

Supporting Information

Modulation of Ligands Conjugation for Efficient FAPbBr₃ based Green Light-Emitting Diodes

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Experiment Section

Materials. Lead bromide (PbBr_2 , 99.5%, Alfa Aesar); Formamidinium bromide (FABr, $\geq 99.5\%$, four times purification, Xi'an Polymer Light Technology Co. Ltd.); 1-(1-naphthyl)ethylamine (NEA, $\geq 98.5\%$, Alfa Aesar); Hydrobromic acid (HBr, 49 wt.% in water, Alfa Aesar); N, N-dimethylformamide (DMF, ultra-dry solvent, J&K Scientific Ltd.); Chlorobenzene (ultra-dry solvent, J&K Scientific Ltd.); Toluene (analytical grade, Beijing Chemical Reagent Co. Ltd., China); Absolute ethanol (analytical grade, Beijing Chemical Reagent Co., Ltd., China); Diethyl ether (analytical grade, Beijing Chemical Reagent Co., Ltd., China); Acetone (analytical grade, Beijing Chemical Reagent Co., Ltd., China); Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS, Xi'an Polymer Light Technology Co. Ltd.); Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-(4,4'-(N-(p-butylphenyl))diphenylamine)] (TFB, Xi'an Polymer Light Technology Co. Ltd.); 2,2',2''-(1,3,5-Benzinetriyl)-tris(1-phenyl-1-H-benzimidazole) (TPBi, Jilin Optical and Electronic Materials Co. Ltd.); Lithium fluoride (LiF, 99%, Alfa Aesar); Aluminum (Al, Sinopharm Chemical Reagent Co. Ltd.); All reagents were used as received without further purification.

Synthesis of 1-(1-naphthyl)ethylamine bromide. 1-(1-naphthyl)ethylamine bromide (NEABr) was synthesized by reaction of NEA with HBr. Typically, 1 mL of NEA was dispersed in 10 mL of absolute ethanol, which was stirred and cooled to 273 K. 920 μL of HBr was then added into the mixture to initiate the reaction. After stirred for two hours, the reaction solution was rotary evaporated to get rid of the solvent with pressure of -0.1 Mpa at 323 K. The obtained products were dissolved in absolute ethanol and further precipitated by diethyl ether for three times. Finally, the resulted pure white precipitates were collected and dried under vacuum (323 K, 5h) for future use.

Preparation of perovskite precursor solution. 0.2 mmol PbBr_2 , 0.2 mmol FABr, and a certain amount of NEABr were mixed in a 5 mL vial. The molar ratio between PbBr_2 and NEABr was indicated as 1:x, where x was varied from 0.2, 0.3, 0.4 to 0.5. Then, the mixture

was transferred into a glove box with 1 mL of DMF added. The solution was stirred over 2 h at 50 °C for further use.

Fabrication of EL Devices. ITO substrates were sequentially washed with toluene, acetone, ethanol and deionized water, followed by O₂ plasma treatment for 2 min. PEDOT:PSS solution was spin coated on the ITO substrate at 4000 rpm for 1 min, then baked on a hot plate at 150 °C for 15 min. TFB dissolved in chlorobenzene (6 mg/mL) was spin coated on the PEDOT:PSS film at 4000 rpm for 1 min, followed by thermal annealing at 120 °C for 20 min. The TFB film was treated with O₂ plasma for 2 min and transferred into the glove box. FAPbBr₃ precursor solution was spread out on the TFB film and spin coated at 4000 rpm for 1 min. During the spin coating of precursor solution, 0.5 mL toluene was dropped one second before the color change. The obtained FAPbBr₃ film was annealed at 60 °C for 5 min to remove residual solvent and enhance the crystallinity. Then, TPBi (25 nm), LiF (1 nm), and Al (80 nm) layers were thermally deposited in sequence in a high-vacuum chamber (pressure below 8×10^{-5} Pa) with deposition rate of 0.5, 0.05, and 5 Å/s, respectively.

Characterizations and device measurements. The SEM images of FAPbBr₃ PeNCs films were recorded on Hitachi S-4800 microscope, working at 5 kV. X-ray diffraction patterns (XRD) were measured on a Bruker/D8 FOCUS X-ray diffractometer with Cu K α radiation source (wavelength at 1.5406 Å). The samples were scanned from 3° < 2 θ < 60° at an increment of 2°/min. The TEM images were captured on a JEOL-JEM 2100F TEM machine operating at an acceleration voltage of 200 kV. FAPbBr₃ PeNCs films were stripped from TFB substrate and dissolved in chlorobenzene for further TEM measurements. UV-Vis absorption spectra were measured on a UV-6100 UV-Vis spectrophotometer (Shanghai Mapada Instruments Co., Ltd., China). PL spectra were taken using a F-380 fluorescence spectrometer (Tianjin Gangdong Sci. & Tech. Development Co., Ltd., China). Time-resolved PL was collected using fluorescence lifetime measurement system (C11367-11, Hamamatsu Photonics, Japan) with excitation

wavelength of 405 nm. The absolute PLQYs of as fabricated FAPbBr₃ films were determined using a fluorescence spectrometer with integrated sphere (C9920-02, Hamamatsu Photonics, Japan) under blue light emitting diodes (LED) excited at a wavelength of 450 nm. The electrical characteristics, electroluminescence spectra, and luminance of the devices were measured with a Keithley 2400 source meter in conjunction with an absolute EQE measurement system (C9920-12, Hamamatsu Photonics K.K., Japan). All the characterizations were performed at room temperature under ambient laboratory conditions.

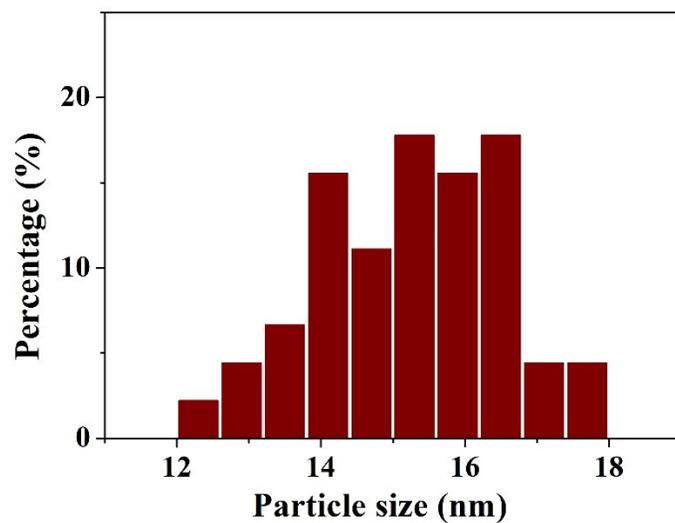


Figure S1. Statistical analysis on particle size corresponding to TEM images of sample 40%.

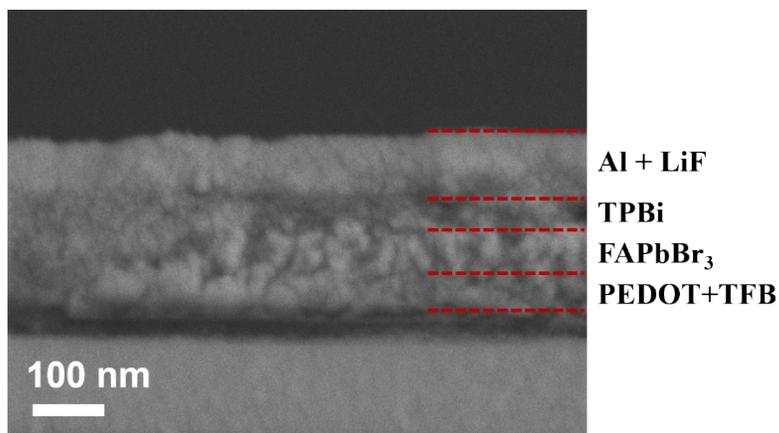


Figure S2. Cross section SEM image of of a typical EL device.

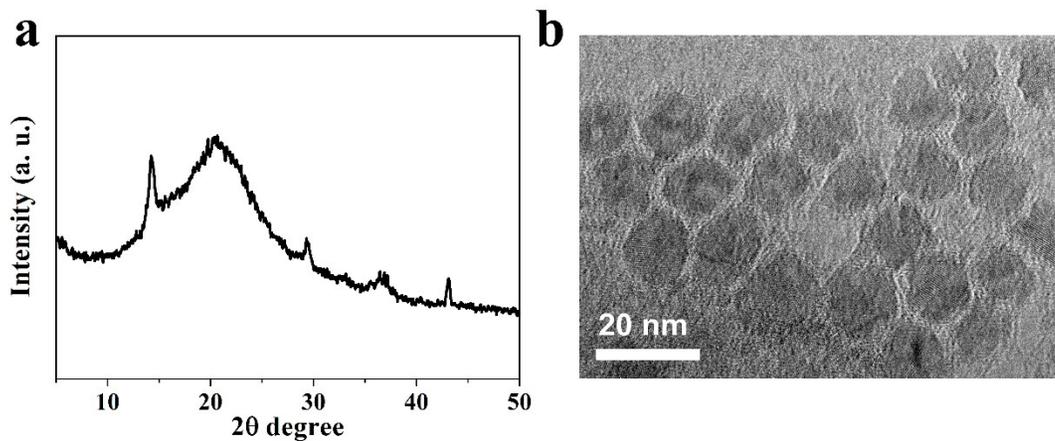


Figure S3. (a) XRD pattern of FAPbBr₃ PeNCs films fabricated by using PEABr molecules. (b) TEM image of FAPbBr₃ PeNCs films fabricated by PEABr.

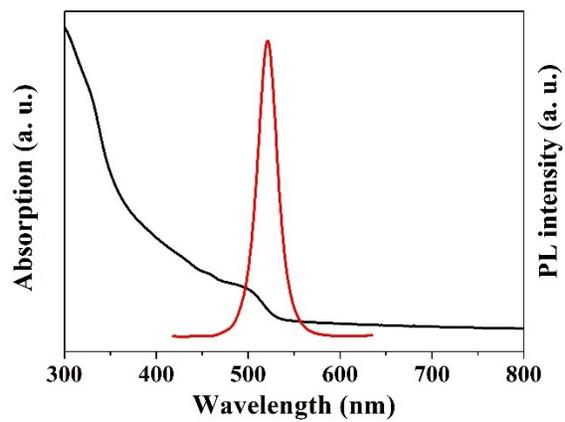


Figure S4. Absorption and emission spectra of FAPbBr₃ PeNCs films fabricated using PEABr.

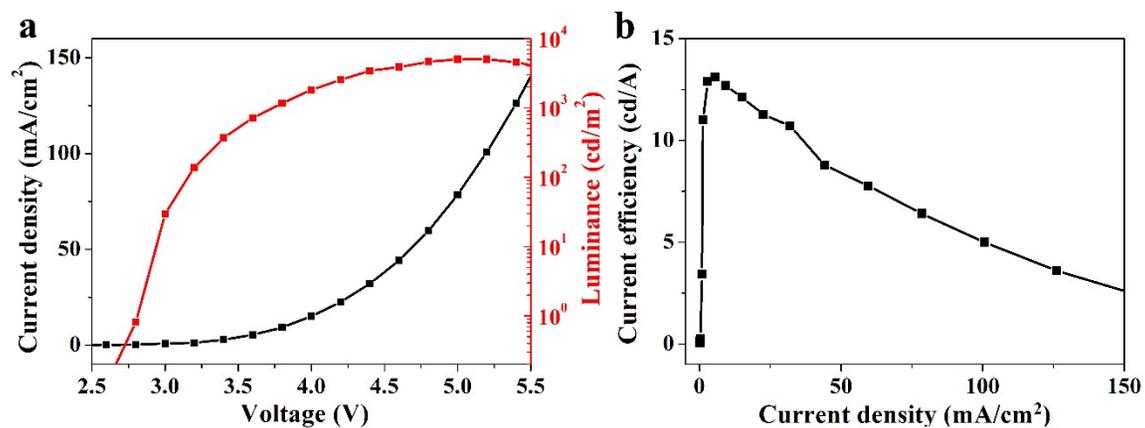


Figure S5. (a) Current density-Voltage-Luminance curves of a typical EL device base on FAPbBr₃ PeNCs films fabricated by using PEABr. (b) The corresponding EQE curve.

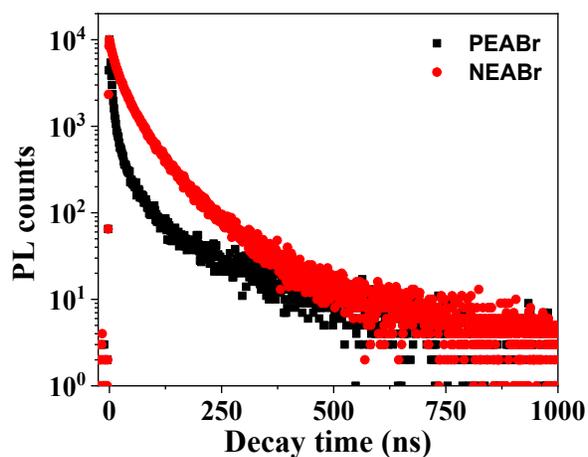


Figure S6. Comparison between time resolved PL decay curves of FAPbBr₃ PeNCs films capped by NEABr and PEABr.

Table S1. The detailed fitting results of sample 20%, 30%, 40% and 50%.

Sample	20%	30%	40%	50%
A_1	9679	4238	3634	3023
A_2	1094	4731	4933	5234
A_3	113	1563	1614	1743
τ_1	3.40	3.85	6.09	7.61
τ_2	22.17	23.80	26.54	28.66
τ_3	151.12	71.73	89.77	90.21
τ_{av}	43.49	44.74	55.77	56.50

Table S2. The operation parameters (turn on voltage (V_T), maximum luminance (L_{max}), EL peak, maximum current efficiency (CE_{max}), and maximum EQE (EQE_{max})) of EL devices based on sample 20%, 30%, 40% and 50%.

Device	V_T (V)	L_{max} (cd/m ²)	EL peak (nm)	CE_{max} (cd/A)	EQE_{max} (%)
20%	3.1	6386	531	5.29	1.32
30%	3.0	14630	529	16.58	3.93
40%	2.8	9944	526	36.83	8.62
50%	2.6	5380	522	24.27	5.78

Table S3. The calculated results of resistance and capacitance of EL devices based on PEABr and NEABr.

Ligands	R (K Ω)	C_{LF} (nF)
PEABr	28.74	24.69
NEABr	12.73	8.10