

Supplementary Information

AI-accelerated scalable synthesis of nanocrystals for cost-effective photovoltaics

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Supplementary Table 5 Summary of labor cost for 1 gram of HI FAPbI₃, LTRI FAPbI₃ and Flow-LTRI FAPbI₃ PNCs.

Supplementary Table 6 Summary of the champion photovoltaic performance.

Supplementary Table 7 Summary of the representative nanocrystal/quantum dot-based photovoltaics.

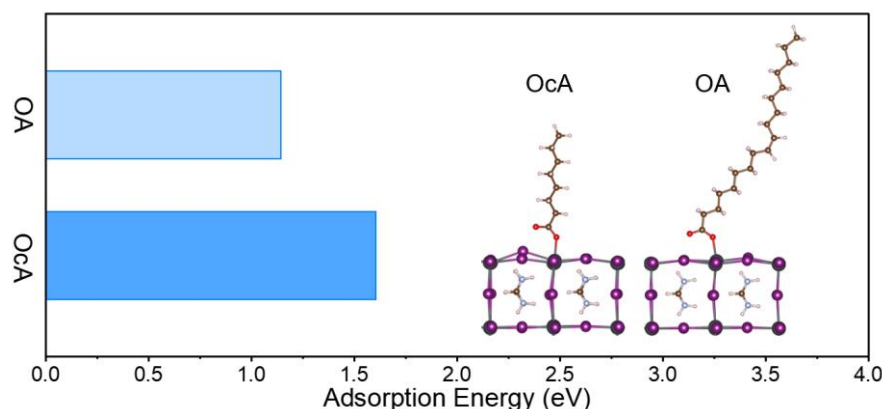
Supplementary Table 8 Summary of photovoltaic performance of the 1-L scale PNC device.

Supplementary Note 1 Comparison of LTRI FAPbI₃ PNC synthesis with different acid chain length.

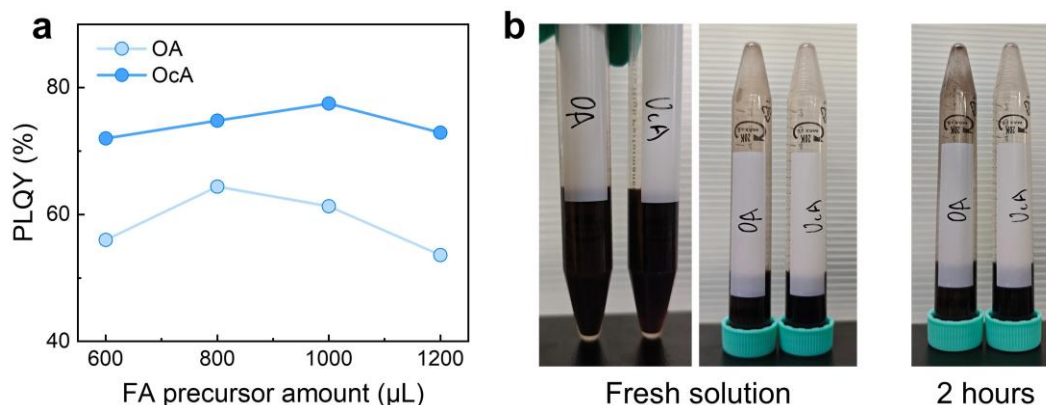
Supplementary Note 2 Machine learning model construction.

Supplementary Note 3 Analysis of ML predicted data.

Supplementary References



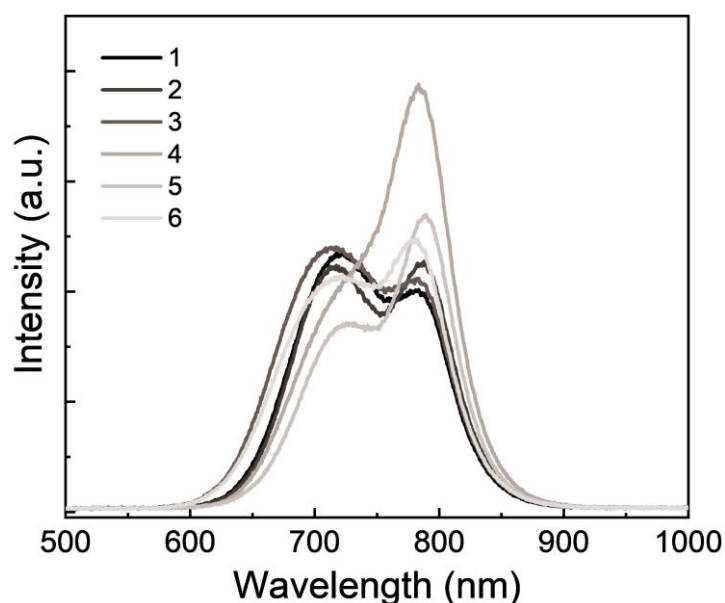
Supplementary Fig. 1 DFT-simulated surface structure and adsorption energy of OA and OcA. DFT-simulated surface structure and adsorption energy of OA and OcA on FAPbI₃ perovskite surface. The DFT calculations were performed by Vienna ab initio simulation package (VASP)¹. The generalized gradient approximation in the form of Perdew-Burke-Ernzerhof (GGA-PBE)² was implemented to describe the exchange-correlation functional, and the interactions between ions and core electrons were included by the projector augmented wave (PAW)³ method. The adsorption energy (E_{ads}) is defined as $E_{\text{ads}} = E_{\text{tot}} - E_{\text{lig}} - E_{\text{per}}$, where E_{tot} denotes the total energy of the passivated slab, while E_{lig} and E_{per} are severally the energy of the isolated ligands (OAc and OA) and perovskite slab before ligand adsorption.



Supplementary Fig. 2 Comparison of LTRI PNC synthesis using OA and OcA. (a) PLQY of FAPbI₃ PNCs synthesized using OA and OcA with varying precursor ratios. An overall enhancement in PLQY value is observed for LTRI PNCs synthesized with OcA compared to OA, indicating that the OcA-regulated LTRI synthesis enables high-quality PNCs. (b) Photographs of fresh PNC solution and 2-hours aged solution, synthesized at the optimal precursor ratio. The photographs reveal that the PNCs synthesized with OcA possess superior colloidal dispersion stability. After 2 hours of static storage in ambient air, the OA-synthesized PNCs exhibit significant sedimentation, which may be attributed to PNC aggregation resulting from poor size uniformity and ligand desorption.

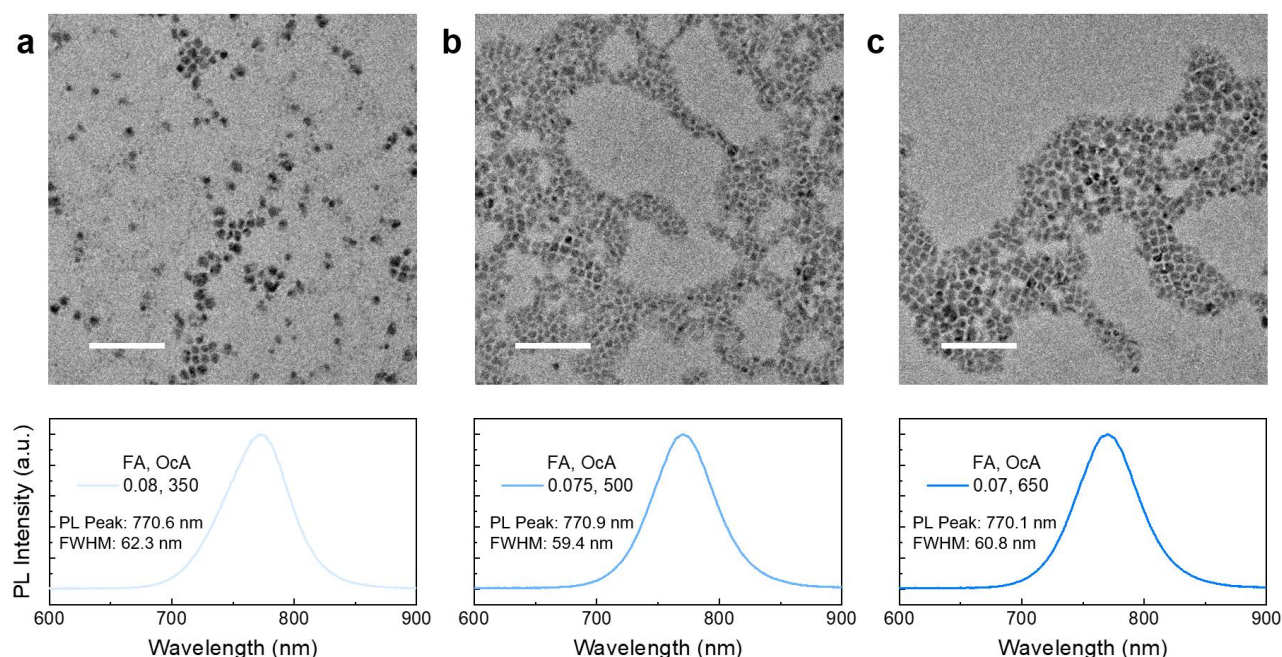


Supplementary Fig. 3 Photograph of the robotic auto-synthesis platform. The platform employs a computer-controlled robotic arm to aspirate precursors and synthesize PNCs in the reaction zone. This system enables high-throughput synthesis across a range of precursor ratios, thereby accelerating the optimization and screening of PNCs.



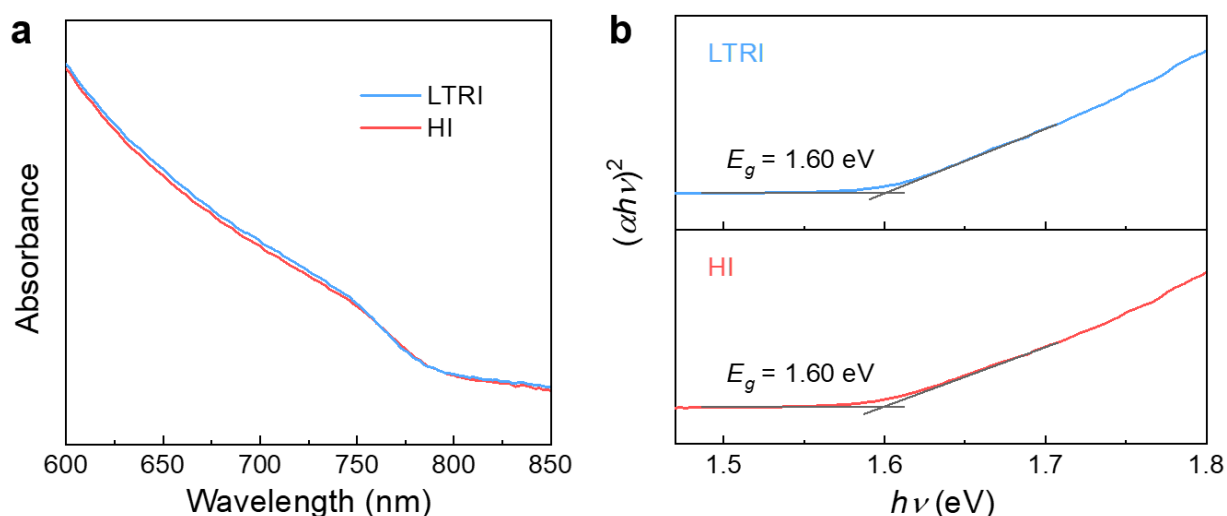
Supplementary Fig. 4 Improper PL spectra of FAPbI₃ PNCs for initial training data. The 1-6 PL spectra tested from the synthesis with **1**: 60 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 250 μ L OcA; **2**: 60 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 500 μ L OcA; **3**: 60 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 750 μ L OcA; **4**: 60 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 1000 μ L OcA; **5**: 120 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 500 μ L OcA; **6**: 180 μ L OA, 60 μ L OAm, 0.03 mmol FAAC, 500 μ L OcA. All the recipe contains 0.06 mmol PbI₂ and 2 mL toluene. Pronounced multi-peak features in the spectral data indicate the formation of low-dimensional nanocrystal structures. Among all PL measurements, these attempts incorporated the smallest amount of FA⁺, which is significantly lower than the 1:1 FA:Pb ratio in the FAPbI₃ perovskite structure^{4,5}. Additionally, certain non-optimal synthesis formulations resulted in complete absence of photoluminescence emission, though these unsuccessful attempts are not

included in the present dataset.



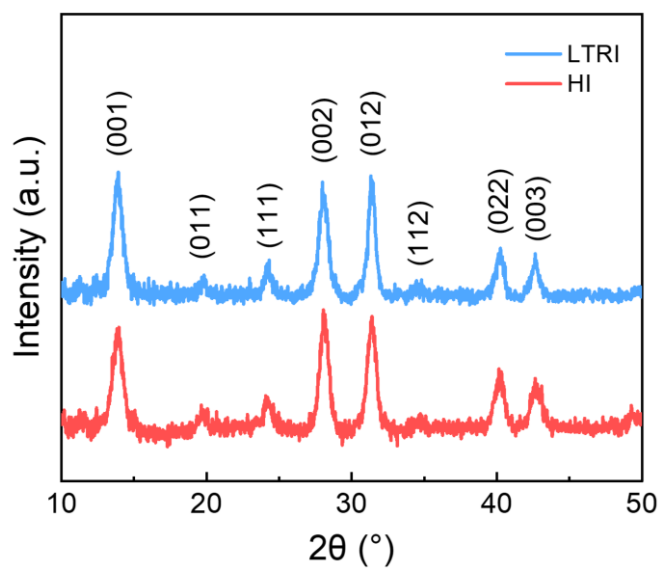
Supplementary Fig. 5 TEM images and PL spectra of LTRI FAPbI₃ PNCs resembling HI samples.

TEM images and correspond PL spectra of LTRI FAPbI₃ PNCs exhibiting PL comparable to those prepared by the HI method. Recipes were selected from 3 datapoints in Fig. 1f, which used 60 μ L OA, 60 μ L OAm, 0.06 mmol PbI₂, 2 mL toluene and (a) 0.08 mmol FAc, 350 μ L OcA; (b) 0.075 mmol FAc, 500 μ L OcA; (c) 0.08 mmol FAc, 350 μ L OcA. Among the three recipes, condition (b) was identified as optimal, as it afforded the most uniform size distribution and the narrowest PL emission peak.

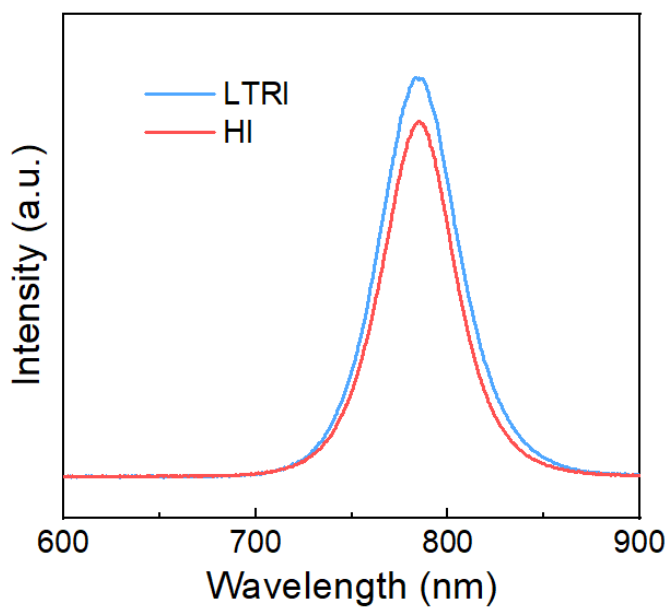


Supplementary Fig. 6 Absorption spectra and Tauc plot of FAPbI₃ PNCs. (a) Absorption spectra and (b) Tauc plot of FAPbI₃ PNCs synthesized by LTRI and HI method. The LTRI synthesis is carried

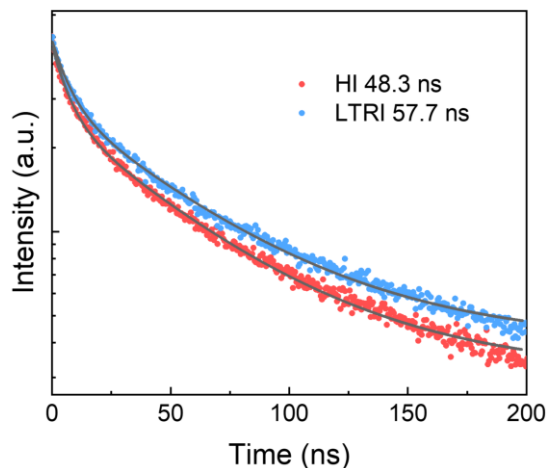
out with 60 μL OA, 60 μL OAm, 0.075 mmol FAc, 500 μL OcA, 0.06 mmol PbI_2 and 2 mL toluene.



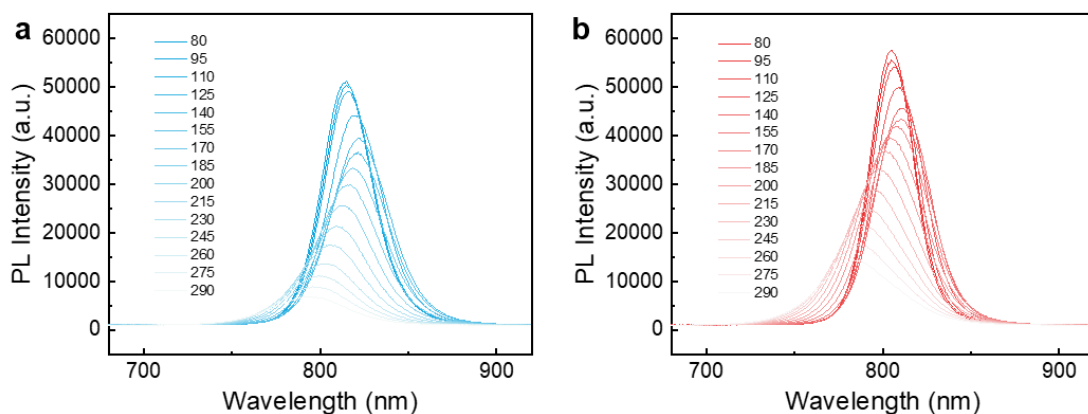
Supplementary Fig. 7 X-ray diffraction spectra of FAPbI_3 PNCs. X-ray diffraction spectra of FAPbI_3 PNC synthesized by LTRI and HI method. The LTRI synthesis is carried out with 60 μL OA, 60 μL OAm, 0.075 mmol FAc, 500 μL OcA, 0.06 mmol PbI_2 and 2 mL toluene.



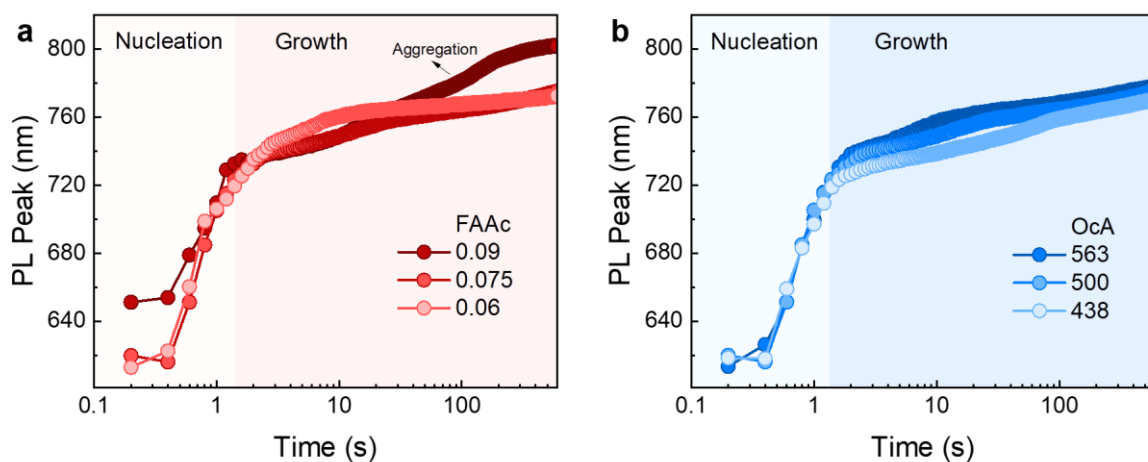
Supplementary Fig. 8 PL spectra of FAPbI_3 PNCs. PL spectra of FAPbI_3 PNCs synthesized by LTRI and HI method.



Supplementary Fig.9 TRPL spectra of FAPbI₃ PNCs. TRPL spectra of FAPbI₃ PNCs synthesized by LTRI and HI method.

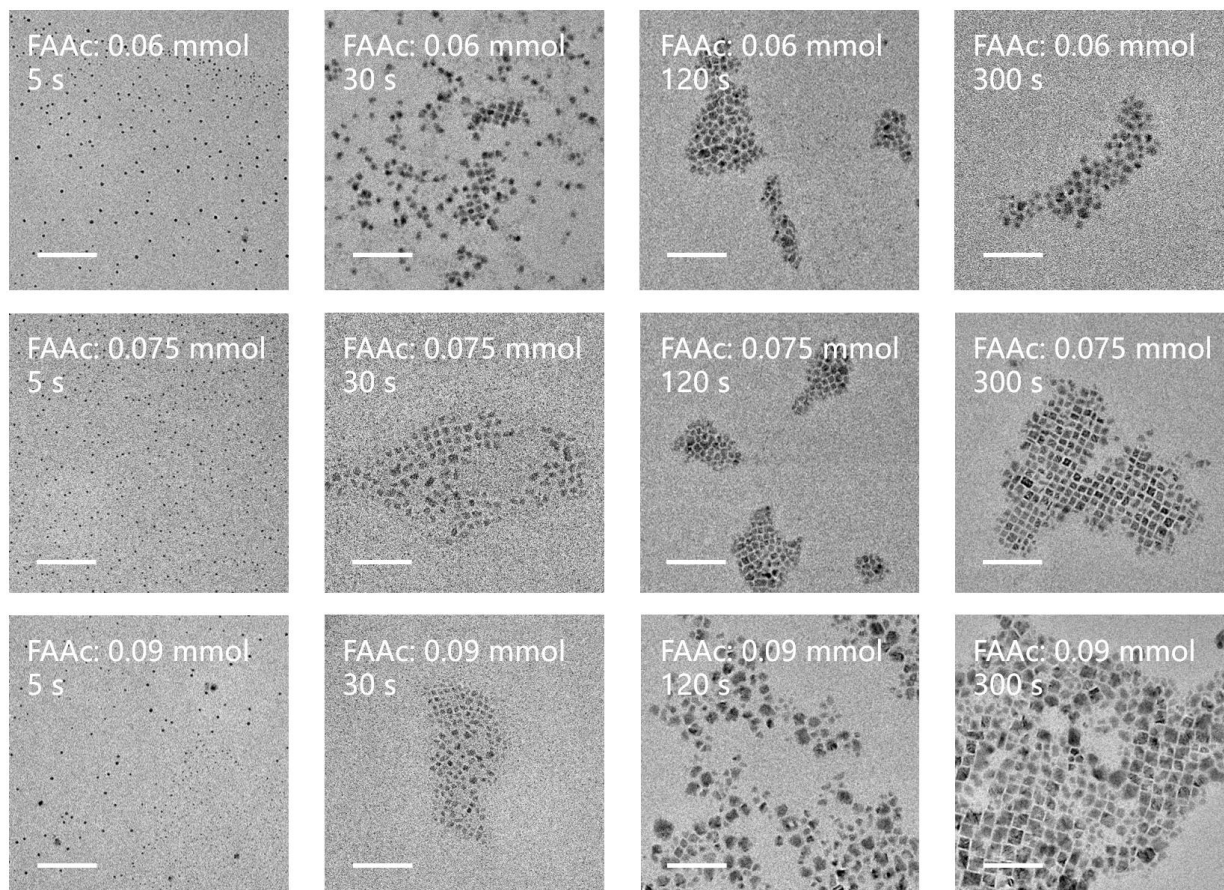


Supplementary Fig. 10 Temperature-dependent PL spectra of FAPbI₃ PNCs. Temperature-dependent PL spectra of FAPbI₃ PNCs synthesized by (a) LTRI and (b) HI method.

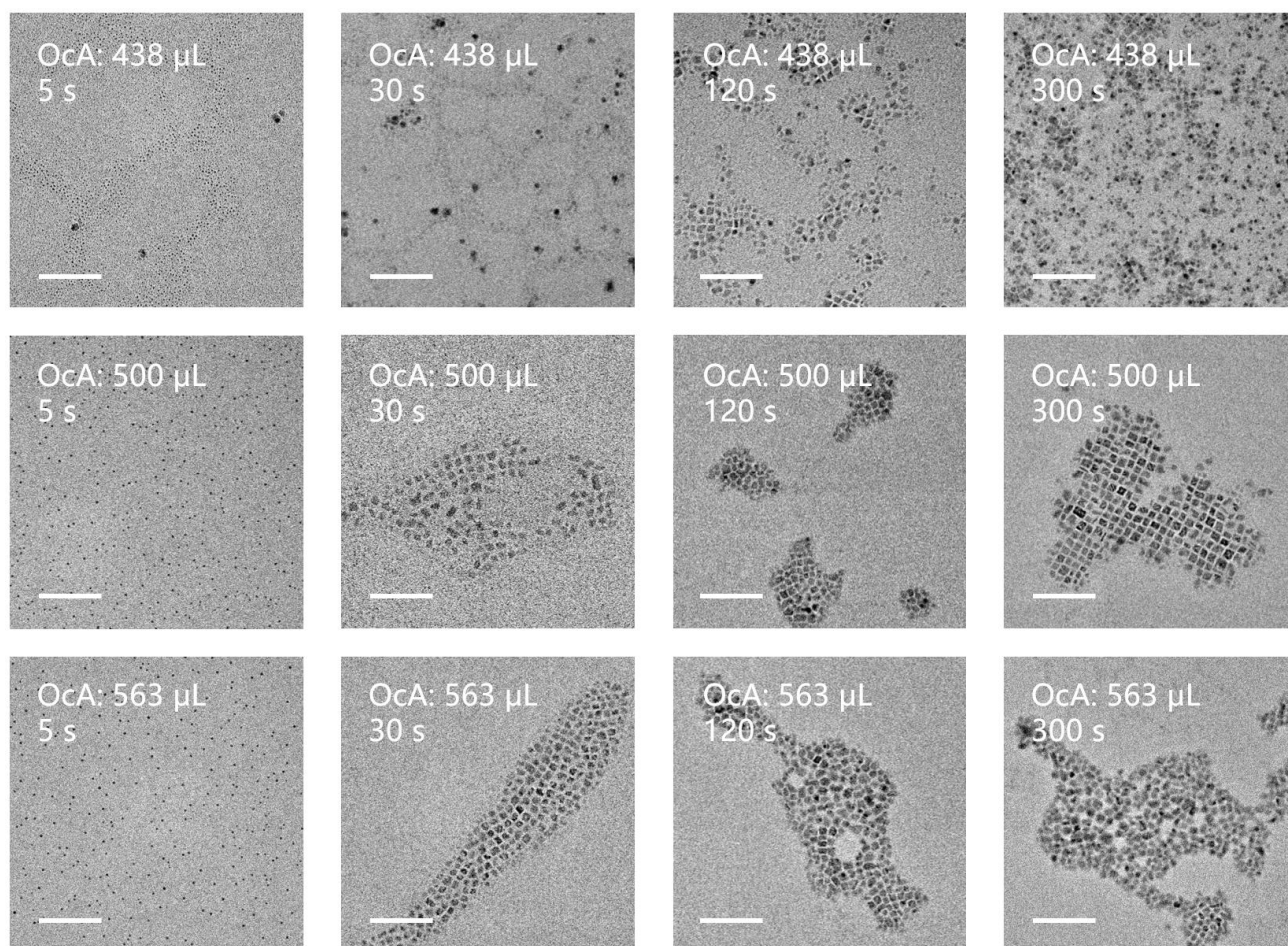


Supplementary Fig. 11 Time evolution curves of PL peak from in-situ PL spectra of LTRI synthesis. Time evolution curves of PL peak from in-situ PL spectra of LTRI synthesis with different

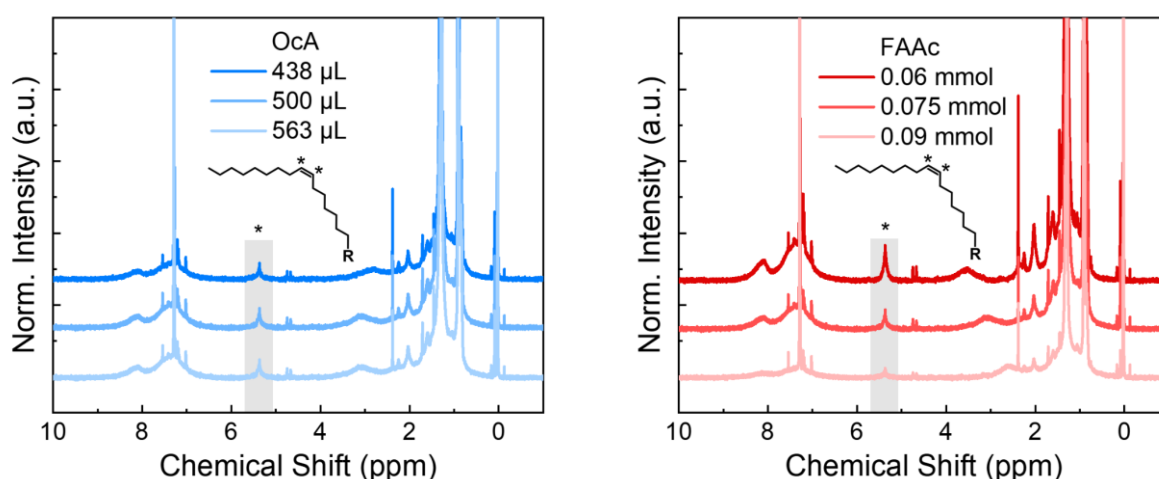
(a) FAAC and (b) OcA. The LTRI synthesis is carried out with 60 μL OA, 60 μL OAm, 0.06 mmol PbI_2 and 2 mL toluene. For (a), the amount of OcA was fixed at 500 μL in all recipes. As the concentration of FAAC increased, the PL peak shifted more slowly during the initial 20 seconds of the reaction and exhibited a more pronounced redshift thereafter. For (b), the FAAC content was held constant at 0.075 mmol in all recipes. With increasing OcA concentration, the PL peak shifted more rapidly during the initial 20 seconds and showed less PL redshift thereafter.



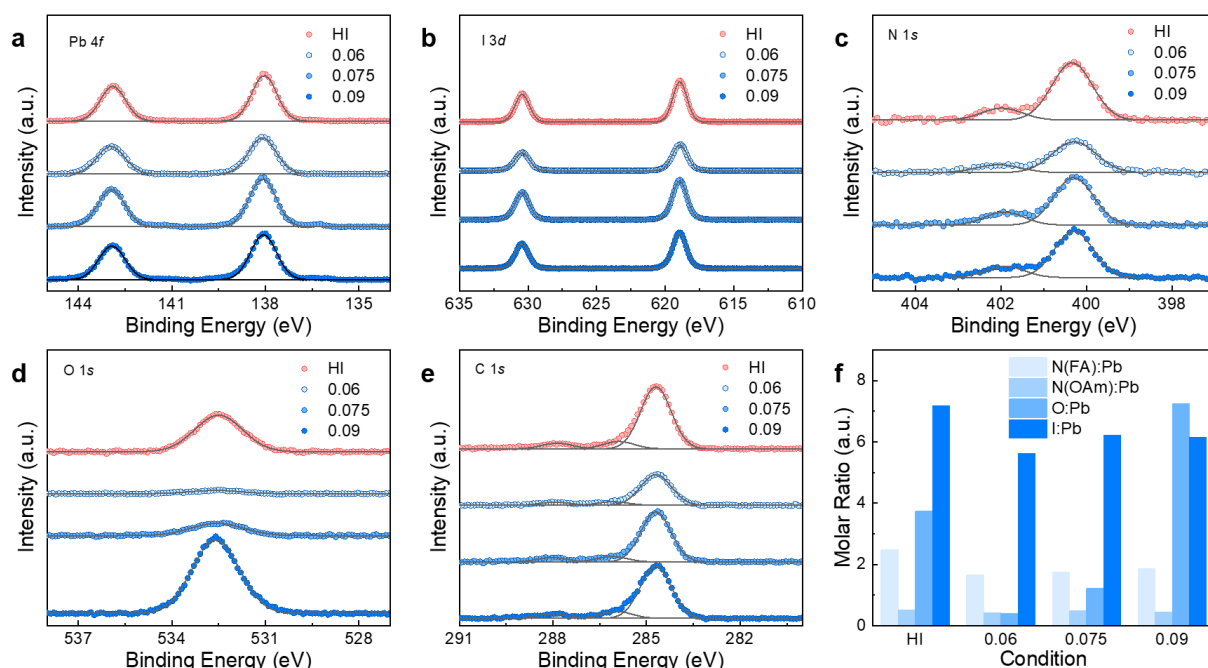
Supplementary Fig. 12 Time-dependent TEM images of LTRI FAPbI₃ PNCs with different FAAC. TEM images of LTRI FAPbI₃ crude solution with 0.06 mmol, 0.075 mmol and 0.09 mmol of FAAC at 5 s, 30 s, 120s and 300 s, respectively (scale bar, 100 nm). The LTRI synthesis is carried out with 60 μL OA, 60 μL OAm, 500 μL OcA, 0.06 mmol PbI_2 , 2 mL toluene and different FAAC.



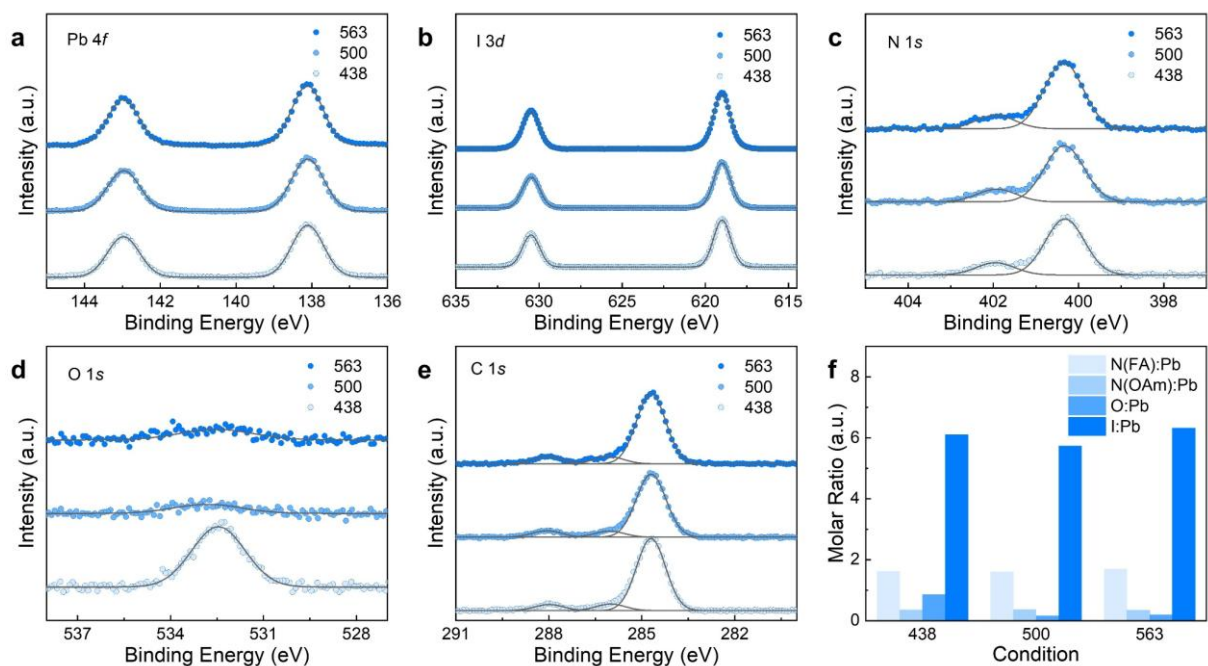
Supplementary Fig. 13 Time-dependent TEM images of LTRI FAPbI₃ PNCs with different OcA. TEM images of LTRI FAPbI₃ crude solution with 438 μ L, 500 μ L and 563 μ L of OcA at 5 s, 30 s, 120s and 300 s, respectively (scale bar, 100 nm). The LTRI synthesis is carried out with 60 μ L OA, 60 μ L OAm, 0.075 mmol FAAC, 0.06 mmol PbI₂, 2 mL toluene and different OcA.



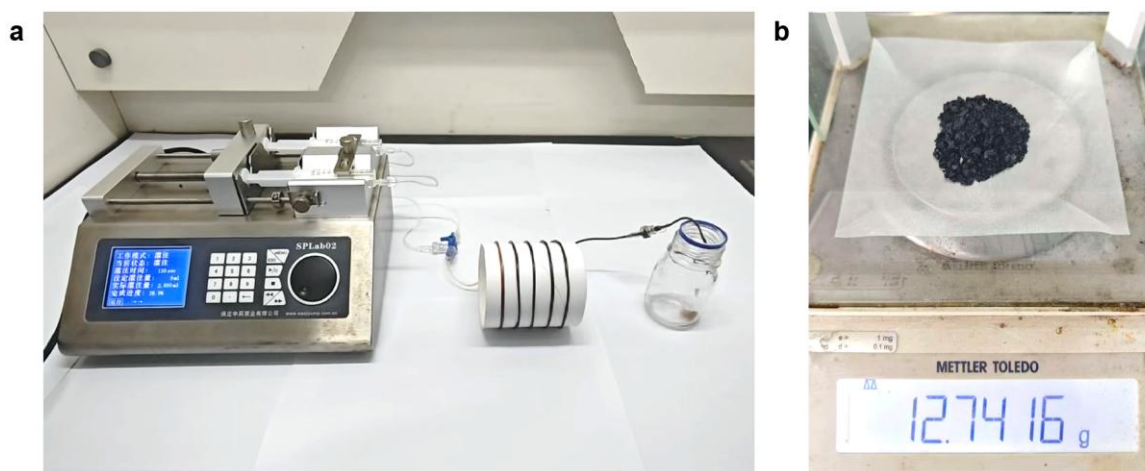
Supplementary Fig. 14 ¹H NMR spectra of LTRI FAPbI₃ PNCs with varying amount of OcA and FAAC. The gray area represents the characteristic peak of oleyl group. All spectra is tested with 20 mg/mL PNC solution in CDCl₃.



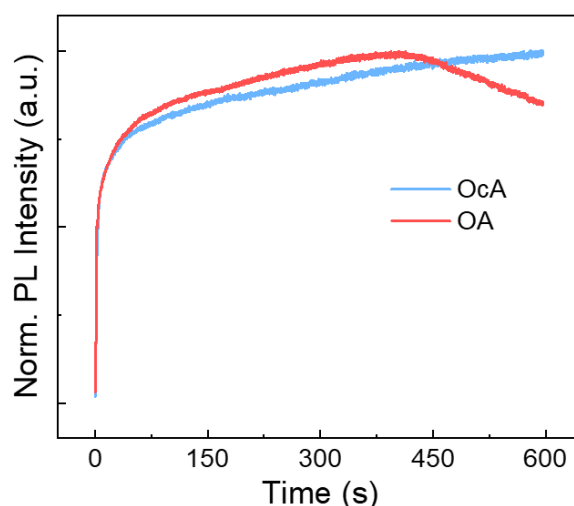
Supplementary Fig. 15 XPS measurements of HI and LTRI FAPbI₃ PNCs with different FAAC. XPS core-level spectra of (a) Pb 4f, (b) I 3d, (c) N 1s, (d) O 1s, (e) C 1s, where the legend shows the FAAC amount (mmol) in the synthesis recipe. The LTRI synthesis is carried out with 60 μ L OA, 60 μ L OAm, 500 μ L OcA, 0.06 mmol PbI₂, 2 mL toluene and different FAAC. To quantitatively evaluate elemental composition, we normalized the Pb signal intensity as a constant reference and calculated relative molar ratios between Pb and other constituent elements across all experimental conditions (f). N(FA) and N(OAm) represent the nitrogen signal from FA and OAm, respectively. A sharp rise in the O:Pb molar ratio from 1.22 to 7.24 can be observed in (d) when increasing FAAC loading. The ratio area of different amount of FAAC covered 3.74 observed in the HI PNCs, indicating a precise control over carboxylic acid ligand density is available in LTRI method.



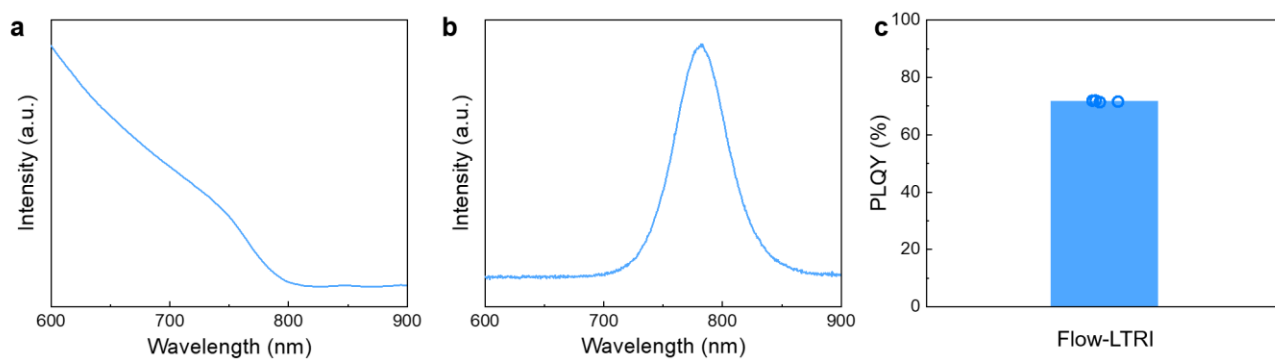
Supplementary Fig. 16 XPS measurements of LTRI FAPbI₃ PNCs with different OcA. XPS core-level spectra of (a) Pb 4f, (b) I 3d, (c) N 1s, (d) O 1s, (e) C 1s. The LTRI synthesis is carried out with 60 μ L OA, 60 μ L OAm, 0.075 mmol FAAC, 0.06 mmol PbI₂, 2 mL toluene and different OcA, which is presented in the legend (μ L). To quantitatively evaluate elemental composition, we normalized the Pb signal intensity as a constant reference and calculated relative molar ratios between Pb and other constituent elements across all experimental conditions (f). N(FA) and N(OAm) represent the nitrogen signal from FA and OAm, respectively. Comparative analysis reveals minimal variation in the N(OAm):Pb ratio across different experimental conditions, indicating that modifications in OcA concentration do not substantially influence the surface coverage of long-chain OAm ligands.



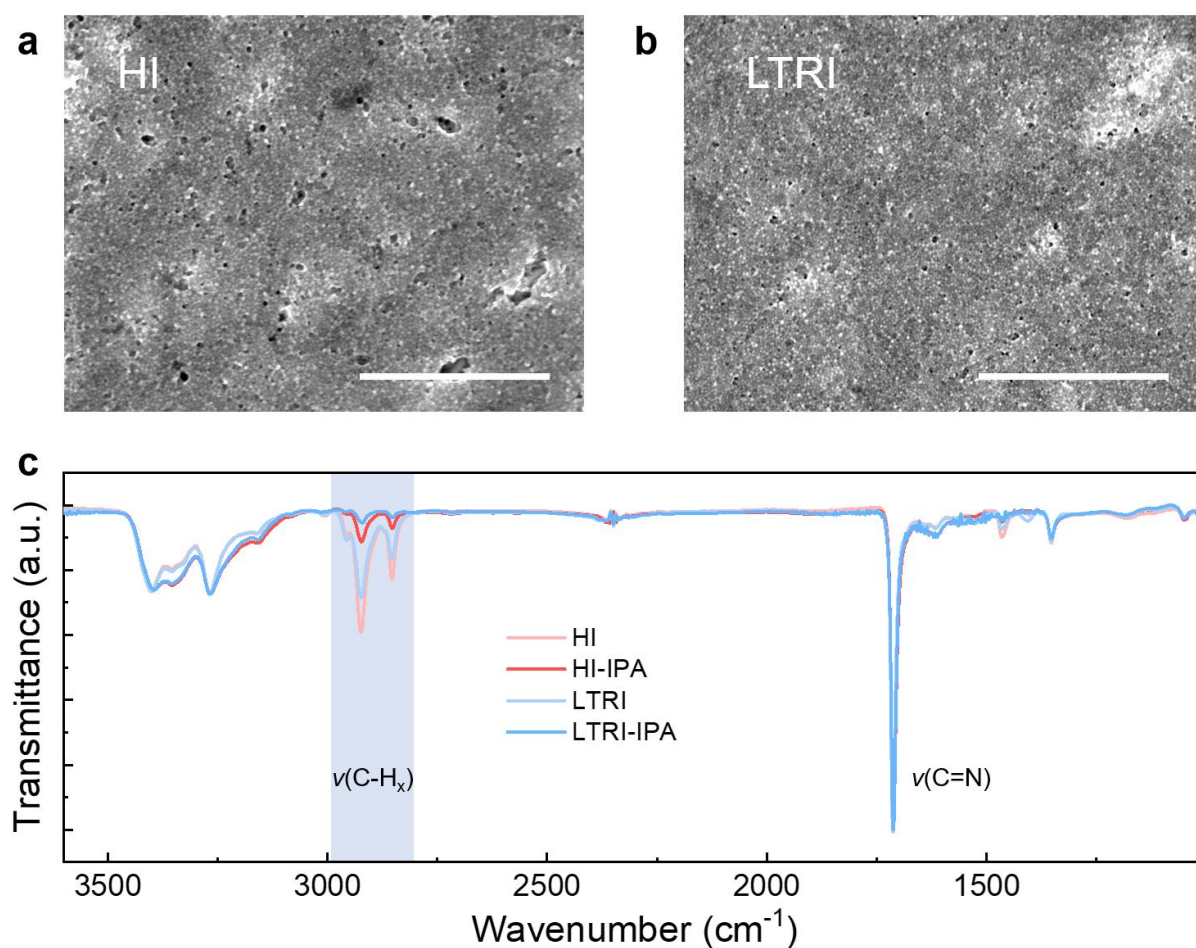
Supplementary Fig. 17 Photograph of FAPbI₃ PNC flow synthesis. (a) The photograph of the flow-synthesis platform. (b) The photograph of purified FAPbI₃ PNC solid from 1 L-scale flow synthesis.



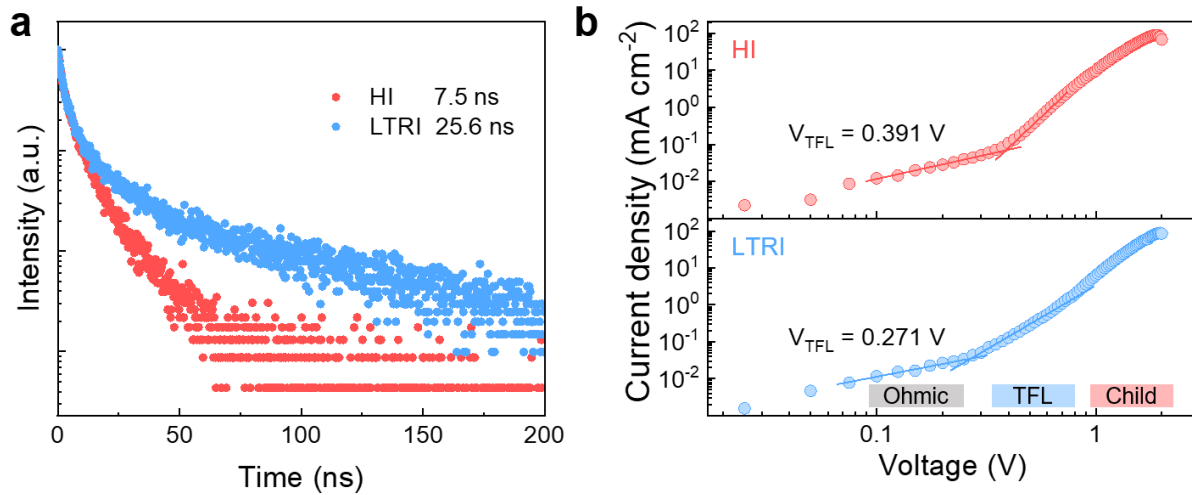
Supplementary Fig. 18 Time-evolution curves of the PL intensity. Time-evolution curves of the PL intensity from in-situ PL spectra of FAPbI₃ PNCs by LTRI synthesis with OA and OcA in Fig. 3b.



Supplementary Fig. 19 Optical properties of flow-synthesis FAPbI₃ PNCs. (a) Absorption, (b) PL spectra and (c) PLQY of flow-synthesis FAPbI₃ PNCs.



Supplementary Fig. 20 Film deposition of HI and LTRI FAPbI₃ PNCs. Top-view SEM images of (a) HI and (b) LTRI FAPbI₃ PNC films. Scale bar, 1 μm . (c) FTIR spectrum of HI and LTRI PNC film with and without treatment of IPA dissolved with 3 mg mL^{-1} MAI, following the film preparation procedure in Methods section. Notably, LTRI PNCs exhibit a lower initial ligand content than their HI counterparts prior to IPA treatment. Consequently, the LTRI films undergo less pronounced shrinkage during IPA processing, ultimately yielding a more uniform and structurally intact film morphology.

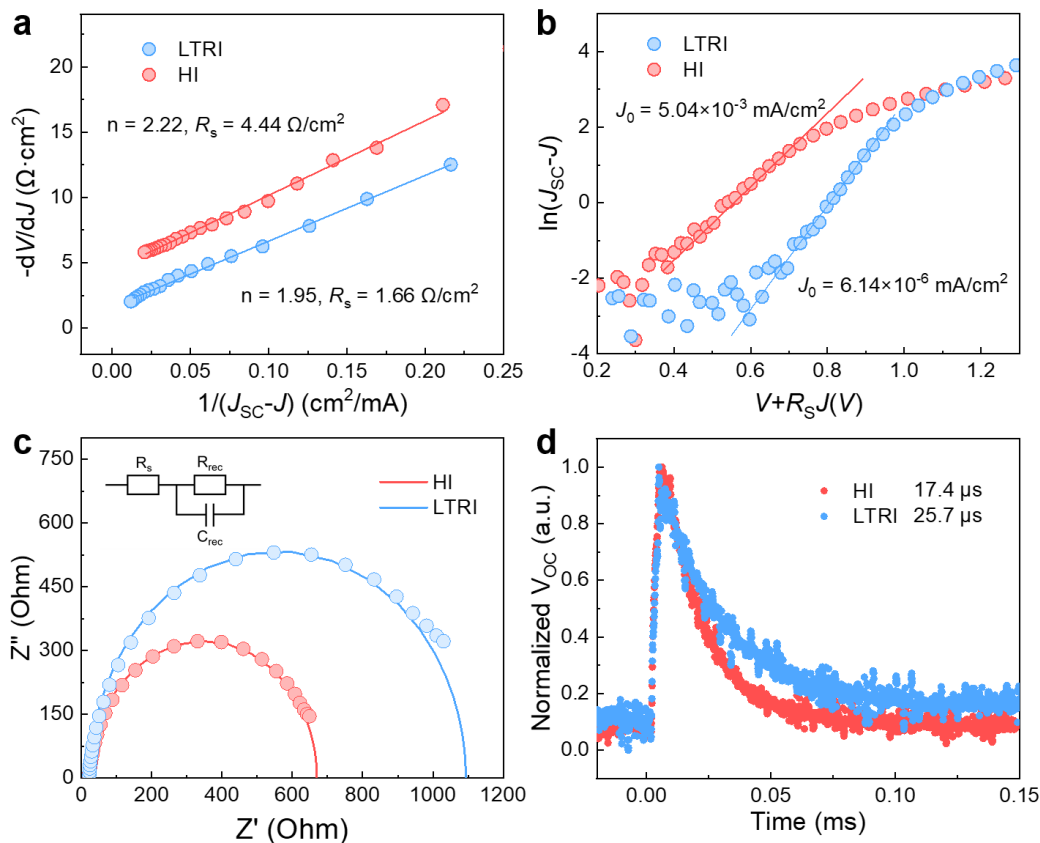


Supplementary Fig. 21 Defects related electrical characteristic of HI and LTRI FAPbI₃ PNC devices. (a) TRPL spectra of PNC films and (b) SCLC curves of electron-only HI and LTRI FAPbI₃ PNC devices. Compared to the HI PNCs, the LTRI PNC films exhibit significantly prolonged carrier lifetime (a) and lower trap-filling voltage (V_{TFL}) (b), suggesting a reduced trap state density and suppressed defect-induced non-radiative recombination in the LTRI PNC films.

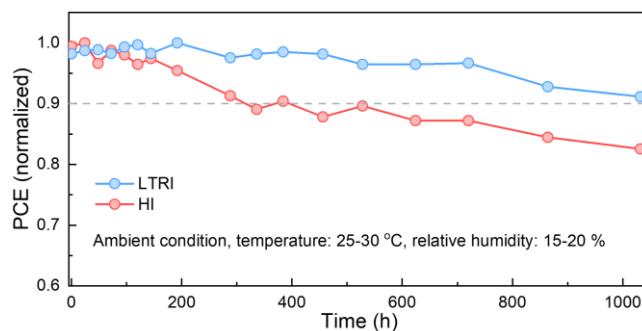
SCLC measurement with an electron-only device structure of FTO/TiO₂/FAPbI₃ PNCs/PCBM/Ag was recorded by Keithley 2400 and measured under dark condition. The electronic trap density (N_e) of FAPbI₃ PNC film was calculated by the following equation:

$$N_e = \frac{2\varepsilon_0\varepsilon_r V_{TFL}}{eL^2}$$

Where ε_0 , ε_r , V_{TFL} , e and L are vacuum permittivity, the dielectric constant, trap-filled limit voltage, elementary charge and film thickness, respectively. Compared to HI device ($N_e = 2.24 \times 10^{16} \text{ cm}^{-3}$), LTRI device shows a lower trap density of $1.55 \times 10^{16} \text{ cm}^{-3}$.



Supplementary Fig. 22 Conductivity related electrical characteristic of HI and LTRI FAPbI₃ PNC devices. (a) $-dV/dJ$ against $(J_{SC}-J)^{-1}$, and (b) $\ln(J_{SC}-J)$ against $V + R_s J$ derived from $J-V$ curves. (c) Nyquist plots and (d) TPV decay spectra of HI and LTRI FAPbI₃ PNC solar cells. $J-V$ characterization analysis (a and b) demonstrates that, in contrast to HI device, LTRI device shows a lower ideal factor (n , signifying reduced trap states), reduced series resistance and a lower initial current density (J_0), suggesting more favorable carrier transport. Nyquist plots (c) of HI and LTRI devices were collected by electrochemical impedance spectroscopy (EIS) and fitted with a semicircle model (RCR circuit), the series resistance (R_s) and carrier recombination resistance (R_{rec}) were extracted at the high- and low-frequency region, respectively. The LTRI device possesses a decreased R_s and increased R_{rec} , indicating effective charge transfer at the heterointerface of devices. Additionally, the carrier extraction dynamics were further studied by transient photovoltage (TPV) decay (d), the LTRI device has a prolonged carrier-extraction lifetime, improving the J_{SC} and FF.⁶



Supplementary Fig. 23 Long-term stability of FAPbI₃ PNC solar cell. The unencapsulated devices were stored under ambient conditions with temperature of 25-30 °C and relative humidity of 15-20%.

Initial PCE of the LTRI and HI device is 18.92% and 16.85%, respectively. LTRI PNC device retains over 90% of initial PCE after 1000 hours, significantly outperforming HI devices which suffered ~20% degradation over the same aging period.

Supplementary Table 1. Synthesis recipe and correspond PL spectra information for ML training. All the recipe is synthesized with 2 mL Toluene and 0.06 mmol PbI₂ under ambient condition. The PL is tested from the crude solution after 2 minutes of reaction. No. 1 to 109 are used to train G1 model, and No. 110 to No. 154 are additional data for G2 model training.

NO.	OA (μL)	OAm (μL)	FAAc (mg)	OcA (μL)	PL Peak	PL FWHM
1	36	36	0.03	250	754.28	78.07
2	36	36	0.06	250	741.71	72.69
3	36	36	0.09	250	769.51	74.93
4	36	36	0.12	250	769.96	71.34
5	36	36	0.03	500	796.31	53.39
6	36	36	0.06	500	764.58	61.02
7	36	36	0.09	500	769.96	74.03
8	36	36	0.12	500	767.72	69.99
9	36	36	0.15	500	769.96	82.56
10	36	36	0.03	750	799.87	50.70
11	36	36	0.06	750	788.73	63.71
12	36	36	0.09	750	772.64	65.96
13	36	36	0.12	750	769.96	85.25
14	36	36	0.15	750	783.81	76.28
15	36	36	0.03	1000	789.62	52.50
16	36	36	0.06	1000	793.19	52.50
17	36	36	0.09	1000	776.67	62.37
18	36	36	0.12	1000	775.77	63.26
19	36	36	0.15	1000	769.51	66.40
20	60	60	0.06	250	752.48	76.28
21	60	60	0.09	250	764.58	78.97
22	60	60	0.12	250	775.32	63.26
23	60	60	0.15	250	775.77	60.57
24	60	60	0.18	250	764.14	72.69
25	60	60	0.06	500	746.65	72.69
26	60	60	0.09	500	786.05	107.23
27	60	60	0.12	500	754.28	74.48
28	60	60	0.15	500	780.69	63.71

29	60	60	0.18	500	781.13	60.12
30	60	60	0.06	750	770.85	61.02
31	60	60	0.09	750	764.14	61.92
32	60	60	0.12	750	786.05	56.98
33	60	60	0.15	750	789.17	56.53
34	60	60	0.18	750	782.03	64.61
35	60	60	0.06	1000	786.05	58.78
36	60	60	0.09	1000	769.51	57.43
37	60	60	0.12	1000	780.24	61.02
38	60	60	0.15	1000	782.03	61.92
39	60	60	0.18	1000	782.47	62.82
40	36	60	0.06	500	756.97	69.55
41	36	60	0.09	500	748.89	71.34
42	36	60	0.12	500	759.21	68.65
43	36	60	0.15	500	781.13	62.82
44	36	60	0.18	500	776.67	64.61
45	120	60	0.06	500	762.35	65.06
46	120	60	0.09	500	775.77	63.26
47	120	60	0.12	500	775.32	66.40
48	120	60	0.15	500	776.22	66.85
49	120	60	0.18	500	781.13	65.06
50	180	60	0.06	500	766.82	59.23
51	180	60	0.09	500	769.96	63.26
52	180	60	0.12	500	773.54	65.06
53	180	60	0.15	500	780.69	62.82
54	180	60	0.18	500	775.77	67.75
55	36	48	0.06	250	758.31	70.44
56	36	48	0.09	250	782.47	63.71
57	36	48	0.12	250	775.77	61.02
58	36	48	0.15	250	770.85	68.20
59	36	48	0.18	250	744.85	87.49
60	36	48	0.06	500	753.38	64.16

61	36	48	0.09	500	781.13	65.51
62	36	48	0.12	500	783.81	64.61
63	36	48	0.15	500	775.32	62.82
64	36	48	0.18	500	779.79	73.58
65	36	48	0.06	750	778.45	56.53
66	36	48	0.09	750	774.88	61.47
67	36	48	0.12	750	781.58	65.96
68	36	48	0.15	750	774.88	65.96
69	36	48	0.18	750	775.32	69.10
70	36	60	0.06	250	748.44	74.93
71	36	60	0.09	250	769.96	74.03
72	36	60	0.12	250	778.45	63.26
73	36	60	0.15	250	781.13	58.33
74	36	60	0.18	250	754.28	83.01
75	36	60	0.06	750	770.40	62.37
76	36	60	0.09	750	764.14	60.57
77	36	60	0.12	750	778.90	60.12
78	36	60	0.15	750	787.39	63.26
79	36	60	0.18	750	782.03	61.47
80	36	72	0.06	250	754.28	76.72
81	36	72	0.09	250	769.51	75.38
82	36	72	0.12	250	777.11	57.43
83	36	72	0.15	250	776.67	58.33
84	36	72	0.18	250	759.66	75.83
85	36	72	0.06	500	737.22	76.28
86	36	72	0.09	500	759.21	66.85
87	36	72	0.12	500	771.30	66.40
88	36	72	0.15	500	782.92	55.64
89	36	72	0.18	500	786.94	56.09
90	36	72	0.06	750	762.79	67.30
91	36	72	0.09	750	758.76	64.16
92	36	72	0.12	750	774.88	62.37

93	36	72	0.15	750	786.94	57.43
94	36	72	0.18	750	787.39	54.29
95	60	72	0.06	250	741.71	79.87
96	60	72	0.09	250	768.61	70.44
97	60	72	0.12	250	775.32	64.16
98	60	72	0.15	250	782.47	56.98
99	60	72	0.18	250	754.28	88.39
100	60	72	0.06	500	759.66	70.44
101	60	72	0.09	500	758.31	67.30
102	60	72	0.12	500	775.32	58.33
103	60	72	0.15	500	787.39	56.53
104	60	72	0.18	500	788.28	53.84
105	60	72	0.06	750	763.24	65.96
106	60	72	0.09	750	763.69	61.92
107	60	72	0.12	750	772.19	64.16
108	60	72	0.15	750	781.13	56.09
109	60	72	0.18	750	792.29	53.84
110	132	54	0.045	350	754.27	75.55
111	180	54	0.045	350	760.1	70.19
112	84	66	0.06	950	781.58	60.93
113	168	66	0.06	950	782.92	62.39
114	168	36	0.06	900	787.83	55.57
115	48	48	0.06	900	781.58	57.03
116	168	42	0.06	500	769.06	62.39
117	108	36	0.06	450	776.66	59.96
118	108	54	0.06	450	765.03	65.8
119	60	36	0.06	550	771.29	64.34
120	132	36	0.06	600	765.03	67.27
121	120	66	0.06	850	774.42	62.39
122	168	36	0.06	450	778	62.39
123	168	42	0.075	800	774.87	58.98
124	144	48	0.075	700	771.74	60.44

125	60	66	0.075	450	763.68	70.19
126	96	66	0.075	650	769.5	62.39
127	96	72	0.075	400	770.4	63.37
128	156	66	0.075	550	765.03	65.32
129	168	60	0.075	500	771.74	63.86
130	132	72	0.075	950	769.95	64.83
131	84	60	0.075	700	776.21	61.42
132	36	60	0.09	450	765.48	69.7
133	84	54	0.09	300	778.45	64.83
134	36	66	0.09	300	764.13	74.09
135	60	72	0.09	1000	777.55	60.44
136	132	66	0.105	600	759.65	70.68
137	36	72	0.105	600	772.19	64.34
138	132	72	0.105	650	776.21	58.49
139	48	60	0.105	750	769.5	62.39
140	60	72	0.105	750	764.13	65.8
141	132	66	0.12	900	777.11	59.47
142	132	72	0.12	550	778	61.42
143	60	66	0.12	300	776.66	60.44
144	36	66	0.12	650	770.85	62.39
145	168	36	0.135	650	789.17	61.42
146	84	54	0.135	550	794.07	56.06
147	168	66	0.15	1000	784.26	58.01
148	180	42	0.15	650	793.18	55.08
149	72	54	0.15	500	788.72	56.54
150	120	48	0.165	900	794.07	56.06
151	144	36	0.165	750	788.72	58.98
152	120	42	0.165	600	787.38	58.01
153	132	54	0.165	500	787.83	56.06
154	48	48	0.18	1000	788.27	61.91

Supplementary Table 2. PL data of PNCs from ML predicted synthesis recipe. All the recipe is picked up randomly from the predicted data, which is synthesized with 2 mL Toluene and 0.06 mmol PbI₂ under ambient condition. The PL is tested from the crude solution after 2 minutes of reaction.

NO.	OA (μL)	OAm (μL)	FAAc (mg)	OcA (μL)	Predicted PL Peak	Predicted FWHM	Tested PL Peak	Tested PL FWHM
1	60	66	0.01	500	757.0888	63.53062	754.2772	63.1942
2	96	72	0.01	450	757.6126	65.36654	759.6568	64.53876
3	180	66	0.025	950	778.7646	58.55355	773.088	56.9196
4	132	60	0.02	600	765.6858	60.88434	759.6568	64.53876
5	180	54	0.025	650	772.2561	58.93974	769.9563	58.26416
6	48	54	0.025	550	762.1565	66.0693	764.1367	64.09058
7	144	60	0.045	900	786.3483	57.68938	789.618	58.26416
8	132	72	0.015	300	762.9852	69.8012	762.793	71.26155
9	144	72	0.03	550	771.0598	62.24881	772.6407	62.29783
10	48	60	0.02	350	757.4743	74.29506	746.6492	74.84704
11	180	54	0.05	850	786.9781	57.36209	788.2792	60.95328
12	60	66	0.06	950	785.1457	60.36321	787.8329	60.95328
13	72	72	0.05	750	785.4461	56.16287	793.187	56.02323
14	84	48	0.045	650	781.3844	61.9497	787.8329	59.60872
15	132	48	0.06	850	789.6424	56.75448	789.618	56.02323
16	156	42	0.055	700	787.8622	60.1666	787.8329	60.95328
17	108	36	0.05	600	783.0301	65.47118	781.5812	67.67606
18	168	36	0.06	600	787.4911	64.04742	787.8329	63.1942
19	60	48	0.04	300	774.0087	66.8438	775.7711	69.91699
20	168	48	0.045	300	775.6819	66.09545	776.2182	68.57243

Supplementary Table 3. Chemical list and price for FAPbI₃ PNC synthesis. Material prices are sourced from public procurement platform, www.tansoole.com.

	Materials	Supplier	Purity (%)	Price (\$)
Lab-scale	PbI ₂	Adamas	99	0.249/g
	ODE	Sigma-Aldrich	90	0.0969/mL
	OA	Alfa	90	0.0821/mL
	OAm	Aladdin	80-90	0.0460/mL
	OcA	TCI	98	0.0354/mL

	Hexane (anhydrous)	Adamas	97	0.0382/mL
	MeOAc (anhydrous)	J&K	99	0.131/mL
	Toluene	Enox	99	0.00506/mL
	FAAc	Aladdin	99	0.0982/g
	PbI ₂	Adamas	99	0.216/g
	ODE	Sigma-Aldrich	90	0.0969/mL
	OA	Alfa	90	0.0570/mL
	OAm	Aladdin	80-90	0.0411/mL
Industry-scale	OcA	Adamas	99	0.0106/mL
	Hexane (anhydrous)	Adamas	97	0.0382/mL
	MeOAc (anhydrous)	J&K	99	0.131/mL
	Toluene	Enox	99	0.00506/mL
	FAAc	Aladdin	99	0.0544/g

Supplementary Table 4. Summary of material cost for 1 gram of HI FAPbI₃, LTRI FAPbI₃ and Flow-LTRI FAPbI₃ PNCs. Material cost of HI and LTRI FAPbI₃ is calculated with lab-scale chemical price, and the material cost of Flow-LTRI FAPbI₃ PNCs is calculated with industry-scale chemical price. No solvent recycling concluded.

		1 g HI FAPbI ₃			1 g LTRI FAPbI ₃			1 g Flow-LTRI FAPbI ₃		
	Materials	Amount used	Cost (\$)	Total material cost (\$/g)	Amount used	Cost (\$)	Total material cost (\$/g)	Amount used	Cost (\$)	Total material cost (\$/g)
Synthesis	PbI ₂	0.860 g	0.21	8.60	1.29 g	0.32	2.01	1.29 g	0.28	1.29
	ODE	66.7 mL	6.46		0	0.00		0	0.00	
	OA	20.0 mL	1.64		2.79 mL	0.23		2.79 mL	0.16	
	OAm	5.00 mL	0.23		2.79 mL	0.13		2.79 mL	0.11	
	OcA	0	0.00		23.3 mL	0.82		23.3 mL	0.25	
	Toluene	0	0.00		93.0 mL	0.47		93.0 mL	0.47	
	FAAc	0.512 g	0.05		0.367 g	0.04		0.367 g	0.02	
Purification	Hexane	20.0 mL	0.76	5.14	14.0 mL	0.53	0.78	14.0 mL	0.53	0.78
	MeOAc	33.3 mL	4.38		1.86 mL	0.24		1.86 mL	0.24	

Supplementary Table 5. Summary of labor cost for 1 gram of HI FAPbI₃, LTRI FAPbI₃ and Flow-LTRI FAPbI₃ PNCs. The labor cost is determined by the number of operators, average labor wages and process throughput. Here, all the synthesis process is estimated with one operator and the lowest labor wages in the literature (27 \$/h/person).⁷ The PNC production of HI and LTRI methods are measured from the experiment, which is 1.2 g and 1.29 g, respectively. The production rate of MF LTRI method is estimated from LTRI FAPbI₃. Since the PbI₂ precursor in the LTRI method is prepared simply by room-temperature stirring and the solution is stable, the 12-hour dissolution step proceeds without human oversight and thus is not factored into the labor cost. The temporal investment required for the synthesis procedure is considered negligible, as the automated nature of the process minimizes necessary human intervention and oversight. For purification steps, 18 L crude solution could be purified at once, which yields 193.5 g PNC solid.

HI FAPbI ₃ PNC			
Operation	Time (min)	Synthesis throughput (g/h)	Labor cost (\$/g)
Preparation for synthesis equipment	15	0.257	105.06
FA-OA precursor synthesis: preparation	15		
Gas removal	90		
FAPbI ₃ synthesis: preparation	20		
Gas removal	60		
PbI ₂ dissolution and gas removal	30		
Reaction and ice bath	10		
Purification	30		
Clean the equipment	10		
LTRI FAPbI ₃ PNC			
Operation	Time (min)	Synthesis throughput (g/h)	Labor cost (\$/g)
Preparation for synthesis equipment	10	0.968	27.92
Precursor synthesis: preparation	20		
FAPbI ₃ synthesis reaction	10		
Purification	30		
Clean the equipment	10		
Flow-LTRI FAPbI ₃ PNC			
Operation	Time (min)	Synthesis throughput (g/h)	Labor cost (\$/g)
Purification	30	290.25	0.09
Clean the equipment	10		

Supplementary Table 6. Summary of photovoltaic performance.

Sample	Scanning direction	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)	
HI	Champion	Reverse	1.128	20.80	73.4	17.22
		Forward	1.121	20.89	72.3	16.93
	Average*	1.115±0.016	20.50±0.66	72.6±2.8	16.58±0.40	
LTRI	Champion	Reverse	1.129	21.39	80.7	19.37
		Forward	1.126	21.35	79.8	19.11
	Average*	1.131±0.005	20.97±0.29	80.8±1.4	18.98±0.19	

*The data were collected from 30 individual cells.

Supplementary Table 7. Summary of the representative nanocrystal/quantum dot-based photovoltaics.

Year	Materials	Synthesis temperature (°C)	PCE (%)	Ref.
2016	CsPbBr ₃ PNC	25*	5.4	<i>Nat. Energy</i> 2 , 16194 (2016)
2016	CsPbI ₃ PNC	170	10.77	<i>Science</i> 354 , 92 (2016)
2017	CsPbI ₃ PNC	185	13.4	<i>Sci. Adv.</i> 3 , eaao4204 (2017)
2020	Cs _{0.5} FA _{0.5} PbI ₃ PNC	170	16.6	<i>Nat. Energy</i> 5 , 79 (2020)
2024	FAPbI ₃ PNC	80	18.94	<i>Nat. Energy</i> 9 , 324 (2024)
2025	FAPbI ₃ PNC	80	19.01	<i>Adv. Mater.</i> 37 , e12201 (2025)
2025	FAPbI ₃ PNC	80	19.14	<i>Energy Environ. Sci.</i> 18 , 8964 (2025)
2026	FAPbI ₃ PNC	80	19.37	<i>Energy Environ. Sci.</i> 19 , 2213, (2026)
2024	FAPbI ₃ PNC	80	16.61	<i>Nat. Energy</i> 9 , 1378 (2024)
2025	FA _{0.47} Cs _{0.53} PbI ₃ PNC	180	18.37	<i>Nat. Commun.</i> 16 , 8612 (2025)
2014	PbS QD	150	9.2	<i>Nat. Mater.</i> 13 , 796 (2014)
2019	PbS QD	120	12.6	<i>Nature</i> 570 , 96 (2019)
2019	PbS QD	120	13.1	<i>Nat. Energy</i> 4 , 969 (2019)
2019	PbS QD	25*	10.1	<i>Nat. Commun.</i> 10 , 5136 (2019)
2025	FAPbI₃ PNC	25	19.37	This work

*The reported work only describes synthesis at room temperature, which we define as 25 °C.

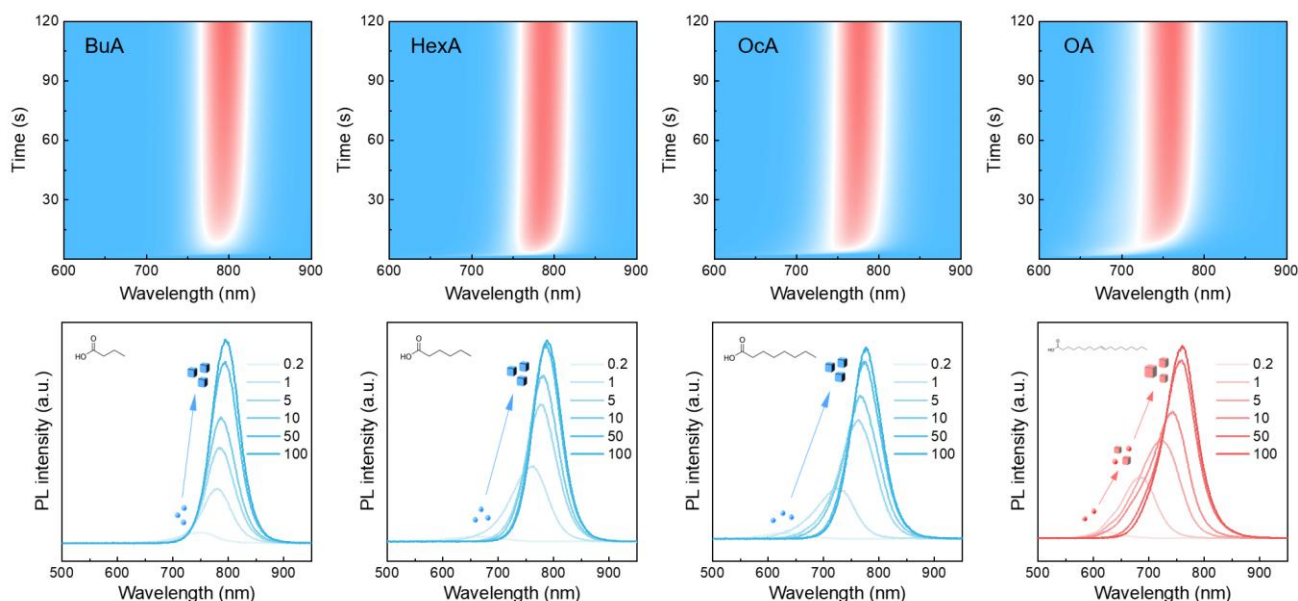
Supplementary Table 8. Summary of photovoltaic performance of the 1-L scale PNC device.

Sample	Scanning direction	V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF (%)	PCE (%)	
1 L scale	Champion	Reverse	1.126	21.05	79.6	18.87

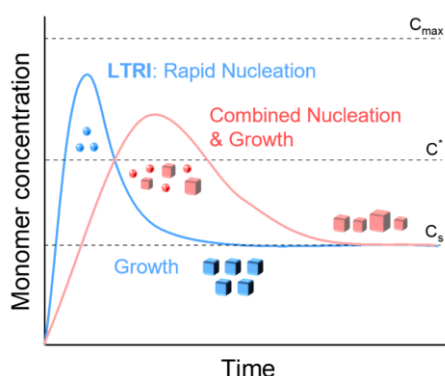
	Forward	1.124	20.81	79.0	18.49
Average*		1.123±0.002	20.73±0.31	77.6±1.7	18.49±0.14

*The data were collected from 12 individual cells.

Supplementary Note 1. Comparison of LTRI FAPbI₃ PNC synthesis with different acid chain length.



In this work, we compared acid ligands with different chain lengths (butyric acid (BuA), hexanoic acid (HexA), OcA, and OA) for the LTRI synthesis of FAPbI₃ PNCs. The synthesis is carried out with 60 μ L OA, 60 μ L OAm, 0.075 mmol FAc, 0.06 mmol PbI₂, 2 mL toluene and 3.16 mmol acid (289 μ L for BuA, 396 μ L for HexA, 500 μ L for OcA, 1001 μ L for OA) at room-temperature. Figure above shows the in-situ PL spectra in 2 minutes (up) and the extracted PL spectra at 0.2 s, 1 s, 5 s, 10 s, 50 s and 100 s (down). It was observed that the use of shorter carboxylic acids in the LTRI synthesis leads to a more rapid redshift of the photoluminescence (PL) peak during the reaction. After 100 s of reaction, the PL peak positions of the PNC solutions were 795 nm, 787 nm, 776 nm, and 759 nm for BuA, HexA, OcA, and OA, respectively, with corresponding FWHM values of 60 nm, 60 nm, 62 nm, and 68 nm.



Notably, the OA sample exhibited a significantly asymmetric PL spectrum during the first 50 s of the reaction, a feature not observed in the other samples. This indicates that the introduction of OA leads

to combination nucleation and growth, resulting in less uniform PNC formation at room-temperature. In contrast, the use of shorter-chain carboxylic acids markedly accelerates the reaction and yields PNCs with narrower PL FWHM. Considering that longer ligand chain lengths enhance product stability through steric hindrance, octanoic acid was identified as the optimal choice for the synthesis in this study.

Supplementary Note 2. Machine learning model construction

1. Data Preprocessing

To enhance the linear correlation between the synthesis parameters and the optical properties, the target variables (PL peak and FWHM) were physically transformed from the wavelength domain (λ , nm) to the energy domain (E , eV) prior to model training, utilizing the relation $E \approx 1240 / \lambda$. Furthermore, the four input features (OA, OAm, FA, OcA) were standardized using a StandardScaler of scikit-learn package.

2. Hyperparameter Optimization (HPO)

The model architectures and hyperparameters were optimized using the Tree-structured Parzen Estimator (TPE) algorithm via the Optuna⁸ framework. The search space encompassed five advanced tree-based algorithms: Random Forest⁹, Gradient Boosting Regressor (GBR)¹⁰, XGBoost¹¹, LightGBM¹², and CatBoost¹³. In the HPO, 30 evaluation trials were conducted using 3-fold cross-validation, with the negative root mean squared error (-RMSE, calculated in the eV domain) serving as the maximized objective metric. The single best-performing model framework and its associated optimal hyperparameters from the study were selected.

$$-\text{RMSE} = -\sqrt{\frac{1}{n} \sum_{i=0}^{n-1} (y_i - \hat{y}_i)^2}$$

Search range of the model frameworks and corresponding hyperparameters (default values are omitted)

Model framework	Hyperparameter range
Random forest ⁹	Number of trees: [50,200] Maximum depth of the individual trees: [3, 10] Minimum samples per leaf: [1, 4] Max features: {'sqrt','log2',1.0}

Gradient boosting regressor ¹⁰	Number of boosting stages: [50,200] Learning rate (log scale): [0.01, 0.2] Maximum depth of the individual estimators: [3, 6] Subsample ratio: [0.6, 1]
XGBoost ¹¹	Number of boosting stages: [50,200] Learning rate (log scale): [0.01, 0.2] Maximum depth of the individual estimators: [3, 6] Subsample ratio: [0.6, 1.0] Colsample by tree: [0.6, 1.0]
LightGBM ¹²	Number of boosting stages: [50,200] Learning rate (log scale): [0.01, 0.2] Maximum leaves: [15, 63] Colsample by tree: [0.6, 1.0]
CatBoost ¹³	Number of boosting stages: [100,300] Learning rate (log scale): [0.01, 0.2] Maximum depth of the individual estimators: [3, 6] L2 leaf regularization (log scale): [0.001, 10]

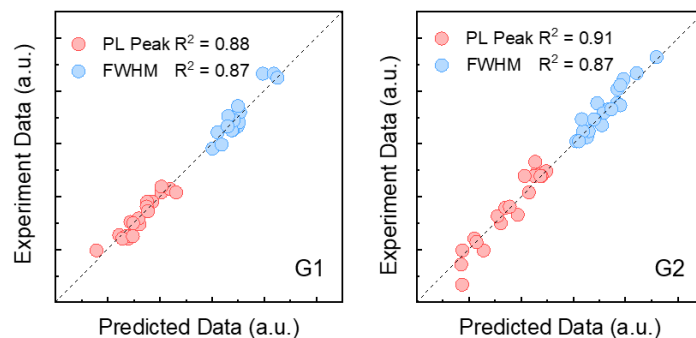
Searched optimal framework-hyperparameter combinations

Prediction target	Optimal framework-hyperparameter combination
PL	Framework: CatBoost Number of boosting stages: 271 Learning rate: 0.0340281674759088 Maximum depth of the individual estimators: 3 L2 leaf regularization: 0.03707156538704712
FWHM	Number of boosting stages: 50 Learning rate: 0.18035629556200522 Maximum depth of the individual estimators: 3 Subsample ratio: 0.6008141686889802 Colsample by tree: 0.8623884766975469

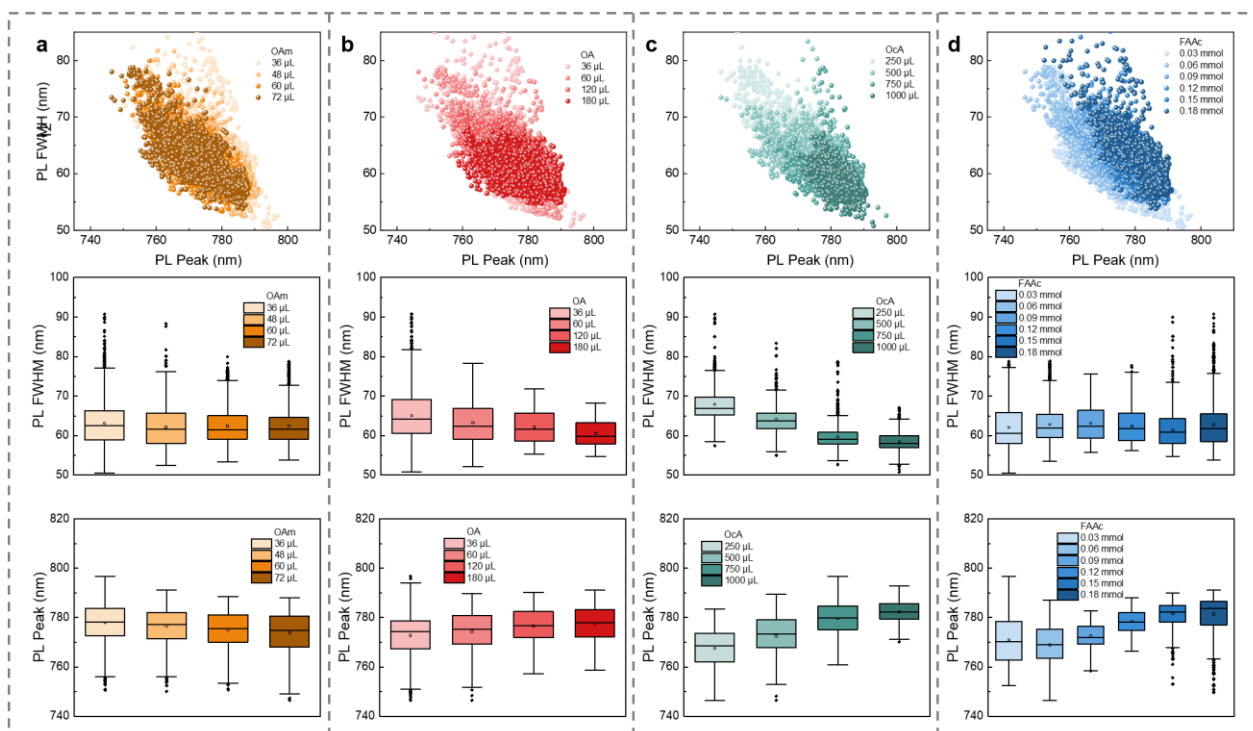
3. SHAP Analysis and Physical Interpretability

To decipher the decision-making process of the dynamically optimized "black-box" model, Shapley Additive exPlanations (SHAP)¹⁴ were employed. Since the model was fundamentally trained to output energy, a custom prediction wrapper function ($f(X) = 1240/\text{Model}(X)$) was utilized, allowing SHAP to directly calculate feature impacts in the optical wavelength domain.

Supplementary Note 3. Analysis of ML predicted data



To ensure the predictive accuracy of the model, we augmented the training dataset with additional experimental data after establishing the G1 model, leading to the updated G2 model. 20 synthesis conditions within the prediction domain (FAAc: 0.03-0.18 mmol, OcA: 250-1000 μ L, OA: 36-180 μ L, OAm: 36-72 μ L, with 2 mL toluene and 0.06 mmol PbI_2) and performed the corresponding experiments. The accuracy of the models was then assessed by comparing the measured PL data with the predicted values. As shown in the figure above, we compared the predicted values with the experimental values for both models. For both the PL peak and PL FWHM, the R^2 values are close to 0.9, indicating good predictive accuracy. Moreover, the iterative refinement of G2 yields only a marginal improvement in prediction performance over G1. Therefore, we consider the predictive accuracy of G2 to be sufficient for the subsequent analyses, and no further iterative training is required.



With the assistance of machine learning, we generated approximately 16,000 sets of synthesis

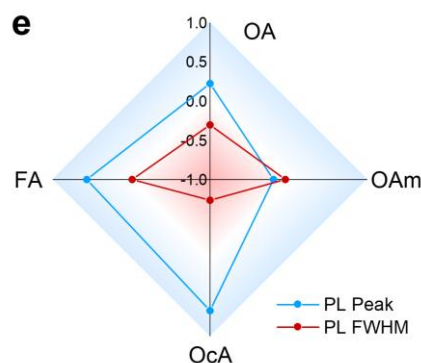
formulations with potential viability, along with the corresponding PL peak positions and FWHM of the resulting products. Here, we conducted statistical analyses for four synthesis variables. Taking **Figure a** as an example, the top panel displays the distribution of PL peak positions and FWHM for all possible products when the amount of OAm in the formulation is fixed at 36, 48, 60, and 72 μL , while the other three variables are allowed to vary freely. The middle and bottom panels present the corresponding box plots for the PL peak positions and FWHM of the synthesized products, respectively. All the box plots have 25-75% box line, $1.5\times$ interquartile range whiskers, median line and mean point. These statistical plots reveal qualitative relationships between the four variables and the properties of the room-temperature synthesized products:

OAm: **Figure a** show the PL distribution statistics related to oleylamine. When the amount of OAm is varied in the synthesis, neither the PL peak position nor the FWHM shows a significant difference.

OA: **Figure b** presents the PL distribution statistics related to oleic acid. It can be observed that when the amount of OA is increased, the PL peak position will slightly increase and PL FWHM will slight decrease.

OcA: **Figure c** shows the PL distribution statistics related to octanoic acid. As the OcA content in the reaction system increases, the PL peak position demonstrates a distinct red-shift trend, while the FWHM tends to decrease.

FAAc: **Figure d** presents the PL distribution statistics related to FFAc. The relationship between FA precursor quantity and PL spectral properties displays notable complexity rather than simple linear correlation. Within the optimal concentration range of 0.06-0.15 mmol, increasing FFAc content systematically induces a redshift in PL emission peak. However, when the FFAc content is excessively high (0.18 mmol) or low (0.03 mmol), the synthesized products exhibit irregular distributions of PL. These observations are consistent with the conclusion in Supplementary Fig. 4, where insufficient FA concentration promotes formation of irregular low-dimensional structures while excess FA leads to substantial nanocrystal aggregation.



To quantitatively analyze the influence of each synthesis variable, we employed the Pearson correlation coefficient r to characterize the relationships between the four variables and the PL peak position and FWHM of the synthesized products in **Figure e**. The formula is shown below:

$$r = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^n (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^n (Y_i - \bar{Y})^2}}$$

It can be found that the FAAc and OcA show significantly stronger correlations with a coefficient of 0.57 and 0.67 for PL peak position; and -0.01 and -0.74 for PL FWHM. Although OA displayed 0.22 correlation coefficient, the SHAP analysis presented in Fig. 1e indicates that its overall influence remains considerably weaker than that of the other variables. These findings suggest that FAAc and OcA emerge as more influential parameters compared to OA and OAm in determining the optical properties of the resulting PNCs.

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