

Supporting Information

Achieving 18.92 % efficiency of non-fullerene organic solar cells with active layer morphology optimization by regulating solvent evaporation dynamics

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Experimental Section:

1. Materials:

Polymer donor D18, non-fullerene acceptor L8-BO and cathode buffer layer material PDINN were purchased from Solarmer Material Inc. Anode buffer layer PEDOT: PSS was obtained from Heraeus (Clevios P A14083). Solvent chloroform (CF) and toluene (Tol) were obtained from J&K Scientific Ltd. The pre-patterned indium tin oxide (ITO) coated glass substrates (sheet resistance of $15 \Omega/\text{Sq}$) were obtained from Huananxiangcheng Technology Co. High-purity argentine (purity > 99.99%) was used for the evaporation of electrode. All the materials were used as received without any further treatment.

2. Solution Preparation:

D18:L8-BO were dissolved in CF or CF:Tol solvent at a concentration of 7.2 mg/ml with weight ratio of 1:1, and then the blend solution was stirred at least 6 h at 50 °C. The cathode buffer layer solution was prepared by dissolving PDINN in methanol (2 mg/ml) and then stirred overnight at room temperature.

3. Device Fabrication:

Patterned ITO electrode was cleaned by sequential sonication in deionized water, acetone, ethyl alcohol each for 30 min, then dried by high-purity nitrogen gas. After 8 min ultraviolet-ozone treatment for the ITO substrate, anode buffer layer was prepared by spin-coating PEDOT:PSS aqueous solution with speed of 3500 rpm and then thermal-annealed at 150 °C for 30 min, then the PEDOT: PSS anode buffer layer was obtained with the thickness of about 30 nm. After that, the treated ITO/PEDOT:PSS films were transferred into a high-purity nitrogen-filled glove box (<0.01 ppm O² and H₂O) to fabricate active layers and cathode interlayers. The D18:L8-BO blend films were spin-coated onto the PEDOT:PSS layer with a thickness of about 100 nm. Subsequently, PDINN interlayer was obtained by spin-casting on top of active layers with the thickness of about 10 nm. Finally, Ag of about 100 nm was thermally deposited

on the PDIN layer under the vacuum of 2×10^{-4} Pa, and the deposition rate and thickness of Ag was in situ recorded with a quartz crystal oscillator monitor. The effective area of organic solar cells is 0.045 cm^2 , which is defined by the overlap of ITO anode and Ag cathode.

4. Instruments and Characterization:

The J - V characteristics of the OSCs were measured in a nitrogen glove box with a Keithley 2410 Source Measure under 100 mW/cm^2 illumination with AM 1.5 solar simulator (San-Ei Electric). AM 1.5 G solar simulator was calibrated by standard silicon solar cells (purchased from Enlitech). The ultraviolet-visible-near infrared (UV-Vis-NIR) absorption spectra were conducted with Hatachi-U3900H spectrophotometer. The photoluminescence (PL) spectra of the films were performed with fluorescence spectrometer (Spex Fluorolog-3). The external quantum efficiency (EQE) was conducted with a solar cell QE/IPCE measurement system (Zolix solar cell scan100). Transient photovoltage (TPV), transient photocurrent (TPC) and photo-induced charge extraction linear increasing voltage (Photo-CELIV) were conducted with the Paios system (FLUXiM AG, Switzerland). The integrated power of the LED for the Paios system is 720 W/m^2 . AFM measurements were performed with a Bruker-Fast scan ultrafast DI AFM. The GIWAXS data were obtained at 1W1A Diffuse X-ray Scattering Station, Beijing Synchrotron Radiation Facility (BSRF-1W1A). The contact angle images were obtained with contact angle measurement system (Dataphysics OCA15Pro). The optimized thickness of the active layer is $\sim 100 \text{ nm}$, which was measured by Bruker Stylus Profile (Dektak XT, Bruker Corporation).

5. Additional experimental results:

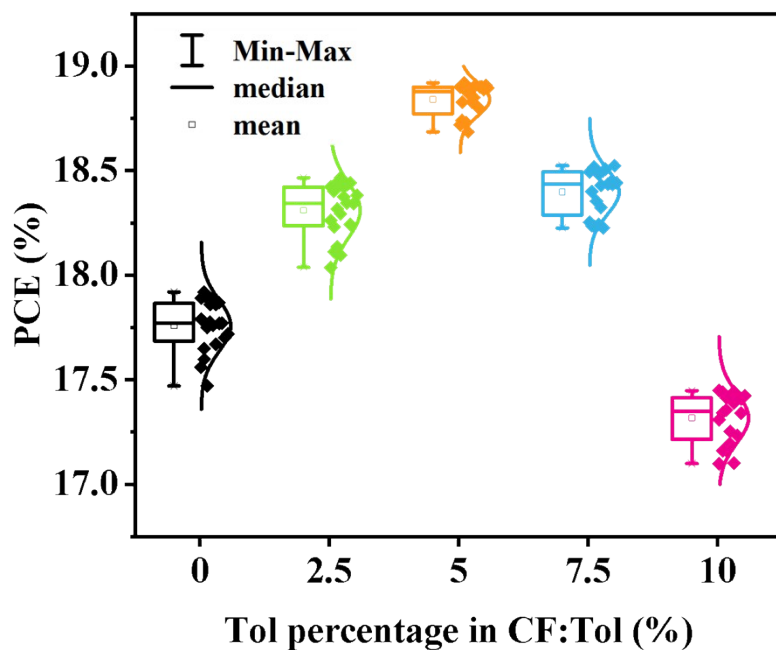


Figure S1. Statistical results of PCE for the OSCs with different CF:Tol ratio.

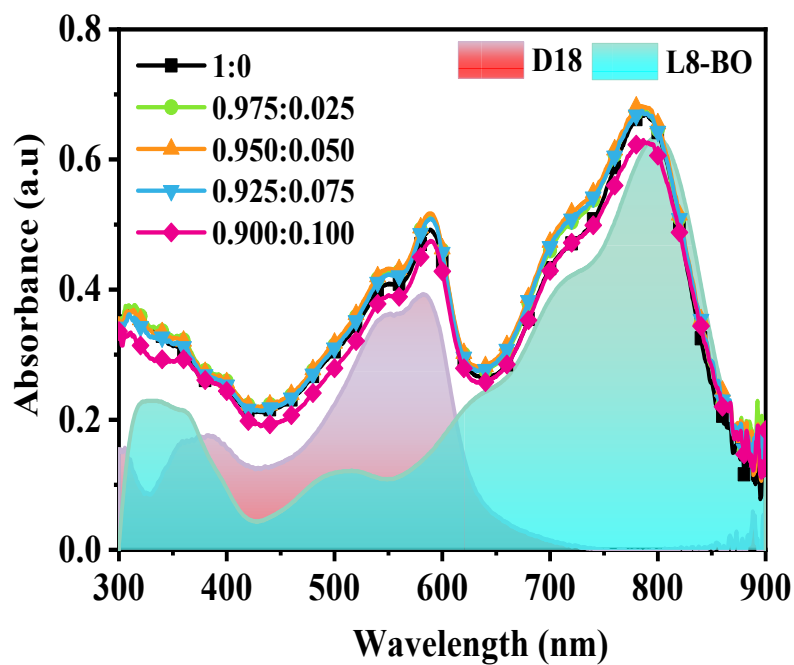


Figure S2. The absorbance curves of D18:L8-BO blend films with different CF:Tol ratio.

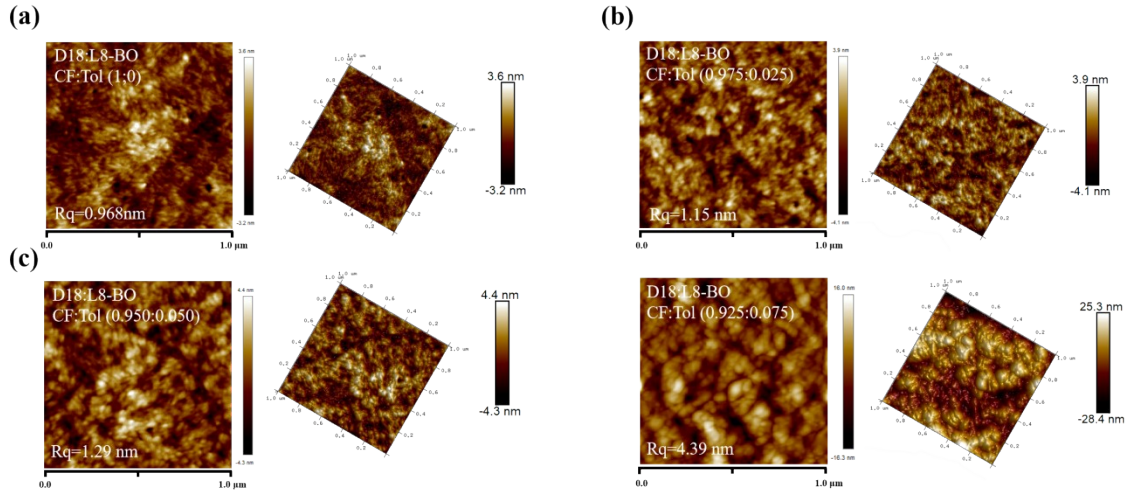


Figure S3. AFM height images of D18:L8-BO films obtained from (a) CF and (b-d) CF:Tol mixed solvent.

Table S1. Summary of the photovoltaics parameters of OSCs prepared with different CF:Tol ratio under illumination of AM 1.5G, 100 mA/cm².

CF:Tol	J_{SC} (mA/cm ²)	J_{cal}^a (mA/cm ²)	V_{OC} (V)	FF (%)	PCE (%)
1:0	25.90	24.62	0.923	74.99	17.89 ^b (17.76 ± 0.16) ^c
0.975:0.025	26.17	24.91	0.927	76.08	18.47 ^b (18.31 ± 0.17) ^c
0.950:0.050	26.43	25.28	0.927	77.24	18.92 ^b (18.83 ± 0.08) ^c
0.925:0.075	26.19	24.95	0.921	76.77	18.52 ^b (18.40 ± 0.13) ^c
0.900:0.100	25.60	24.47	0.911	74.82	17.45 ^b (17.32 ± 0.12) ^c

^a The integral current density from EQE spectra, ^b the maximum values of the devices,

^c the average values and deviation obtained from 20 devices.

Table S2. GIWAXS parameters of the OSCs prepared different CF:Tol ratio.

CF:Tol	In plane			Out of plane		
	$q(\text{\AA}^{-1})$	$d_{\text{spacing}}(\text{\AA})$	CCL(\AA)	$q(\text{\AA}^{-1})$	$d_{\text{spacing}}(\text{\AA})$	CCL(\AA)

1:0	0.3170	19.82	18.17	1.7186	3.66	15.09
0.95:0.05	0.3270	19.21	18.08	1.7353	3.62	18.16

Table S3. Water contact angle related parameters.

film	D18	L8-BO	D18:L8-BO CF	D18:L8-BO CF:Tol(0.95:0.05)
contact angle (°)	106.9	94	103.9	101.15
L8-BO surface content (%)	/	/	22.8	44.1