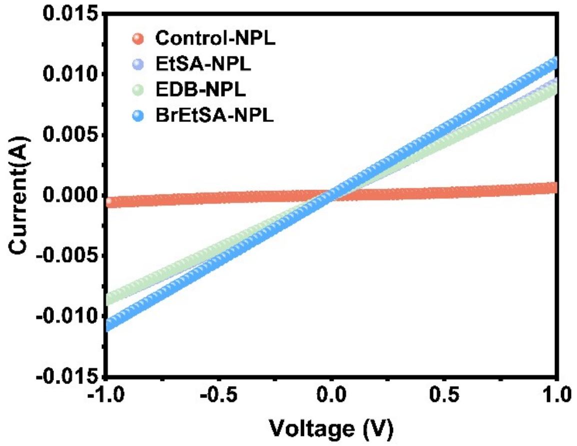

Figure S11. I-V curves of NPL film.

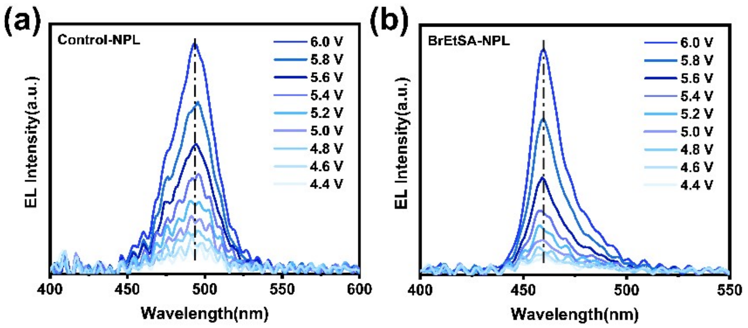

Figure S12. EL spectra of the device at different operating voltages.

Table S1. PL lifetime characteristics of Control-NPL, EtSA-NPL, EDB-NPL, and BrEtSA-NPL.

Sample	τ_1(ns)	A_1(%)	τ_2(ns)	A_2(%)	τ_3(ns)	A_3(%)	τ_{ave}(ns)
Control-NPL	1.09	18.16	2.86	63.17	10.41	18.67	6.49
EtSA-NPL	0.88	30.29	2.92	56.90	11.96	12.81	6.77
EDB-NPL	1.03	31.05	3.01	54.05	11.41	17.97	6.76
BrEtSA-NPL	1.18	25.78	3.22	58.12	12.55	16.10	7.56

τ_1 (fast lifetime component): Attributed to defect-assisted non-radiative recombination, primarily reflecting the rapid capture and annihilation of charge carriers by deep-level defects at the surface or grain boundaries.

τ_2 (medium lifetime component): Attributed to shallow defect-induced recombination or interface-assisted recombination processes. This component may involve exciton dissociation, diffusion of carriers to non-radiative centers, or surface-state-modulated recombination.

τ_3 (slow lifetime component): Attributed to band-edge radiative recombination, representing the radiative recombination of free excitons, which serves as the main channel for efficient light emission.

All *K*r and *K*nr of the sample were calculated according to the following formula:

$\tau_{ave} = 1/(K\mathrm{r}+K\mathrm{nr})$ and $\mathrm{PLQY} = K\mathrm{r}/(K\mathrm{r}+K\mathrm{nr})$

where k_r and k_{nr} represent the radiative and nonradiative recombination rate constants, respectively.

Table S2. Performance parameters of blue PeLEDs.

Devices	**V_{on} (V)**	**L (cd m^{-2})**	**EQE (%)**	**EL (nm)**
Control-NPL	4.4	291	0.25	493
BrEtSA-NPL	4.4	50	0.80	460