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Supporting Information

Rational Design of One-dimensional Triarylamine-based Covalent Organic Frameworks for Perovskite Solar Cells with Improved Efficiency and Stability

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Section S1: Materials and General Methods

1.1 Chemicals

Mesitylene, and nitrobenzene were purchased from Acros Organic. Imidazole, Trifluoroacetic anhydride, Tri(4-aminophenyl) amine, *p*-Toluidine, Aniline, *p*-Fluoroaniline, 4-Trifluoromethylamine were purchased from Aladdin. Dichloromethane (CH_2Cl_2) and Petroleum ether (PE) was purchased from Admas. Trifluoroacetic acid, conc. Hydrochloric acid (36 wt % in water), $NaHCO_3$, $MgSO_4$ and Toluene were purchased from Jiangtian huagong (Tianjin, China). Acetone (> 99%), Chlorobenzene (> 99.8%), Tetrahydrofuran (> 99%), 1,4-dioxane (> 99%), Dimethyl sulfoxide (DMSO, > 99.5%), N, N-Dimethylformamide (DMF, > 99.8%), Acetonitrile (>99%), Methanol (>99%), 2-Propanol (>99.5%), hydrobromic acid (47 wt % in water), hydroiodic acid (57 wt % in water), *d6*-DMSO, were purchased from Sigma Aldrich. Methylamine hydrochloride (MACl), PbI_2 (> 99.9%), $PbBr_2$ (> 99.9%), $PbCl_2$ (> 99.9%), Spiro-MeOTAD (> 98%), PEDOT:PSS and $PC_{61}BM$ were pursued from Xi'an Yuri Solar Co., Ltd. FTO glass, Formamidinium iodide (FAI), 4-tert-butylpyridine (t-BP, > 98%) and lithium bis(trifluoromethylsulphonyl)imide (LiTFSI, >99.95%) were pursued from Yingkou Youxuan Technology Co., Ltd. SnO_2 colloidal solution (15 wt% in H_2O) was purchased from Alfa Aesar.

1.2 Analytical techniques

Fourier-transform infrared spectroscopy (**FTIR**) spectra were recorded on FTIR-650 (Tianjin Donggang). Powder X-ray diffraction (**PXRD**) patterns were collected from Mini Flex 600, Rigaku, X-ray diffraction analysis platform with Cu Kα radiation (λ = 1.5418 Å). Samples were observed at a scan speed of 10.0 deg min^{-1} from 2-35° for COF and 2-60° for PbI_2 or perovskite film on FTO. Ultraviolet-visible (**UV-vis**) absorption spectrum was obtained from the UV2600. Ultraviolet-visible-near IR (**UV-vis-NIR**) absorption spectrum was obtained from the PerkinElmer Lambda 950. Nuclear magnetic resonance (**NMR**) spectra were obtained on an NMR Bruker 500 MHz operated at room temperature. Transmission electron microscopy (**TEM**) and high-resolution transmission electron microscopy（HR-TEM）images of the powder was taken by JEOL F2001 operating at 300 kV for morphology and JEOL F200 for mapping. The powder dispersed in ethanol. After ultrasonication for 15min, the solution was dropped on TEM grids for testing. Cross-sectional Scanning Electron Microscope (**SEM**) and top-view SEM images were taken by a field emission scanning electron microscopy Hitachi UHR FE-SEM SU8000. X-ray photoelectron spectroscopy (**XPS**) and ultraviolet photoelectron spectroscopy (**UPS**) were measured using a photoelectron spectrometer Kratos Analytical, ESCALAB-250Xi and the He(I) excitation was 21.22 eV. Steady-state photoluminescence (**PL**) was measured with HORIBA Scientific FlouroMax-4 with excitation wavelength 500 nm. Time-resolved photoluminescence (**TRPL**) was measured using a HORIBA Fluorolog-3 spectrometer equipped with a 450 W Edinburgh Xe900 Xenon lamp as the exciting light source. ***J-V* curves** were obtained using a Keithley 2400 source under one simulated sun illumination. The AM 1.5G spectrum was obtained from an Oriel 300 W solar simulator and calibrated to 100 mW cm^{-2} using a standard Si solar cell (NREL, Newport). During the test, the active area of the devices was controlled at 0.04 cm^2, and the scanning speed was 100 mV s^{-1}. The incident light-to-electron conversion efficiency (**IPCE**) was obtained through the IPCE test system

(E0201a, Chinese Academy of Sciences)_under DC mode condition, where monochromatic beam was generated by a CHF-XM-500 W Xenon lamp. Electrochemical impedance spectroscopy (**EIS**) was measured with an electrochemical workstation (Vertex. +One. EI, Ivium) via a bias voltage -0.8 V. Film thickness were determined by Alpha-Step D-300 Stylus Profiler. Atomic force microscopy (**AFM**) images were recorded in tapping mode on a Bruker Dimension icon. The **Contact Angles** were measured using a JC 2000D contact angle instrument. Particle size analysis was tested by Delsa nano C particle analyzer (Beckman Counter). Solid state NMR (**ssNMR**) spectra were collected using AVANCE II 400M. Low-pressure **N_2 adsorption measurements** were carried out on a Micromeritics ASAP 2420 surface area analyzer. A liquid N_2 bath was used for measurements at 77 K.

Section S2: Synthesis of COFs

2.1 Synthesis of TPB-CHO linker[1,2]

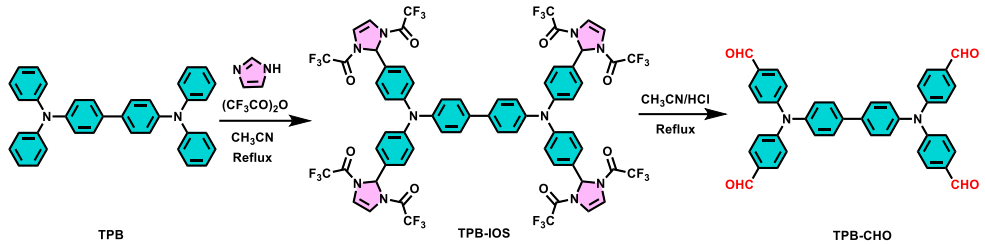

Figure S1. Schematic route to the synthesis of the TPB-CHO.

*1,1',1'',1''',1'''',1''''',1''''''-((([1,1'-biphenyl]-4,4'-diylbis(azanetriyl))tetrakis(benzene-4,1-diyl))tetrakis(1H-imidazole-2,1,3(2H)-triyl))octakis(2,2,2-trifluoroethan-1-one) (**TPB-IOS**)* : To a solution of imidazole (1.36 g, 20.0 mmol) in acetonitrile (30.0 mL) was added dropwise trifluoroacetic anhydride (10.5 g, 50.0 mmol) under an argon atmosphere. The mixture was refluxed for 1 h, and then cooled by removal of the oil bath. *N*,*N*,*N*',*N*'-tetraphenylbenzidine (TPB, 1.96 g, 4.0 mmol) was added to the mixture, and then the reaction mixture was refluxed for 20 h. After cooling to room temperature, the reaction mixture was treated with ice to give a green precipitate, which was filtrated and washed with water and ethanol. The precipitate was dissolved in CH_2Cl_2, washed with saturated aqueous $NaHCO_3$, and dried over $MgSO_4$, and the solvent was removed under reduced pressure to afford a greenish-yellow solid (, 6.10 g), which was used for the next step without further purification.

*4,4',4'',4'''-([1,1'-biphenyl]-4,4'-diylbis(azanetriyl))tetrabenzaldehyde (**TPB-CHO**)*: To a suspension of this crude product in acetonitrile (200 mL) was added a dilute hydrochloric acid (20 mL of conc. hydrochloric acid and 100 mL of water) under an argon atmosphere. The mixture was refluxed for 6 h, after cooling and neutralization with saturated aqueous $NaHCO_3$ to PH = 7. The flittered dark red participation was dissolved in CH_2Cl_2, and the residue was chromatographed on silica gel (CH_2Cl_2:PE = 3:1 as eluent) to afford TPB-CHO (1.98g, 83%) as a bright-yellow solid: ^{1}H NMR (400 MHz, *d6*-DMSO) δ (ppm) 9.92 (s, 4H), 7.81 (d, J = 8.6 Hz, 8H), 7.62 (d, J = 8.5 Hz, 4H), 7.25 (dd, J = 8.1, 3.0 Hz, 12H). ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 122.25, 126.26, 127.61, 130.43, 130.91, 137.72, 151.16, 189.63. MALDI-TOF-MS m/z: 647.115.

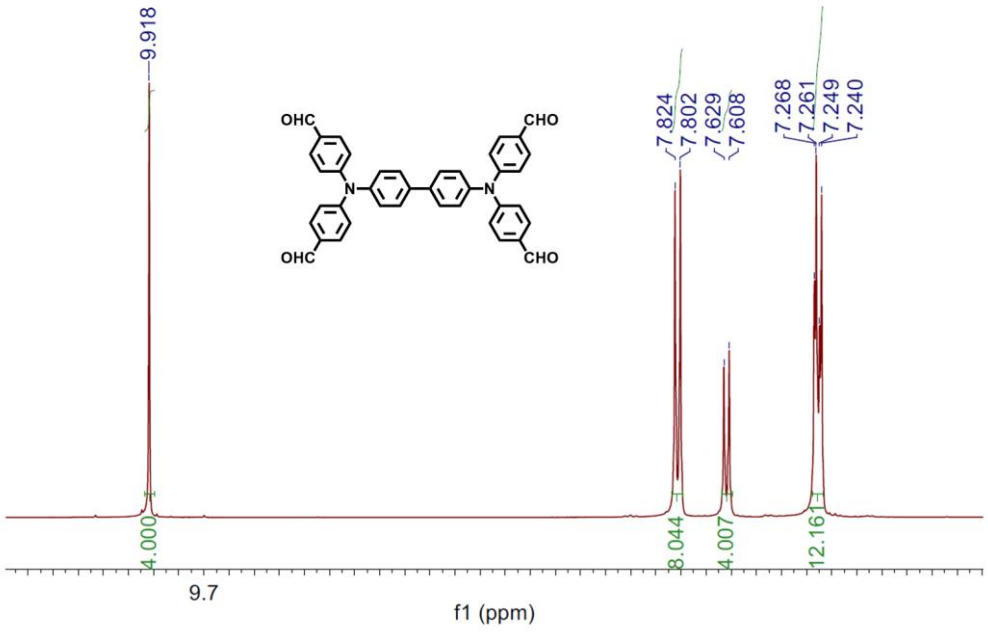

Figure S2. ^{1}H NMR spectrum of TPB-CHO.

2.2 Synthesis of $[(TPA)_2(TPB)_1]$-*C=N*-[3]

12.0 mg TPB-CHO (0.02 mmol), 12.0 mg tri(4-aminophenyl) amine (TPA-NH_2) (0.04 mmol) and *p*-toluidine (45.0 mg, 0.42 mmol) were added to 1.5 mL nitrobenzene, and then completely dissolved by ultrasound for 10 min. Then, 0.5 mL methylene and 4 μL trifluoroacetic acid (TFA)were added, sealed and reacted at 85 °C for 120 h. After centrifugation and precipitation with ethanol (× 3 times) and THF (× 3 times), 16.9 mg of orange solid powder was obtained after vacuum drying. The theoretical yield was 22.2 mg ($C_{304}H_{224}N_{40}$, 4437.29 g mol^{-1}), and the yield was 76.1%.

2.3 Synthesis of $[(TPA)_2(TPB)_1]$-*C=N*-X

$[(TPA)_2(TPB)_1]$-*C=N*- (22.0 mg, 0.02 mmol) was dispersed in 5 mL THF, concentrated hydrochloric acid (2.0 mg, 0.05 mmol) was added, the mixture was vigorously stirred at room temperature for 30 min. After centrifugation and precipitation with ethanol for 3 times, 22.4 mg of dark black solid was obtained after vacuum drying. The theoretical yield was 23.6 mg ($C_{304}H_{232}N_{40}Cl_8$, 4728.98 g mol^{-1}), and the yield was 94.9%.

$[(TPA)_2(TPB)_1]$-*C=N*- (22.0 mg, 0.02 mmol) was dispersed in 5 mL THF, hydrobromic acid 47 wt.% in H_2O (9 mg, 0.05 mmol) was added, the mixture was vigorously stirred at room temperature for 30 min. After centrifugation and precipitation with ethanol for 3 times, 25.0 mg of dark black solid was obtained after vacuum drying. The theoretical yield was 25.4 mg ($C_{304}H_{232}N_{40}Br_8$, 5084.59 g mol^{-1}), and the yield was 98.4%.

$[(TPA)_2(TPB)_1]$-*C=N*- (22.0 mg, 0.02 mmol) was dispersed in 5 mL THF, hydriodic acid 57 wt.% in H_2O (11 mg, 0.05 mmol) was added, the mixture was vigorously stirred at room temperature for 30 min. After centrifugation and precipitation with ethanol for 3 times, 27.0 mg of dark black solid was obtained after vacuum drying. The theoretical yield was 27.3 mg ($C_{304}H_{232}N_{40}I_8$, 5460.59 g mol^{-1}), and the yield was 98.9%.

Section S3: Computational details

3.1 COF structure simulation

Computational modeling of the $[(TPA)_2(TPB)_1]$-*C=N*- structure was carried out using the Materials Studio. The calculated PXRD pattern was generated with the Reflex Plus module using Pseudo-Voigt function. Finally, Pawley refinement was applied for profile fitting, producing the refined PXRD profile.

3.2 The binding energy and electron interaction of heterostructures

All calculations were conducted using the Vienna *Ab initio* Simulation Package (VASP)[4,5]. The COF adsorbed on perovskite (COF@perovskite) was simulated in a superlattice model, with lateral dimension **a** = 20.002 Å, **b** = 13.006 Å and containing 358 atoms. The Spri-OMeTAD adsorbed on COF structure was simulated in a superlattice model, with lateral dimension **a** = 41.078 Å, **b** = 52.000 Å and containing 445 atoms.

The projector-augmented wave (PAW)[6,7] method was adopted to describe the core-valence electron interaction, and the generalized gradient approximation (GGA) formulated by Perdew-Burke-Ernzerhof (PBE)[8], was employed to treat the exchange correlation between electrons. The plane-wave cutoff energy was set to 400 eV. The energy criterion was set to 10^{-4} eV in iterative solution of the Kohn-Sham equation. A vacuum layer of 15 Å is added perpendicular to the surface to avoid artificial interaction between periodic images, and dipole correction[9] was employed to improve the convergence.

2×3×1 and 1×1×1 Gamma-centered k-meshes were used for COF@perovskite and COF@Spiro-OMeTAD models, respectively, to calculate their electronic properties. All the structures were relaxed until the residual forces on the atoms declined to be less than 0.03 eV/Å.

Section S4: Preparation of PSCs

4.1 Fabrication of planar n-i-p PSCs

Fluorine-doped SnO_2 (FTO) conductive substrate was cleaned with deionized water, acetone, isopropanol and ethanol, each step taking 20 minutes. Oxygen plasma was treated for 10 min, 100W to clean further. The SnO_2 layer was deposited on the cleaned FTO substrate by spin coating using a SnO_2 colloidal solution diluted with water (1:5 v/v%) and annealing at 150 °C for 30 min at ambient atmosphere. A 1.5 M of PbI_2 solution was prepared by dissolving 691.5 mg of PbI_2 in 900 μL of DMF and 100 μL of DMSO. The PbI_2layer was spin-coated on the SnO_2-coated FTO substrate at 1500 rpm for 30 s, and annealing at 90°C for 5 min. Organic salts of FAI: MACl (172 mg: 42 mg in 2mL IPA) with/without COF-I were spin-coated on PbI_2 films at a rate of 2000 rpm for 30 s, followed with thermal annealing at 150 °C for 12 min in ambient air with a humidity (30~40%). After cooled to room temperature, the perovskite films were transferred into glovebox for hole transporting layer deposition. A spiro-MeOTAD layer was spin-coated at 4000 rpm for 30 s using the solution of 72.3 mg of spiro-MeOTAD, 28.8 μL of 4-tert-butylpyridine and 17.5 μL of LiTFSI (520 mg dissolved in 1 mL of acetonitrile) in 1 mL chlorobenzene. A gold electrode was deposited on the spiro-MeOTAD layer by thermal evaporation at an evaporation rate of 0.1~0.8 Å s^{-1} for 80 nm thickness of Au metal contact.

4.2 Preparation of saturated COF-I IPA dispersion

Firstly, 5 mg of COF-I powder was dispersed into 20 mL of IPA and then sonicated for more than 24 hours to obtain the COF-I suspension. Then the solution was centrifuged at 6000 rpm for 5 mins, and the transparent supernatant fluid was collected. The insoluble solid after centrifugation was vacuum dried, the weight was about 1.0 mg. Thus, the concentration of the stable COF-I powder dispersions was about 0.2 mg mL^{-1}. Then 10, 20, 30, 40 μL, 50 μL, 0.4 mg mL^{-1} COF-I IPA dispersion mixed with 90 μL, 80 μL, 70 μL, 60 μL, and 50 μL 0.5 M FAI/MACl IPA solution afforded a solution with concentration of COF-I in IPA 0.02, 0.04, 0.06, 0.08 and 0.10 mg mL^{-1}, respectively.

Section S5: Figures

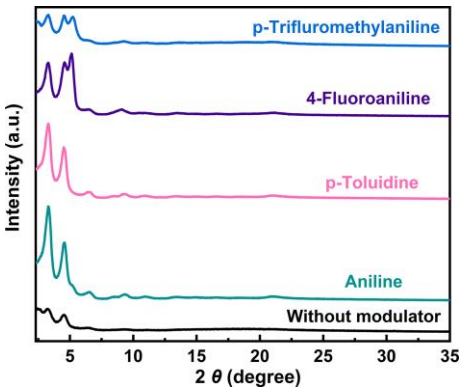

Figure S3. PXRD patterns of $[(TPA)_2(TPB)_1]$-*C=N*- with different anilines modulators.

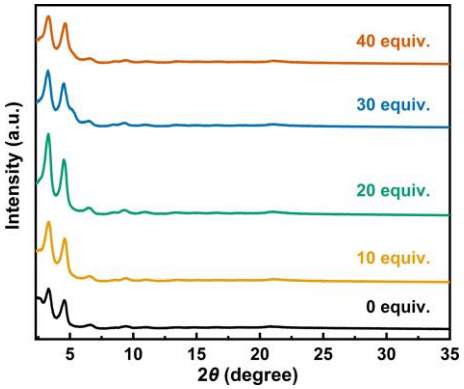

Figure S4. PXRD patterns of $[(TPA)_2(TPB)_1]$-*C=N*- with different equivalent aniline.

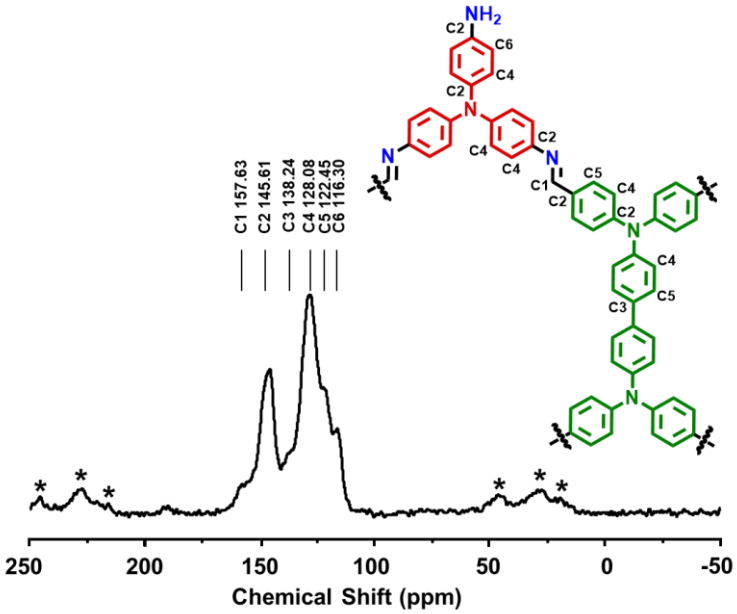

Figure S5. Solid-state ^{13}C CP-MAS NMR spectrum of $[(TPA)_2(TPB)_1]$-*C=N*-. The assignments of ^{13}C chemical shifts are indicated in the chemical structure, which classified by their different chemical environment. Spinning sidebands are denoted with asterisks.

Characteristic C Assignment	Signal (ppm)/Comments
C1	158 /Imine C=N carbons
C2	146 /α-amino carbons

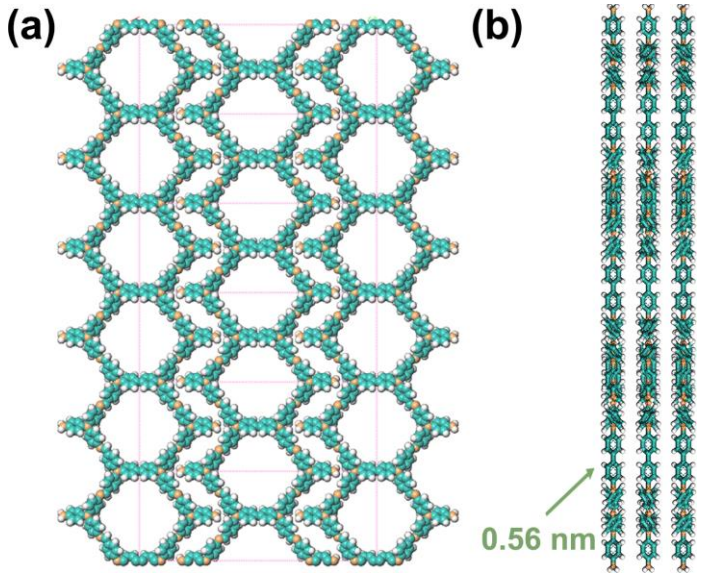

Figure S6. (a) The top-view and (b) side-view of the crystal structure of $[(TPA)_2(TPB)_1]$-*C=N*-.

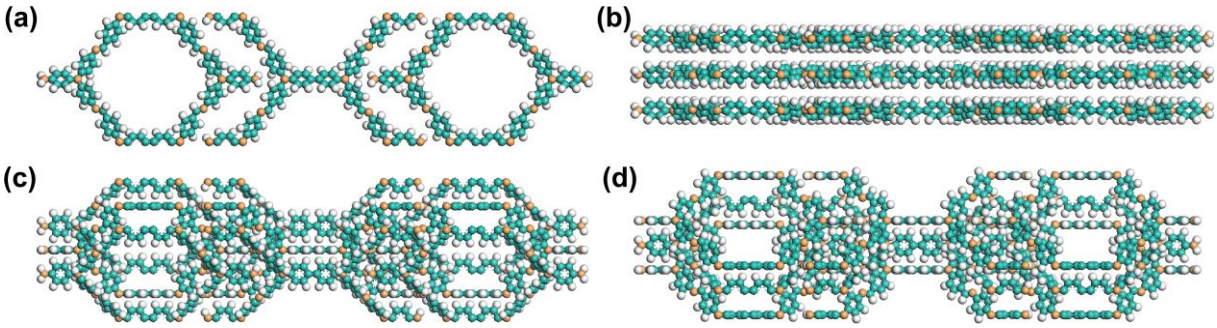

Figure S7. The original cell of [$(TPA)_2(TPB)_1$]-*C=N*-.

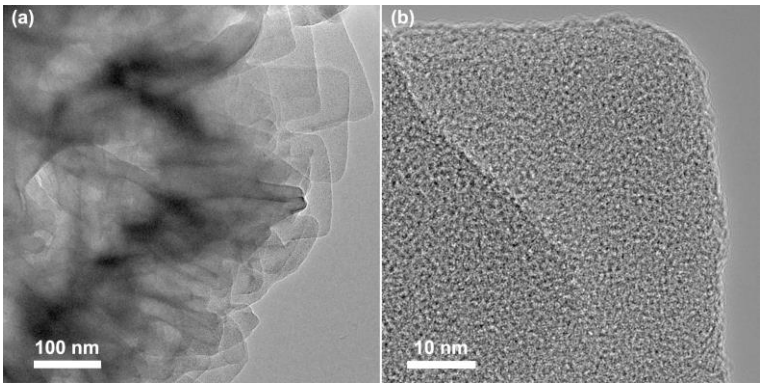

Figure S8. TEM images of [$(TPA)_2(TPB)_1$]-*C=N*-.

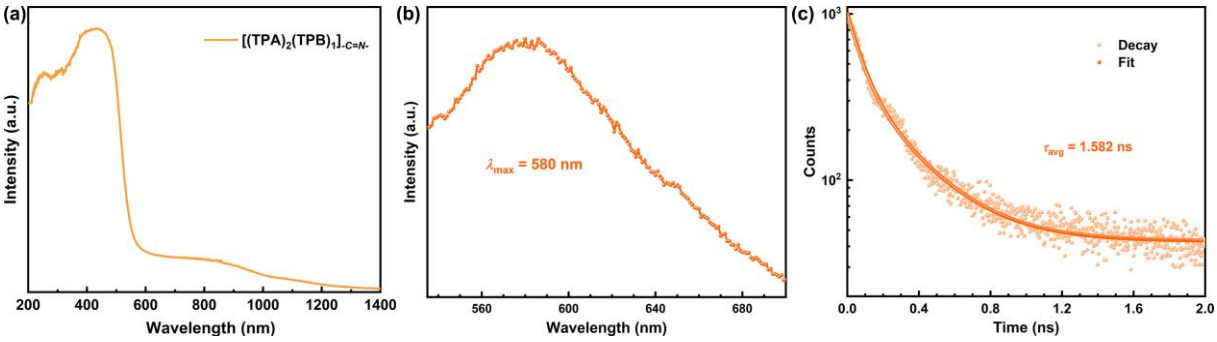

Figure S9. (a) UV-vis-NIR spectrum (b) Steady-state photoluminescence (PL) spectrum and (c) time-resolved photoluminescence (TRPL) spectrum of [$(TPA)_2(TPB)_1$]-*C=N*-.

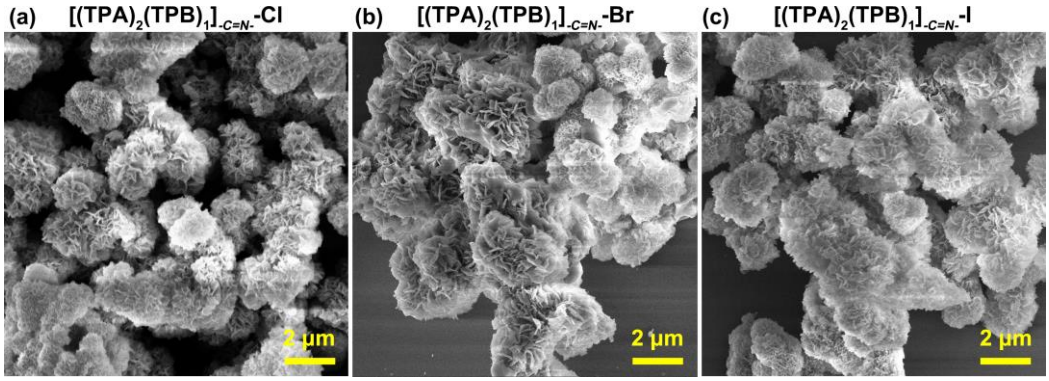

Figure S10. SEM images of COF-X (a) $[(TPA)_2(TPB)_1]$-*C=N*--Cl, (b) $[(TPA)_2(TPB)_1]$-*C=N*--Br, and (c) $[(TPA)_2(TPB)_1]$-*C=N*--I.

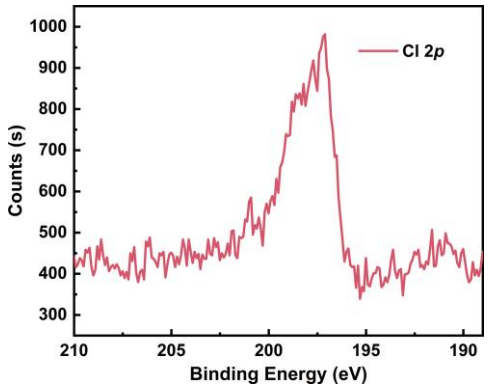

Figure S11. The Cl 2*p* spectra of $[(TPA)_2(TPB)_1]$-*C=N*--Cl powder.

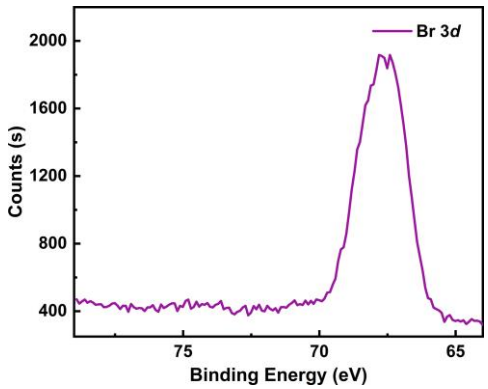

Figure S12. The Br 3*d* spectra of $[(TPA)_2(TPB)_1]$-*C=N*--Br powder.

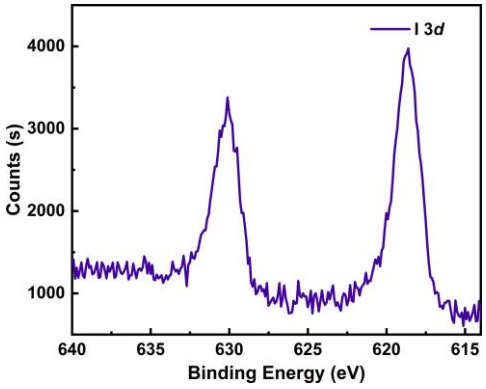

Figure S13. The I 3*d* spectra of $[(TPA)_2(TPB)_1]$-*C=N*-I powder.

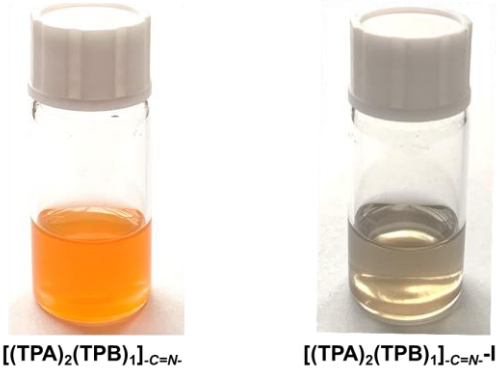

Figure S14. The 0.1 mg/mL supernatant of $[(TPA)_2(TPB)_1]$-*C=N*- and COF-I powders in IPA.

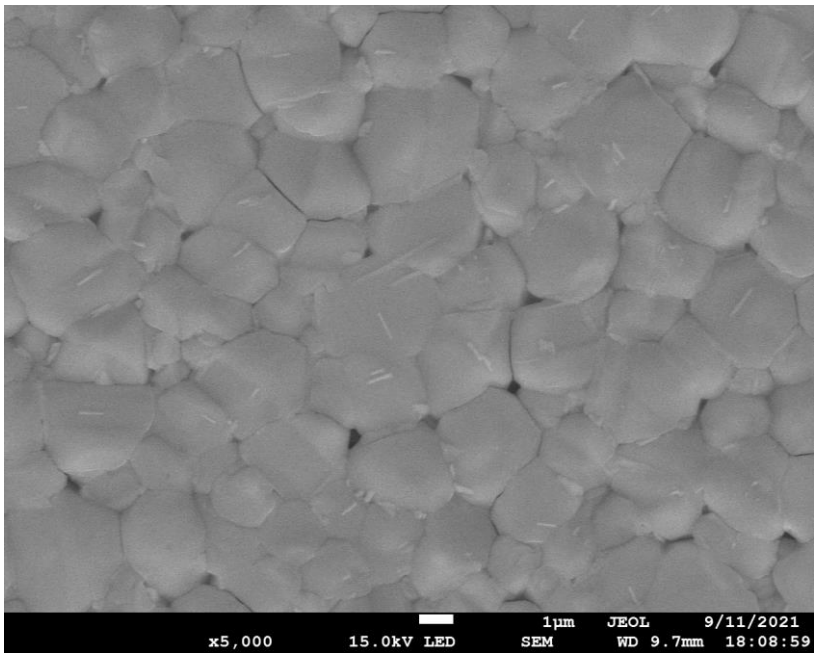

Figure S15. SEM images of the target perovskite film.

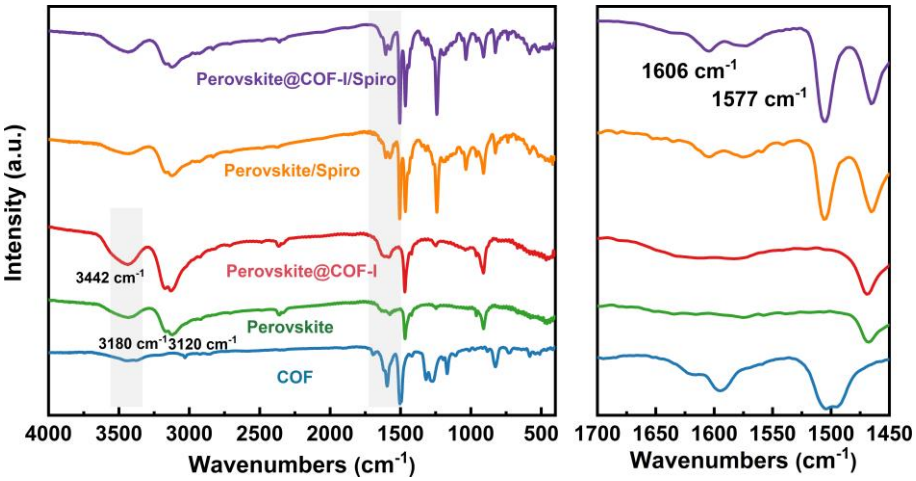

Figure S16. FT-IR spectra of perovskite, perovskite@COF-I, perovskite/Sprio-OMeTAD, and perovskite@COF-I/Sprio-OMeTAD films.

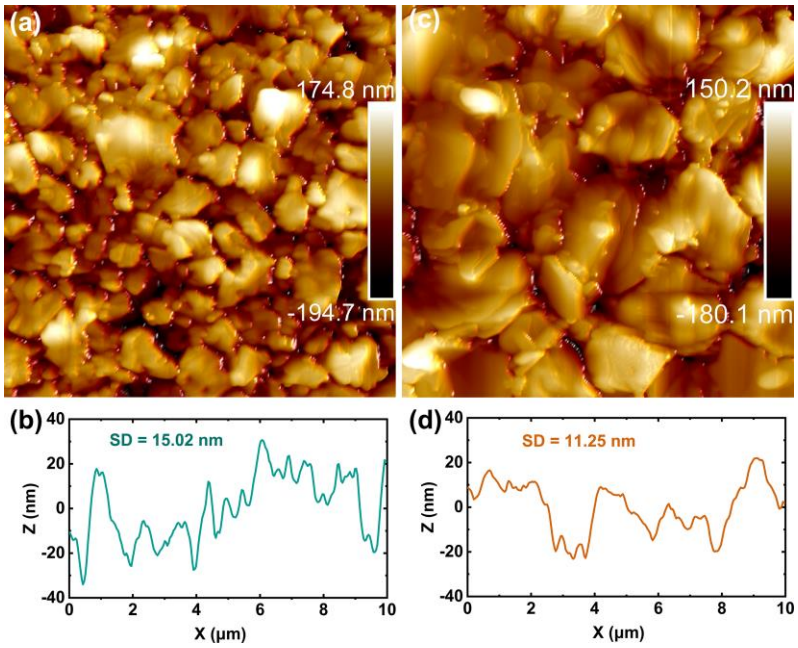

Figure S17. (a) AFM image of the perovskite film, (B) surface potential variations of the perovskite across the center line in a. (c) standard deviation AFM image of the target perovskite film. (d) surface potential variations of the target perovskite film across the center line in c.

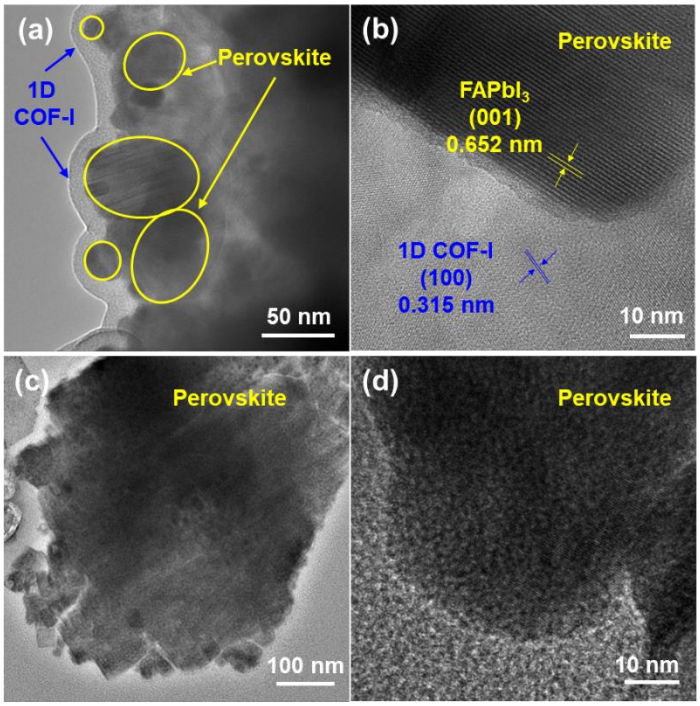

Figure S18. (a)TEM and (b) HRTEM images of the scraped powders from the perovskite@COF-I film, (c)TEM and (d) HRTEM images of the scraped powders from the perovskite film.

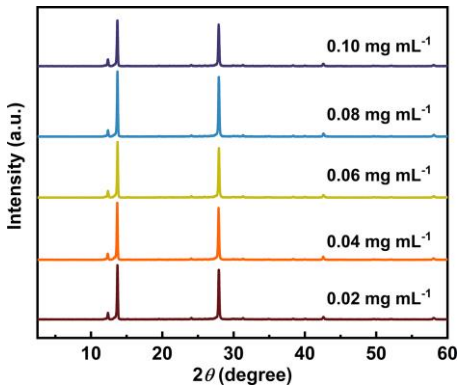

Figure S19. XRD patterns of perovskite films with different concentrations of COF-I.

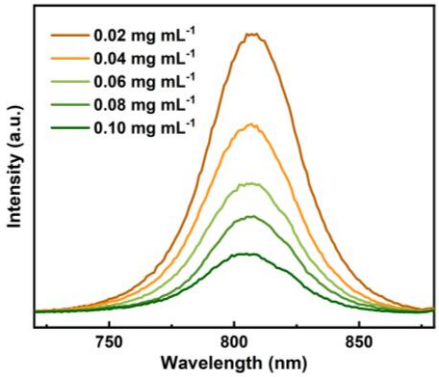

Figure S20. PL spectra of perovskite films with different concentrations of COF-I.

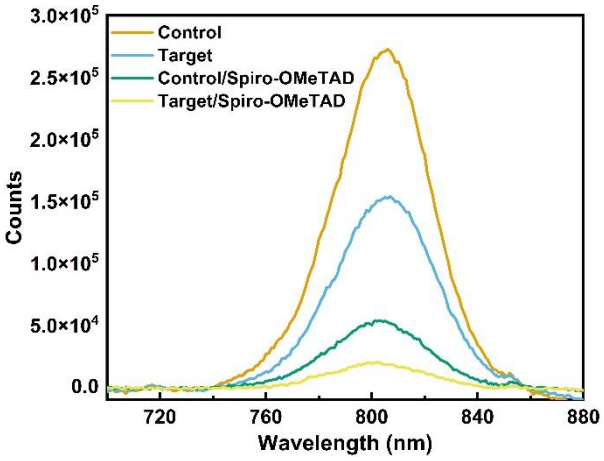

Figure S21. PL spectra of the control, target, control/Sprio-OMeTAD, and target/Sprio-OMeTAD films.

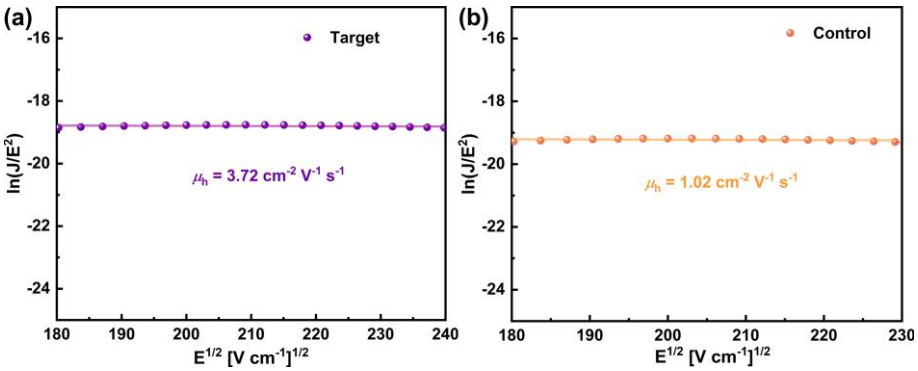

Figure S22. Fitting curves of hole-only devices.

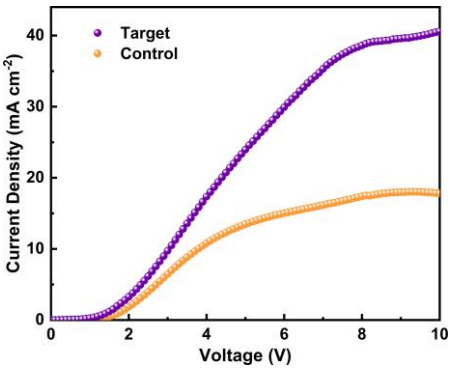

Figure S23. *J-V* curves of hole-only devices.

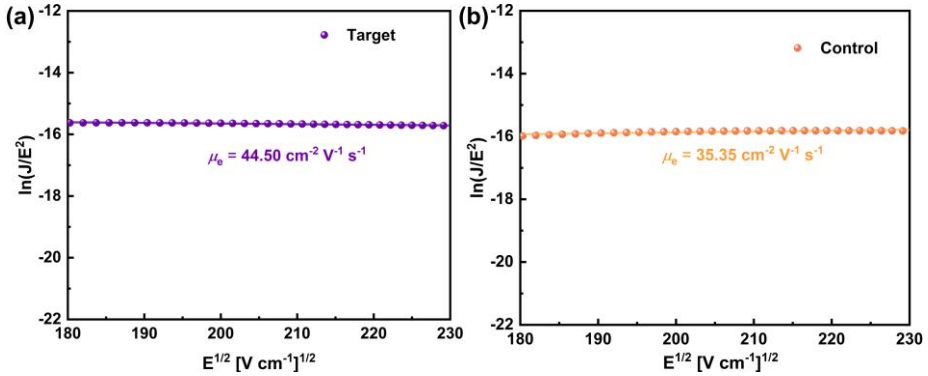

Figure S24. Fitting curves of electron-only devices.

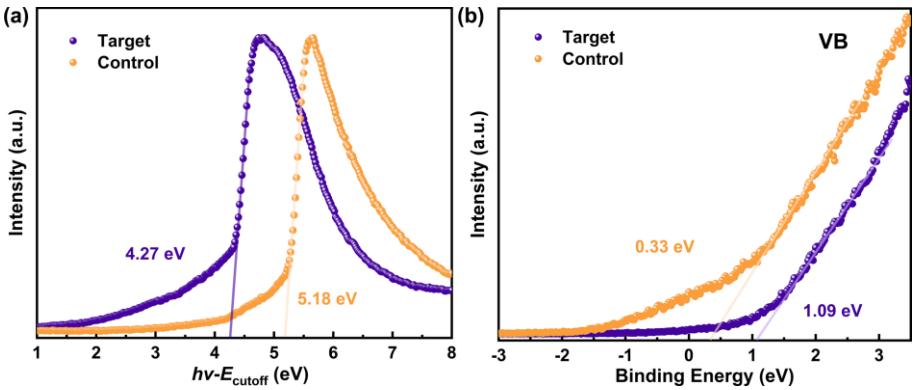

Figure S25. Characterization of (a) the working function and (b) valence band of the control and target perovskite films by UPS spectra. The valance band maximum (VBM) for perovskite films can be calculated through formula as $E_{VBM} = h\nu - (E_{cutoff} - E_F)$, where E_{cutoff} can be received from high-binding energy secondary electron cutoff region as shown in Figure S22a; E_F is fermi energy level, which can be obtained from VB edge region as Figure S22b.. Thus, the VBM of the control and target perovskite film was calculated to be -5.51 and -5.36 eV, respectively.

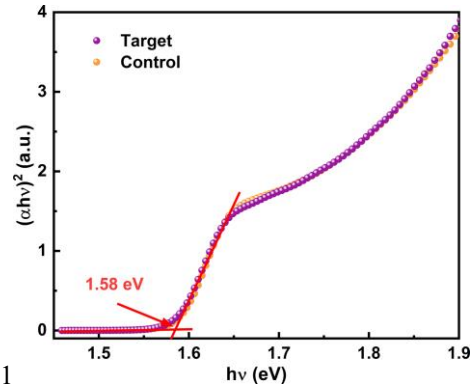

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Figure S26. The E_g of the control and target perovskite films calculated from the Tauc plots.

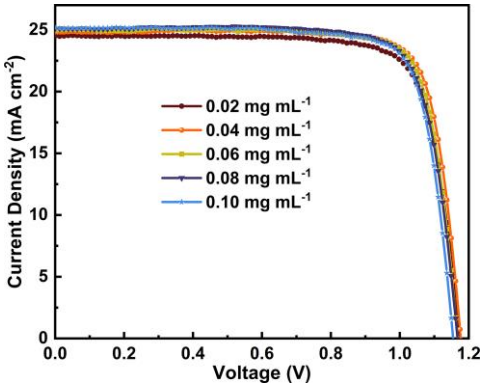

Figure S27. *J-V* curves of the PSCs based on different concentrations of COF-I.

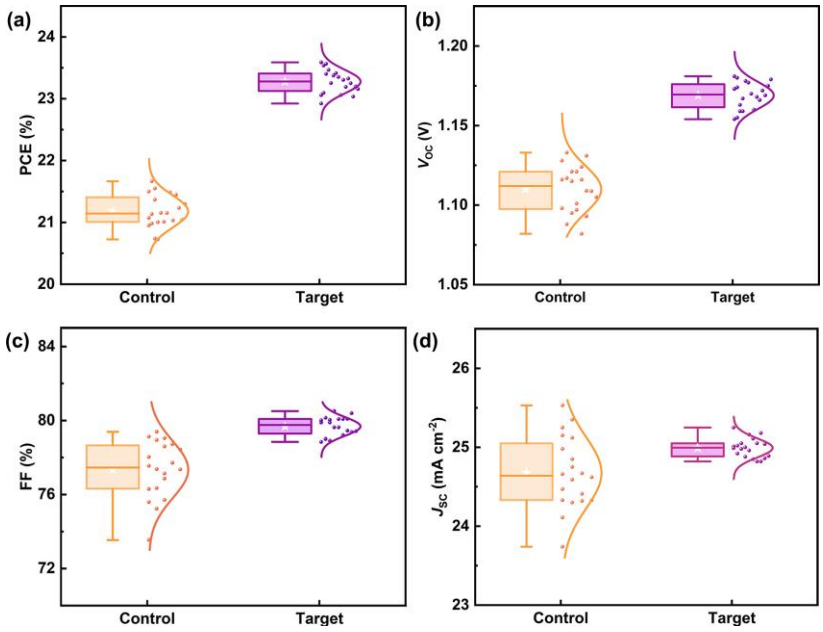

Figure S28. Device parameter statistics for 20 individual control and target PSCs. (a) PCE; (b) V_{OC}; (c) FF; (d) J_{SC}. The center line represents the median value, the white pentagram represents the average value, the bounds of box indicate upper and lower quartiles and the whiskers represent the minimum and maximum values.

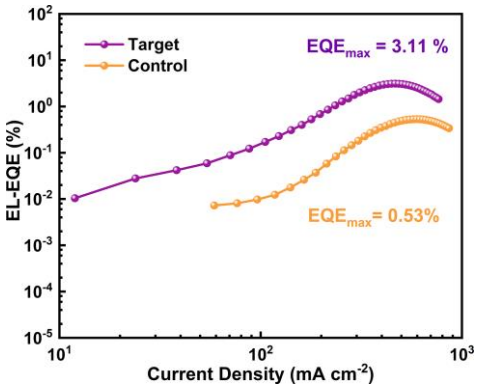

Figure S29. The EL-EQE curves for the control and target PSCs while operating as LEDs.

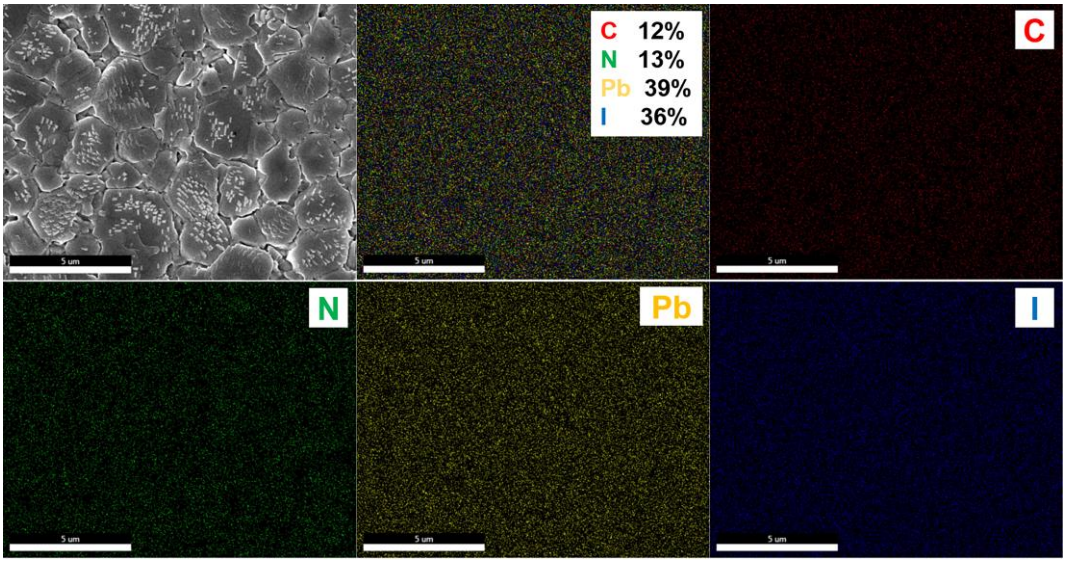

Figure S30. Top-view SEM image and EDS mapping of the target perovskite film after storage in air for 1000 hours.

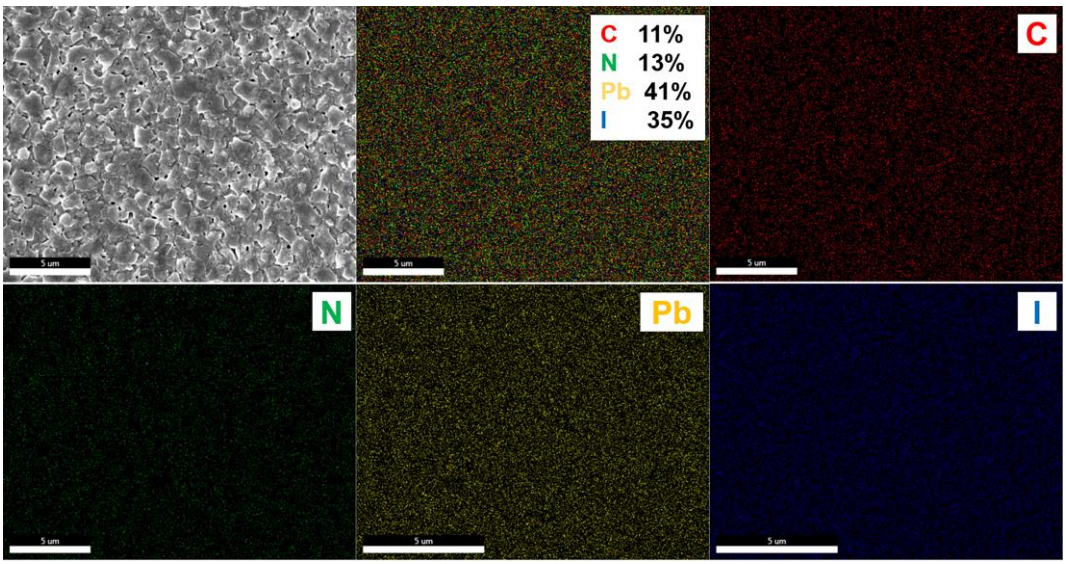

Figure S31. Top-view SEM image and EDS mapping of the control perovskite film after storage in air for 1000 hours.

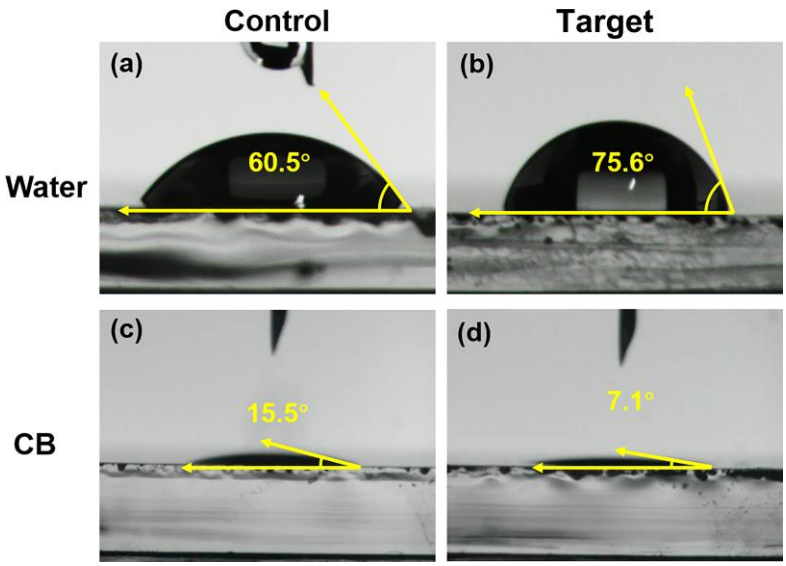

Figure S32. The contact angle measurements of the control and target perovskite films. (a) Water as solution for the control film; (b) Water as solution for the target perovskite film; (c) Chlorobenzene as solution for the control film, (d) Chlorobenzene as solution for the target perovskite film.

Section S5: Tables

Table S1. Atomic coordinates and refined unit cell parameters of $[(TPA)_2(TPB)_1]$-*C=N*-.

Space Group	*CMCM* (No. 63)	**a** (Å)	54.5387	b (Å)	20.5392	c (Å)	11.2291
Unit Cell Volume (Å^3)	12578.6	α (°)	90	β (°)	90	γ (°)	90
Atom name	X	y	z	**Atom name**	x	y	z
C1	0.02725	0.95841	0.92301	C42	0.39632	0.5602	0.99317
C2	0.97275	0.04159	0.07699	C43	0.39632	0.5602	0.50683
C3	0.97275	0.04159	0.42301	C44	0.60368	0.4398	0.49317
C4	0.02725	0.95841	0.57699	C45	0.39632	0.4398	0.49317
C5	0.97275	0.95841	0.57699	C46	0.60368	0.5602	0.50683
C6	0.02725	0.04159	0.42301	C47	0.60368	0.5602	0.99317
C7	0.02725	0.04159	0.07699	C48	0.39632	0.4398	0.00683
C8	0.97275	0.95841	0.92301	C49	0.09548	0.88816	0.0834
C9	0.52725	0.45841	0.92301	C50	0.90452	0.11184	0.9166
C10	0.47275	0.54159	0.07699	C51	0.90452	0.11184	0.5834
C11	0.47275	0.54159	0.42301	C52	0.09548	0.88816	0.4166
C12	0.52725	0.45841	0.57699	C53	0.90452	0.88816	0.4166
C13	0.47275	0.45841	0.57699	C54	0.09548	0.11184	0.5834
C14	0.52725	0.54159	0.42301	C55	0.09548	0.11184	0.9166
C15	0.52725	0.54159	0.07699	C56	0.90452	0.88816	0.0834
C16	0.47275	0.45841	0.92301	C57	0.59548	0.38816	0.0834
C17	0.05293	0.95852	0.92239	C58	0.40452	0.61184	0.9166
C18	0.94707	0.04148	0.07761	C59	0.40452	0.61184	0.5834
C19	0.94707	0.04148	0.42239	C60	0.59548	0.38816	0.4166
C20	0.05293	0.95852	0.57761	C61	0.40452	0.38816	0.4166
C21	0.94707	0.95852	0.57761	C62	0.59548	0.61184	0.5834
C22	0.05293	0.04148	0.42239	C63	0.59548	0.61184	0.9166
C23	0.05293	0.04148	0.07761	C64	0.40452	0.38816	0.0834
C24	0.94707	0.95852	0.92239	C65	0.10763	0.82613	0.09048
C25	0.55293	0.45852	0.92239	C66	0.89237	0.17387	0.90952
C26	0.44707	0.54148	0.07761	C67	0.89237	0.17387	0.59048
C27	0.44707	0.54148	0.42239	C68	0.10763	0.82613	0.40952
C28	0.55293	0.45852	0.57761	C69	0.89237	0.82613	0.40952
C29	0.44707	0.45852	0.57761	C70	0.10763	0.17387	0.59048
C30	0.55293	0.54148	0.42239	C71	0.10763	0.17387	0.90952
C31	0.55293	0.54148	0.07761	C72	0.89237	0.82613	0.09048
C32	0.44707	0.45852	0.92239	C73	0.60763	0.32613	0.09048
C33	0.10368	0.9398	0.00683	C74	0.39237	0.67387	0.90952
C34	0.89632	0.0602	0.99317	C75	0.39237	0.67387	0.59048
C35	0.89632	0.0602	0.50683	C76	0.60763	0.32613	0.40952
C36	0.10368	0.9398	0.49317	C77	0.39237	0.32613	0.40952
C37	0.89632	0.9398	0.49317	C78	0.60763	0.67387	0.59048
C38	0.10368	0.0602	0.50683	C79	0.60763	0.67387	0.90952
C39	0.10368	0.0602	0.99317	C80	0.39237	0.32613	0.09048

C40	0.89632	0.9398	0.00683	C81	0.12909	0.81382	0.02459
C41	0.60368	0.4398	0.00683	C82	0.87091	0.18618	0.97541
C83	0.87091	0.18618	0.52459	C132	0.14119	0.75183	0.46072
C84	0.12909	0.81382	0.47541	C133	0.85881	0.75183	0.46072
C85	0.87091	0.81382	0.47541	C134	0.14119	0.24817	0.53928
C86	0.12909	0.18618	0.52459	C135	0.14119	0.24817	0.96072
C87	0.12909	0.18618	0.97541	C136	0.85881	0.75183	0.03928
C88	0.87091	0.81382	0.02459	C137	0.64119	0.25183	0.03928
C89	0.62909	0.31382	0.02459	C138	0.35881	0.74817	0.96072
C90	0.37091	0.68618	0.97541	C139	0.35881	0.74817	0.53928
C91	0.37091	0.68618	0.52459	C140	0.64119	0.25183	0.46072
C92	0.62909	0.31382	0.47541	C141	0.35881	0.25183	0.46072
C93	0.37091	0.31382	0.47541	C142	0.64119	0.74817	0.53928
C94	0.62909	0.68618	0.52459	C143	0.64119	0.74817	0.96072
C95	0.62909	0.68618	0.97541	C144	0.35881	0.25183	0.03928
C96	0.37091	0.31382	0.02459	C145	0.17637	0.67938	0.9983
C97	0.13738	0.86483	0.94707	C146	0.82363	0.32062	0.0017
C98	0.86262	0.13517	0.05293	C147	0.82363	0.32062	0.4983
C99	0.86262	0.13517	0.44707	C148	0.17637	0.67938	0.5017
C100	0.13738	0.86483	0.55293	C149	0.82363	0.67938	0.5017
C101	0.86262	0.86483	0.55293	C150	0.17637	0.32062	0.4983
C102	0.13738	0.13517	0.44707	C151	0.17637	0.32062	0.0017
C103	0.13738	0.13517	0.05293	C152	0.82363	0.67938	0.9983
C104	0.86262	0.86483	0.94707	C153	0.67637	0.17938	0.9983
C105	0.63738	0.36483	0.94707	C154	0.32363	0.82062	0.0017
C106	0.36262	0.63517	0.05293	C155	0.32363	0.82062	0.4983
C107	0.36262	0.63517	0.44707	C156	0.67637	0.17938	0.5017
C108	0.63738	0.36483	0.55293	C157	0.32363	0.17938	0.5017
C109	0.36262	0.36483	0.55293	C158	0.67637	0.82062	0.4983
C110	0.63738	0.63517	0.44707	C159	0.67637	0.82062	0.0017
C111	0.63738	0.63517	0.05293	C160	0.32363	0.17938	0.9983
C112	0.36262	0.36483	0.94707	C161	0.17127	0.62673	0.0789
C113	0.12471	0.92639	0.93758	C162	0.82873	0.37327	0.9211
C114	0.87529	0.07361	0.06242	C163	0.82873	0.37327	0.5789
C115	0.87529	0.07361	0.43758	C164	0.17127	0.62673	0.4211
C116	0.12471	0.92639	0.56242	C165	0.82873	0.62673	0.4211
C117	0.87529	0.92639	0.56242	C166	0.17127	0.37327	0.5789
C118	0.12471	0.07361	0.43758	C167	0.17127	0.37327	0.9211
C119	0.12471	0.07361	0.06242	C168	0.82873	0.62673	0.0789
C120	0.87529	0.92639	0.93758	C169	0.67127	0.12673	0.0789
C121	0.62471	0.42639	0.93758	C170	0.32873	0.87327	0.9211
C122	0.37529	0.57361	0.06242	C171	0.32873	0.87327	0.5789
C123	0.37529	0.57361	0.43758	C172	0.67127	0.12673	0.4211
C124	0.62471	0.42639	0.56242	C173	0.32873	0.12673	0.4211
C125	0.37529	0.42639	0.56242	C174	0.67127	0.87327	0.5789
C126	0.62471	0.57361	0.43758	C175	0.67127	0.87327	0.9211
C127	0.62471	0.57361	0.06242	C176	0.32873	0.12673	0.0789
C128	0.37529	0.42639	0.93758	C177	0.18557	0.56809	0.0808
C129	0.14119	0.75183	0.03928	C178	0.81443	0.43191	0.9192

C130	0.85881	0.24817	0.96072	C179	0.81443	0.43191	0.5808
C131	0.85881	0.24817	0.53928	C180	0.18557	0.56809	0.4192
C181	0.81443	0.56809	0.4192	C230	0.1967	0.32772	0.42284
C182	0.18557	0.43191	0.5808	C231	0.1967	0.32772	0.07716
C183	0.18557	0.43191	0.9192	C232	0.8033	0.67228	0.92284
C184	0.81443	0.56809	0.0808	C233	0.6967	0.17228	0.92284
C185	0.68557	0.06809	0.0808	C234	0.3033	0.82772	0.07716
C186	0.31443	0.93191	0.9192	C235	0.3033	0.82772	0.42284
C187	0.31443	0.93191	0.5808	C236	0.6967	0.17228	0.57716
C188	0.68557	0.06809	0.4192	C237	0.3033	0.17228	0.57716
C189	0.31443	0.06809	0.4192	C238	0.6967	0.82772	0.42284
C190	0.68557	0.93191	0.5808	C239	0.6967	0.82772	0.07716
C191	0.68557	0.93191	0.9192	C240	0.3033	0.17228	0.92284
C192	0.31443	0.06809	0.0808	C241	0.25651	0.45685	0.92388
C193	0.20538	0.55946	0.002	C242	0.74349	0.54315	0.07612
C194	0.79462	0.44054	0.998	C243	0.74349	0.54315	0.42388
C195	0.79462	0.44054	0.502	C244	0.25651	0.45685	0.57612
C196	0.20538	0.55946	0.498	C245	0.74349	0.45685	0.57612
C197	0.79462	0.55946	0.498	C246	0.25651	0.54315	0.42388
C198	0.20538	0.44054	0.502	C247	0.25651	0.54315	0.07612
C199	0.20538	0.44054	0.998	C248	0.74349	0.45685	0.92388
C200	0.79462	0.55946	0.002	C249	0.75651	0.95685	0.92388
C201	0.70538	0.05946	0.002	C250	0.24349	0.04315	0.07612
C202	0.29462	0.94054	0.998	C251	0.24349	0.04315	0.42388
C203	0.29462	0.94054	0.502	C252	0.75651	0.95685	0.57612
C204	0.70538	0.05946	0.498	C253	0.24349	0.95685	0.57612
C205	0.29462	0.05946	0.498	C254	0.75651	0.04315	0.42388
C206	0.70538	0.94054	0.502	C255	0.75651	0.04315	0.07612
C207	0.70538	0.94054	0.998	C256	0.24349	0.95685	0.92388
C208	0.29462	0.05946	0.002	C257	0.2822	0.45657	0.92418
C209	0.21096	0.61316	0.92421	C258	0.7178	0.54343	0.07582
C210	0.78904	0.38684	0.07579	C259	0.7178	0.54343	0.42418
C211	0.78904	0.38684	0.42421	C260	0.2822	0.45657	0.57582
C212	0.21096	0.61316	0.57579	C261	0.7178	0.45657	0.57582
C213	0.78904	0.61316	0.57579	C262	0.2822	0.54343	0.42418
C214	0.21096	0.38684	0.42421	C263	0.2822	0.54343	0.07582
C215	0.21096	0.38684	0.07579	C264	0.7178	0.45657	0.92418
C216	0.78904	0.61316	0.92421	C265	0.7822	0.95657	0.92418
C217	0.71096	0.11316	0.92421	C266	0.2178	0.04343	0.07582
C218	0.28904	0.88684	0.07579	C267	0.2178	0.04343	0.42418
C219	0.28904	0.88684	0.42421	C268	0.7822	0.95657	0.57582
C220	0.71096	0.11316	0.57579	C269	0.2178	0.95657	0.57582
C221	0.28904	0.11316	0.57579	C270	0.7822	0.04343	0.42418
C222	0.71096	0.88684	0.42421	C271	0.7822	0.04343	0.07582
C223	0.71096	0.88684	0.07579	C272	0.2178	0.95657	0.92418
C224	0.28904	0.11316	0.92421	C273	0.06631	0	0
C225	0.1967	0.67228	0.92284	C274	0.93369	0	0
C226	0.8033	0.32772	0.07716	C275	0.93369	0	0.5
C227	0.8033	0.32772	0.42284	C276	0.06631	0	0.5

C228	0.1967	0.67228	0.57716	C277	0.56631	0.5	0
C229	0.8033	0.67228	0.57716	C278	0.43369	0.5	0
C279	0.43369	0.5	0.5	N24	0.59138	0.5	0.5
C280	0.56631	0.5	0.5	N25	0.21815	0.5	0
C281	0.98685	0	0	N26	0.78185	0.5	0
C282	0.01315	0	0	N27	0.78185	0.5	0.5
C283	0.01315	0	0.5	N28	0.21815	0.5	0.5
C284	0.98685	0	0.5	N29	0.71815	0	0
C285	0.48685	0.5	0	N30	0.28185	0	0
C286	0.51315	0.5	0	N31	0.28185	0	0.5
C287	0.51315	0.5	0.5	N32	0.71815	0	0.5
C288	0.48685	0.5	0.5	N33	0.31952	0.5	0
C289	0.24317	0.5	0	N34	0.68048	0.5	0
C290	0.75683	0.5	0	N35	0.68048	0.5	0.5
C291	0.75683	0.5	0.5	N36	0.31952	0.5	0.5
C292	0.24317	0.5	0.5	N37	0.81952	0	0
C293	0.74317	0	0	N38	0.18048	0	0
C294	0.25683	0	0	N39	0.18048	0	0.5
C295	0.25683	0	0.5	N40	0.81952	0	0.5
C296	0.74317	0	0.5	H1	0.01936	0.92635	0.86436
C297	0.29506	0.5	0	H2	0.98064	0.07365	0.13564
C298	0.70494	0.5	0	H3	0.98064	0.07365	0.36436
C299	0.70494	0.5	0.5	H4	0.01936	0.92635	0.63564
C300	0.29506	0.5	0.5	H5	0.98064	0.92635	0.63564
C301	0.79506	0	0	H6	0.01936	0.07365	0.36436
C302	0.20494	0	0	H7	0.01936	0.07365	0.13564
C303	0.20494	0	0.5	H8	0.98064	0.92635	0.86436
C304	0.79506	0	0.5	H9	0.51936	0.42635	0.86436
N1	0.16288	0.73644	0.98821	H10	0.48064	0.57365	0.13564
N2	0.83712	0.26356	0.01179	H11	0.48064	0.57365	0.36436
N3	0.83712	0.26356	0.48821	H12	0.51936	0.42635	0.63564
N4	0.16288	0.73644	0.51179	H13	0.48064	0.42635	0.63564
N5	0.83712	0.73644	0.51179	H14	0.51936	0.57365	0.36436
N6	0.16288	0.26356	0.48821	H15	0.51936	0.57365	0.13564
N7	0.16288	0.26356	0.01179	H16	0.48064	0.42635	0.86436
N8	0.83712	0.73644	0.98821	H17	0.06201	0.92789	0.86455
N9	0.66288	0.23644	0.98821	H18	0.93799	0.07211	0.13545
N10	0.33712	0.76356	0.01179	H19	0.93799	0.07211	0.36455
N11	0.33712	0.76356	0.48821	H20	0.06201	0.92789	0.63545
N12	0.66288	0.23644	0.51179	H21	0.93799	0.92789	0.63545
N13	0.33712	0.23644	0.51179	H22	0.06201	0.07211	0.36455
N14	0.66288	0.76356	0.48821	H23	0.06201	0.07211	0.13545
N15	0.66288	0.76356	0.01179	H24	0.93799	0.92789	0.86455
N16	0.33712	0.23644	0.98821	H25	0.56201	0.42789	0.86455
N17	0.09138	0	0	H26	0.43799	0.57211	0.13545
N18	0.90862	0	0	H27	0.43799	0.57211	0.36455
N19	0.90862	0	0.5	H28	0.56201	0.42789	0.63545
N20	0.09138	0	0.5	H29	0.43799	0.42789	0.63545
N21	0.59138	0.5	0	H30	0.56201	0.57211	0.36455

N22	0.40862	0.5	0	H31	0.56201	0.57211	0.13545
N23	0.40862	0.5	0.5	H32	0.43799	0.42789	0.86455
H33	0.08039	0.89545	0.135	H82	0.86908	0.03813	0.12063
H34	0.91961	0.10455	0.865	H83	0.86908	0.03813	0.37937
H35	0.91961	0.10455	0.635	H84	0.13092	0.96187	0.62063
H36	0.08039	0.89545	0.365	H85	0.86908	0.96187	0.62063
H37	0.91961	0.89545	0.365	H86	0.13092	0.03813	0.37937
H38	0.08039	0.10455	0.635	H87	0.13092	0.03813	0.12063
H39	0.08039	0.10455	0.865	H88	0.86908	0.96187	0.87937
H40	0.91961	0.89545	0.135	H89	0.63092	0.46187	0.87937
H41	0.58039	0.39545	0.135	H90	0.36908	0.53813	0.12063
H42	0.41961	0.60455	0.865	H91	0.36908	0.53813	0.37937
H43	0.41961	0.60455	0.635	H92	0.63092	0.46187	0.62063
H44	0.58039	0.39545	0.365	H93	0.36908	0.46187	0.62063
H45	0.41961	0.39545	0.365	H94	0.63092	0.53813	0.37937
H46	0.58039	0.60455	0.635	H95	0.63092	0.53813	0.12063
H47	0.58039	0.60455	0.865	H96	0.36908	0.46187	0.87937
H48	0.41961	0.39545	0.135	H97	0.13298	0.71674	0.09207
H49	0.10058	0.78996	0.145	H98	0.86702	0.28326	0.90793
H50	0.89942	0.21004	0.855	H99	0.86702	0.28326	0.59207
H51	0.89942	0.21004	0.645	H100	0.13298	0.71674	0.40793
H52	0.10058	0.78996	0.355	H101	0.86702	0.71674	0.40793
H53	0.89942	0.78996	0.355	H102	0.13298	0.28326	0.59207
H54	0.10058	0.21004	0.645	H103	0.13298	0.28326	0.90793
H55	0.10058	0.21004	0.855	H104	0.86702	0.71674	0.09207
H56	0.89942	0.78996	0.145	H105	0.63298	0.21674	0.09207
H57	0.60058	0.28996	0.145	H106	0.36702	0.78326	0.90793
H58	0.39942	0.71004	0.855	H107	0.36702	0.78326	0.59207
H59	0.39942	0.71004	0.645	H108	0.63298	0.21674	0.40793
H60	0.60058	0.28996	0.355	H109	0.36702	0.21674	0.40793
H61	0.39942	0.28996	0.355	H110	0.63298	0.78326	0.59207
H62	0.60058	0.71004	0.645	H111	0.63298	0.78326	0.90793
H63	0.60058	0.71004	0.855	H112	0.36702	0.21674	0.09207
H64	0.39942	0.28996	0.145	H113	0.15711	0.63001	0.13704
H65	0.15268	0.85735	0.89685	H114	0.84289	0.36999	0.86296
H66	0.84732	0.14265	0.10315	H115	0.84289	0.36999	0.63704
H67	0.84732	0.14265	0.39685	H116	0.15711	0.63001	0.36296
H68	0.15268	0.85735	0.60315	H117	0.84289	0.63001	0.36296
H69	0.84732	0.85735	0.60315	H118	0.15711	0.36999	0.63704
H70	0.15268	0.14265	0.39685	H119	0.15711	0.36999	0.86296
H71	0.15268	0.14265	0.10315	H120	0.84289	0.63001	0.13704
H72	0.84732	0.85735	0.89685	H121	0.65711	0.13001	0.13704
H73	0.65268	0.35735	0.89685	H122	0.34289	0.86999	0.86296
H74	0.34732	0.64265	0.10315	H123	0.34289	0.86999	0.63704
H75	0.34732	0.64265	0.39685	H124	0.65711	0.13001	0.36296
H76	0.65268	0.35735	0.60315	H125	0.34289	0.13001	0.36296
H77	0.34732	0.35735	0.60315	H126	0.65711	0.86999	0.63704
H78	0.65268	0.64265	0.39685	H127	0.65711	0.86999	0.86296
H79	0.65268	0.64265	0.10315	H128	0.34289	0.13001	0.13704

H80	0.34732	0.35735	0.89685	H129	0.1813	0.53088	0.13971
H81	0.13092	0.96187	0.87937	H130	0.8187	0.46912	0.86029
H131	0.8187	0.46912	0.63971	H178	0.7525	0.57469	0.13265
H132	0.1813	0.53088	0.36029	H179	0.7525	0.57469	0.36735
H133	0.8187	0.53088	0.36029	H180	0.2475	0.42531	0.63265
H134	0.1813	0.46912	0.63971	H181	0.7525	0.42531	0.63265
H135	0.1813	0.46912	0.86029	H182	0.2475	0.57469	0.36735
H136	0.8187	0.53088	0.13971	H183	0.2475	0.57469	0.13265
H137	0.6813	0.03088	0.13971	H184	0.7525	0.42531	0.86735
H138	0.3187	0.96912	0.86029	H185	0.7475	0.92531	0.86735
H139	0.3187	0.96912	0.63971	H186	0.2525	0.07469	0.13265
H140	0.6813	0.03088	0.36029	H187	0.2525	0.07469	0.36735
H141	0.3187	0.03088	0.36029	H188	0.7475	0.92531	0.63265
H142	0.6813	0.96912	0.63971	H189	0.2525	0.92531	0.63265
H143	0.6813	0.96912	0.86029	H190	0.7475	0.07469	0.36735
H144	0.3187	0.03088	0.13971	H191	0.7475	0.07469	0.13265
H145	0.22533	0.60895	0.86701	H192	0.2525	0.92531	0.86735
H146	0.77467	0.39105	0.13299	H193	0.2915	0.4248	0.86919
H147	0.77467	0.39105	0.36701	H194	0.7085	0.5752	0.13081
H148	0.22533	0.60895	0.63299	H195	0.7085	0.5752	0.36919
H149	0.77467	0.60895	0.63299	H196	0.2915	0.4248	0.63081
H150	0.22533	0.39105	0.36701	H197	0.7085	0.4248	0.63081
H151	0.22533	0.39105	0.13299	H198	0.2915	0.5752	0.36919
H152	0.77467	0.60895	0.86701	H199	0.2915	0.5752	0.13081
H153	0.72533	0.10895	0.86701	H200	0.7085	0.4248	0.86919
H154	0.27467	0.89105	0.13299	H201	0.7915	0.9248	0.86919
H155	0.27467	0.89105	0.36701	H202	0.2085	0.0752	0.13081
H156	0.72533	0.10895	0.63299	H203	0.2085	0.0752	0.36919
H157	0.27467	0.10895	0.63299	H204	0.7915	0.9248	0.63081
H158	0.72533	0.89105	0.36701	H205	0.2085	0.9248	0.63081
H159	0.72533	0.89105	0.13299	H206	0.7915	0.0752	0.36919
H160	0.27467	0.10895	0.86701	H207	0.7915	0.0752	0.13081
H161	0.20105	0.71023	0.86549	H208	0.2085	0.9248	0.86919
H162	0.79895	0.28977	0.13451	H209	0.32839	0.46977	0.94833
H163	0.79895	0.28977	0.36549	H210	0.67161	0.53023	0.05167
H164	0.20105	0.71023	0.63451	H211	0.67161	0.53023	0.44833
H165	0.79895	0.71023	0.63451	H212	0.32839	0.46977	0.55167
H166	0.20105	0.28977	0.36549	H213	0.67161	0.46977	0.55167
H167	0.20105	0.28977	0.13451	H214	0.32839	0.53023	0.44833
H168	0.79895	0.71023	0.86549	H215	0.32839	0.53023	0.05167
H169	0.70105	0.21023	0.86549	H216	0.67161	0.46977	0.94833
H170	0.29895	0.78977	0.13451	H217	0.82839	0.96977	0.94833
H171	0.29895	0.78977	0.36549	H218	0.17161	0.03023	0.05167
H172	0.70105	0.21023	0.63451	H219	0.17161	0.03023	0.44833
H173	0.29895	0.21023	0.63451	H220	0.82839	0.96977	0.55167
H174	0.70105	0.78977	0.36549	H221	0.17161	0.96977	0.55167
H175	0.70105	0.78977	0.13451	H222	0.82839	0.03023	0.44833
H176	0.29895	0.21023	0.86549	H223	0.82839	0.03023	0.05167
H177	0.2475	0.42531	0.86735	H224	0.17161	0.96977	0.94833

Table S2. The obtained carrier lifetimes of the control and target perovskite films.

Sample	A_1 (%)	τ_1(ns)	A_2 (%)	τ_2 (ns)	τ_{av} (ns)
Control	1.41	70.5	98.59	984.6	832.2
Target	11.85	73.15	88.15	290.2	214.7

TRPL fitting results obtained using bi-exponential decay equation

$$y = A_1 e^{-\frac{x-x_0}{\tau_1}} + A_2 e^{-\frac{x-x_0}{\tau_1}}$$

where, A_1 and τ_1 are amplitude and time constant for fast decay component and A2 and τ_2 are amplitude and time constant for slow decay component. The average lifetime (τ_{av}) is calculated from

$$\tau_{ave} = \frac{A_1{\tau_1}^2 + A_2{\tau_2}^2}{A_1\tau_1 + A_2\tau_2}$$

The excitation wavelength is 500 nm.

Table S3. Parameters for the SCLC devices

Sample	$V_{TFL\,(h)}$ [V]	$N_{t\,(h)}$ [$\times 10^{15}$ cm^{-3}]	μ_h [cm^{-2} V^{-1} s^{-1}]	$V_{TFL\,(e)}$ [V]	$N_{t\,(e)}$ [$\times 10^{15}$ cm^{-3}]	μ_e [cm^{-2} V^{-1} s^{-1}]
Taget	0.77	6.95	3.72	0.25	2.25	3.88
Control	1.06	9.56	1.02	0.68	6.16	3.14

Table S4. Photovoltaic parameters of PSCs based on different amount of COF-I.

Concentration [mg mL^{-1}]	V_{OC} [V]	FF [%]	J_{SC} [mA cm^{-2}]	PCE [%]
0.02	1.174	78.53	24.54	22.62
0.04	1.177	80.69	24.81	23.56
0.06	1.167	80.39	24.92	23.38
0.08	1.163	79.37	25.03	23.10
0.10	1.155	79.03	25.18	22.98

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