Electronic Supplementary Information

Isomerization of Peripheral Functional Groups Refines Aggregation and Non-Radiative Energy

Loss for Efficient Organic Photovoltaics

Xiaoning Wang,^{ac} Xiangyu Shen,^a Jianxiao Wang,^a Fuzhen Bi, ^{*abcd} Huanxiang Jiang,^e Hao Lu,^e Cheng Sun,^a Chunming Yang,^f Yonghai Li, ^{*abcd} and Xichang Bao^{*abcd}

^{*a*} State Key Laboratory of Photoelectric Conversion and Utilization of Solar Energy, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, China

E-mail: bifz@qibebt.ac.cn; liyh@qibebt.ac.cn; baoxc@qibebt.ac.cn

^b Laboratory of Solar Energy, Shandong Energy Institute, Qingdao 266101, China

^c College of Materials Sciences and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 101408, China

^d Qingdao New Energy Shandong Laboratory, Qingdao 266101, China

^e College of Textiles and Clothing, State Key Laboratory of Bio-fibers and Eco-textiles, Qingdao University, Qingdao 266071, China

^f Shanghai Synchrotron Radiation Facility Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201204, China

Experimental Procedures

Materials and Characterization Techniques

Donor materials D18 was purchased from Shenzhen Ruixun optoelectronic material Technology Co., Ltd. The commercial 5,6-difluoro-2H-benzo[d][1,2,3]triazole, 3,9-diundecyl-12,13-dihydro-[1,2,5] thiadiazolo[3,4-]thieno[2",3":4',5']thieno[2',3':4,5] py rrolo [3,2-]thieno[2',3':4,5]thieno[3,2-b] indole (1), 2F-IC end-caps were purchased from Nanjing Zhiyan Technology Co., Ltd. Other reagents were purchased from Alfa Aesar, Sigma-Aldrich, et al., which were utilized directly unless stated otherwise.

¹H NMR and ¹³C NMR spectra were recorded on Bruker AVANCE III 600 MHz spectrometer at 298 K. The absorption spectra were recorded using a Hitachi U-4100 UV-Vis scanning spectrophotometer. The photoluminescence (PL) spectra and time-resolved photoluminescence (TRPL) spectra were recorded by FLS1000 Edinburgh steady state and transient fluorescence spectrometer with excited wavelength of 700 nm for neat acceptor films and 400 nm for blend films. Cyclic voltammetry (CV) measurements were performed on a CHI660D electrochemical workstation, equipped with a three-electrode cell consisting of a platinum working electrode, a saturated calomel electrode (SCE) as reference electrode and a platinum wire counter electrode. CV measurements were carried out in anhydrous acetonitrile containing 0.1 M n-Bu4NPF6 as a supporting electrolyte under an argon atmosphere at a scan rate of 100 mV s-1 assuming that the absolute energy level of Fc/Fc+ was -4.80 eV. Thin films were deposited from CHCl₃ solution onto the working electrodes. Grazing incidence wide-angle X-ray scattering (GIWAXS) patterns were acquired from Shanghai Synchrotron Radiation Facility at the beam BL6B1. Transmission electron microscopy (TEM) images were obtained by using a HITACHI H-7650 electron microscope with an acceleration voltage of 100kV. Atomic force microscopy (AFM) images were obtained using Agilent 5400 scanning probe microscope in tapping mode with MikroMasch NSC-15 AFM tips. The thickness of films was measured using a Veeco Dektak 150 profilometer. Contact angles (CA) are measured by the contact angle measuring instrument CSCDIC-200S. In-situ absorptions were carried out from the in-situ dynamic spectrometer DU-300, with chloroform as the solvents. The background illumination was provided by the LED light source, and pulsed light was provided by an arbitrary wave generator (AFG322C, Tektronix) to measure Transient photovoltage (TPV) and photocurrent (TPC). The photovoltage traces were registered by the oscilloscope (AFG322C, Tektronix). The photocurrent traces were registered with the resistance of 50 Ω , switching open-circuit mode to short-circuit mode. The integrated TPC signal provides a measure of the total charge generated by the LED light source.

The geometry structure of the BTz-1, BTz-2, PM6/ YBTz-1 complex, PM6/ YBTz-1 complex were comprehensively optimized by employing the B3LYP function with 6-31g(d,p) basis sets. For the optimizations of the complexes systems, Grimme's dispersion with the original D3 damping functional (GD3) was exploited for dispersion correction.^[4] PM6 molecules with two repeating units were selected instead of polymers in this work. The excitation properties calculation were performed by TD-DFT method with CAM-B3LYP(ω =0.01)/6-31g(d,p) /polarizable continuum model (PCM). The dibutylether with dielectric constant (ε)3.0 was used to describe the solvent effect. Electron and hole distributions analysis were implemented using Multiwfn 3.8 ^[1-2] and outputs are visualized using VMD 1.9.3. ^[3] The hole and electron transfer integral for the complex are calculated using the site energy correction method. ^[5]

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Molecular dynamics (MD) simulations were based on the GAFF force field and conducted with the GROMACS 2019 software package.^[1] The atomic charges were fitted using the restrained electrostatic potential (RESP) method by Multiwfn software.^[2] The equilibrium bond lengths and angles were updated based on optimized geometries. 300 YBTz-1/YBTz-2 molecules were used to simulated the acceptor films. 200 YBTz-1/YBTz-2 and 38 D18 pentamer were used to simulated the blend films, to give a 1: 1.2 weight ratio between D18 pentamer and NFAs. The molecular packing morphologies was imitated by the following procedure: (1) the molecules were randomly placed into a cubic box with a density of 0.1 g/cm³ using packmol software;^[3] (2) 5 ns of simulation at 600 K and 100 bar to make

molecules close together quickly; (3) 10 ns of simulation at 600 K and 1 bar, then cooling down to 300 K in 5 ns; (4) 10 ns of equilibration at 300 K and 1 bar and another 10 ns of NPT was performed to obtain the equilibrated configuration. The analyses are performed on the frames extracted from the last 5 ns with the help of MD Analysis package.^[4] The Berendsen barostat and velocity rescaling thermostat under the NPT ensemble were applied to control the pressure and temperature, respectively.

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Device fabrication and Evaluations

The conventional binary and ternary devices structure of glass/ITO/ PEDOT: PSS/ Active layer/ PDINN/ Ag were fabricated. The patterned indium tin oxide (ITO, $\approx 15 \Omega$ / square) glass substrates were sequentially ultrasonicated with detergent, deionized water, acetone, and isopropanol. The washed ITO glass substrates were dried with the high-pressure purity nitrogen and treated in an ultraviolet-ozone chamber (PREEN II-862) for 100 s. Subsequently, the PEDOT: PSS solution was filtrated and spin-coated on ITO substrates at 4000 rpm for 30 s. Then the ITO glass substrates coated with the layer of PEDOT: PSS were baked at 150 °C for 15 min in air. Solution of binary D18/YBTz-1 or YBTz-2 (w/w=1:1.2) and ternary D18/L8BO/YBTz (w/w/w=1:1.2:0.15) in chloroform (5.2 mg/mL for D18) were stirred at 60°C for 2 h before spin-coating on the PEDOT:PSS layer to form the active layers with the thickness of 100±20 nm, which measured by a Veeco Dektak 150 profilometer. Then the active layers are thermal annealed at 100 °C for 1.5 min. PDINO (in CH₃OH, 1mg/mL) was spincoating at 3000 rpm to form the electron transfer layer. Finally, Ag (60 nm) metal electrode was thermal evaporated under about 5×10⁻⁴ Pa and the device area was 0.1 cm² defined by shadow mask.

The current density-voltage (J-V) curves were measured by a Keithley 2400 unit under solar

simulator with light intensity of 100 mw cm⁻². The external quantum efficiencies (EQEs) were analyzed using a certified Newport incident photon conversion efficiency (IPCE) measurement system. The light intensity was calibrated with a standard single-crystal Si photovoltaic cell. The beam size is 5 cm \times 5 cm. The voltage step and delay time were 10 mV and 3 ms, respectively. The scan started from -0.2 V to 1.2 V. The hole mobility and electron mobility were measured by space-charge-limited current (SCLC) method with a device configuration of ITO/PEDOT:PSS/active layer/MoO₃/Al and ITO/ ZnO/ active layer/ PDINO/ Al structure, respectively. The SCLC is described by the Mott–Gurney law:

 $J = 9\varepsilon\mu V^2 / (8L^3)$

where ε represents the dielectric constant of the metal, and μ is the carrier mobility, V is the voltage drop across the device and L is the thickness of the active layer.

Materials Synthesis

The synthesis details are listed below:

(1) Synthesis of compound 2:



3,9-diundecyl-12,13-dihydro-[1,2,5]thiadiazolo[3,4-e]thieno[2",3":4',5']thieno[2',3':4, 5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b]indole (1.0 g, 1.34 mmol), 1-Bromo-2-ethylhexane (258 mg, 1.34 mmol) powered KI(11.2 mg, 0.067mmol) and K₂CO₃ (549.5 mmol, 4.0 mmol) were dissolved in DMF(30 mL) and stirred at 100 °C overnight under nitrogen. Cool to room temperature and spin dry with ethyl acetate and water. Further purification by column chromatography using dichloromethane/petroleum ether (1/2, v/v) as eluent to afford red solid 2 (0.6 g, 52% yield). The compound 2 was used for the next step without further purification.

(2) Synthesis of compound 3:



Compound 2 (500 mg, 0.58 mmol), 1,6-dibromohexane (280.6 mg, 1.16 mmol), KI (4.8 mg, 0.03 mmol) and K_2CO_3 (240.4 mg, 1.74 mmol) were dissolved in NMP (20 ml) and stirred at 100 °C for 4 hours. Cool to room temperature and spin dry with ethyl acetate and water. Then the organic phase was purified by silica gel column chromatography using dichloromethane/petroleum ether (1/4, v/v) as eluent to afford red solid 3 (520 mg, 88% yield).

Compound 3: ¹H NMR (600 MHz, CDCl₃) δ 7.02 (s, 2H), 4.69 – 4.56 (m, 4H), 3.21 (t, J = 6.7 Hz, 2H), 2.83 (t, J = 7.7 Hz, 4H), 1.86 (m, 6H), 1.40 – 1.22 (m, 46H), 0.99 – 0.80 (m, 22H), 0.62 (m, 6H). (3) Synthesis of compound 4:



Phosphorus oxychloride (0.5 mL) was added at 0 °C to anhydrous DMF (1 mL) in a dry 50 mL threeneck flask, and the mixture was then stirred for 2 h. A solution of compound 3 (0.4 g, 0.4 mmol) in 1,2-dichloroethane (15 mL) was added to the mixture dropwise. After stirring for another 30 min at 0 °C and cooling to room temperature, the mixture was heated to 70 °C for overnight. After cooling to room temperature, the mixture was quenched with saturated CH₃COONa solution and extracted with ethyl acetate. The organic phase was dried over Na₂SO₄ and filtered. After removing the solvent, the residue was purified by column chromatography on silica gel using ethyl acetate/petroleum ether (1/8, v/v) as eluent to afford compound 4-1 as a red solid (0.42 g, 96% yield).

Compound 4: ¹H NMR (600 MHz, CDCl₃) δ 10.13 (s, 2H), 4.75 – 4.55 (m, 4H), 3.37 (t, J = 6.5 Hz, 2H), 3.18 (t, J = 7.1 Hz, 4H), 2.02 – 1.80 (m, 8H), 1.73 – 1.55 (m, 3H), 1.53 – 1.13 (m, 44H), 1.13 –

0.79 (m, 16H), 0.67 (t, J = 7.3 Hz, 3H), 0.60 (t, J = 7.2 Hz, 3H).

(4) Synthesis of compounds 5 and 6:



Compound 4 (400 mg, 0.37 mmol), 1H-benzo[d][1,2,3]triazole(88.4 mg, 0.74 mmol), KI (3.1 mg, 0.019 mmol) and K_2CO_3 (153.4 mg, 1.11 mmol) were dissolved in DMF (18 ml) and stirred at 100 °C overnight under nitrogen. Cool to room temperature and spin dry with ethyl acetate and water. Then the organic phase was purified by silica gel column chromatography using ethyl acetate/petroleum (1/7, v/v) as eluent to afford red solid 5 (185.92 mg, 45% yield) and 6 (173.5 mg, 42% yield).

Compound 5: ¹H NMR (600 MHz, CDCl₃) δ 10.13 (d, J = 4.2 Hz, 2H), 7.78 (dd, J = 6.5, 3.1 Hz, 2H), 7.32 (dd, J = 6.5, 3.0 Hz, 2H), 4.66 (t, J = 7.5 Hz, 2H), 4.62 – 4.52 (m, 4H), 3.22 – 3.14 (m, 4H), 2.05 – 1.77 (m, 10H), 1.52 – 1.13 (m, 44H), 1.11 – 0.80 (m, 16H), 0.64 (t, J = 7.4 Hz, 3H), 0.58 (t, J = 7.3 Hz, 3H).

Compound 6:¹H NMR (600 MHz, CDCl₃) δ 10.14 (s, 2H), 8.00 (d, *J* = 8.3 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.36 – 7.33 (m, 1H), 7.33 – 7.29 (m, 1H), 4.66 (t, *J* = 7.4 Hz, 2H), 4.60 (d, *J* = 7.9 Hz, 2H), 4.45 (t, *J* = 7.0 Hz, 2H), 3.19 (t, *J* = 7.7 Hz, 4H), 2.05 – 1.75 (m, 10H), 1.49 – 1.09 (m, 52H), 1.08 – 0.78 (m, 18H), 0.65 (t, *J* = 7.4 Hz, 3H), 0.58 (t, *J* = 7.3 Hz, 3H).

(5) Synthesis of YBTz-1 and YBTz-2:



INCN-F (41.4 mg, 0.18 mmol) and compound 5 (100 mg, 0.09 mmol) were dissolved in chloroform (20 mL), then pyridine (0.5 mL) was added to the mixture and stirred for 2 hrs. The mixture was dropped into methanol and got a blue solid. The blue solid was purified on a silica-gel column chromatography using dichloromethane as eluent to afford YBTz-2 (126.2 mg, 91% yield). The blue solid YBTz-1 were obtained by a similar method with yield of 92%.

Compound YBTz-1:

¹H NMR (600 MHz, CDCl₃) δ 8.92 (s, 1H), 8.72 (s, 1H), 8.44 (ddd, J = 21.1, 9.9, 6.5 Hz, 2H), 8.10 (d, J = 8.3 Hz, 1H), 7.67 (t, J = 7.4 Hz, 1H), 7.52 – 7.43 (m, 3H), 7.35 (t, J = 7.5 Hz, 1H), 4.91 – 4.79 (m, 2H), 4.78 – 4.68 (m, 4H), 3.20 – 2.94 (m, 4H), 2.38 – 1.62 (m, 13H), 1.58 – 0.81 (m, 44H), 0.68 (t, J = 7.2 Hz, 3H), 0.62 (t, J = 7.2 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 185.93, 153.63, 147.29, 146.03, 145.09, 137.11, 133.08, 127.28, 123.88, 120.19, 114.67, 109.08, 47.85, 31.93, 29.85, 29.65, 29.63, 29.52, 29.44, 29.35, 22.70, 14.12, 13.70, 10.29.

Compound YBTz-2:

¹H NMR (600 MHz, CDCl₃) δ 8.91 (s, 1H), 8.74 (s, 1H), 8.43 (ddd, J = 25.0, 9.8, 6.5 Hz, 2H), 7.77 (dd, J = 6.5, 3.1 Hz, 2H), 7.72 (t, J = 7.5 Hz, 1H), 7.63 (t, J = 7.4 Hz, 1H), 7.32 (dd, J = 6.5, 3.0 Hz, 2H), 4.84 – 4.57 (m, 6H), 3.05 (d, J = 7.6 Hz, 4H), 2.45 – 1.61 (m, 14H), 1.52 – 0.78 (m, 44H), 0.67 (t, J = 7.2 Hz, 3H), 0.60 (t, J = 7.2 Hz, 3H). ¹³C NMR (151 MHz, CDCl₃) δ 185.98, 185.91, 158.23, 157.78, 155.10, 153.80, 153.58, 153.33, 147.24, 146.97, 145.18, 145.05, 144.24, 137.08, 137.02, 135.15, 134.56, 134.43, 134.11, 133.47, 133.00, 132.64, 132.35, 130.66, 130.36, 126.34, 119.85, 119.67, 117.81, 114.80, 114.65, 114.45, 113.40, 113.21, 112.44, 112.32, 68.95, 68.80, 56.23, 55.16, 51.49, 40.55, 31.93, 31.04, 30.94, 29.85, 29.81, 29.66, 29.64, 29.52, 29.45, 29.43, 29.36, 26.38, 26.19, 23.29, 22.70, 14.13, 13.71, 10.26.

Supplementary Figures and Tables



Fig. S1 The CV plots deposited on glassy carbon electrodes in 0.1 M Bu₄NPF₆-CH₃CN at a scan rate of 100 mV s⁻¹ and the corresponding molecular frontier orbitals of YBTz-1 and YBTz-2.



Fig. S2 ESP maps of YBTz-1 and YBTz-2 molecules.



Fig. S3 The extinction coefficient of YBTz-1 and YBTz-2 neat films.



Fig. S4 (a) The calculated absorption spectra and molar extinction coefficients of YBTz-1 and YBTz-2 molecules. (b) Simulated oscillator strengths of YBTz-1 and YBTz-2.



Fig. S5. SCLC curves of (a) the hole-only devices and (b) electron-only devices of pristine acceptor films. The supplementary Table includes the maximum values, and average values with deviations based on five individual devices.



Fig. S6 Center-of-mass radial distribution functions between the molecular sleletons of acceptors.



Fig. S7 Thermal stabilities of the two solar cells under continuous heating at 65 °C (unencapsulated devices, in glove box) and the extrapolated $T_{80\%}$ value of D18:YBTz-2 device.



Fig. S8 $J_{\rm ph}$ vs $V_{\rm eff}$ plots of the two optimal solar cells.



Fig. S9 SCLC curves of (a) the hole-only and (b) the electron-only devices of optimal bend films.



Fig. S10 PL spectra of D18, D18: YBTz-1 and D18: YBTz-2 films.



Fig. S11 TRPL spectra of D18: YBTz-1 and D18: YBTz-2 films.



Fig. S12 (a) The J_{SC} versus light intensity and V_{OC} versus light intensity characteristics of D18:YBTz-1 and D18:YBTz-2 devices.



Fig. S13 TRPL spectra of YBTz-1 and YBTz-2 films.



Fig. S14 The optimized molecular configurations of D18/YBTz-1 and D18/YBTz-2 systems. The side chains of D18 were replaced by methyl, and the outer side chains of acceptors were also replaced by methyl to reduce the calculation time.



Fig. S15. The MD snapshots of a D18:YBTz-1 box and a D18:YBTz-2 box with 200 acceptor molecules and 38 D18 pentamer for each box. The YBTz-1, YBTz-2, and D18 are colored by orange, green, and blue respectively, with all alkyl chains hidden for clarity.



Fig. S16. Distribution of delocalized electrons and holes of D18/YBTz-1 and D18/YBTz-2 optimized supramolecular configurations based on DFT calculations (green and blue stand for electron and hole respectively).



Fig. S17. Distribution of delocalized electrons and holes of D18/YBTz-1 and D18/YBTz-2 optimized supramolecular configurations extracted from MD simulations (green and blue stand for electron and hole respectively). The pentamer of D18 was replaced by dimer for simplicity.



Fig. S18 The contact angles of D18, YBTz-1, and YBTz-2 neat films.



Fig. S19 PL spectra of L8BO, L8BO: YBTz-1 and L8BO: YBTz-2 films.



Fig. S20 TRPL spectra of L8BO, L8BO: YBTz-1 and L8BO: YBTz-2 films.



Fig. S21 UV-vis absorption of D18:L8BO, D18:L8BO:YBTz-1 and D18: :L8BO:YBTz-2 blend



Fig. S22 2D-GIWAXS patterns of L8BO, L8BO: YBTz-1 and L8BO: YBTz-2 films.

CH ₂ I ₂	40.90°
H₂O	92.99° /

Fig. S23 The contact angles of L8BO neat films.



Fig. S24 AFM images of the D18:L8BO and D18:L8BO:YBTz-1, D18:L8BO:YBTz-2 optimal blend films.

	$S_1 (eV)$	T ₁ (eV)	$\Delta E_{\text{S1-T1}} \text{ (meV)}$
YBTz-1	1.6881	1.2079	480.2
YBTz-2	1.6876	1.2087	478.9

Table S1. The excited state energies of YBTz-1 and YBTz-2 molecules based on DFT calculations

Table S2. Photovoltaic parameters of the D18:YBTz-1 and D18:YBTz-2 based OSCs.

Blend	Additive	V _{oc}	$J_{ m SC}$	FF	PCE
	(mg/mL)	(V)	(mA cm ⁻²)	(%)	(%)
	As cast	0.811	25.19	67.72	13.8 (13.6±0.2)
D10.DT~ 1	3	0.806	25.31	69.24	14.1 (13.9±0.2)
D18:B12-1	4	0.803	25.37	71.96	14.7 (14.4±0.3)
	5	0.795	25.08	71.84	14.4 (14.1±0.3)
	As cast	0.876	25.93	77.38	17.6 (17.4±0.2)
D18:BTz-2	3	0.874	27.14	78.05	18.5 (18.3±0.2)
	4	0.873	27.83	78.63	19.1 (18.8±0.3)
	5	0.869	27.29	79.29	18.8 (18.6±0.2)

Table S3. The calculated energies of excited states of D18/YBTz-1 and D18/YBTz-2 supramolecular systems based on DFT calculations.

D18/YBTz-1					
En side d state		S.,	Excitation energy	$\Delta E(S1-CT_x)$	$\Delta E(T1-CT_x) (eV)$
Exclied state		Sr	(eV)	(eV)	
1	¹ CT_1	0.13879	1.381		
2	¹ CT_2	0.28011	1.608		
3	¹ CT_3	0.28538	1.659		
4	S ₁ (LE)	0.60226	1.700	0.041	
5	³ CT_1	0.28786	1.376		
6	³ CT_2	0.28835	1.618		
7	³ CT_3	0.12687	1.664		
8	T1		1.251		0.125

D18/YBTz-2					
Excited state		S.a.	Excitation energy	AE(81 CT =) (-V)	$\Delta E(T1-CT_x) (eV)$
		Sr	(eV)	$\Delta E(SI-CI_x)(ev)$	
1	¹ CT_1	0.12256	1.308		
2	¹ CT_2	0.13293	1.544		
3	¹ CT_3	0.19823	1.631		
4	S ₁ (LE)	0.65644	1.644	0.013	
5	³ CT_1	0.28939	1.301		
6	³ CT_2	0.21470	1.545		
7	³ CT_3	0.17388	1.630		
	T1		1.223		0.078

Table S4. The calculated energies of excited states of D18/YBTz-1 and D18/YBTz-2 supramolecular systems extracted from the MD simulations.

D18/YBTz-1					
		S.a.	Excitation	$\Delta E(S1-CT_x)$	$\Delta E(T1-CT_x)$
excited state		Sr	energy (eV)	(eV)	(eV)
1	CT_1	0.15316	1.2486		
2	CT_2	0.36325	1.5277		
3	CT_3	0.44636	1.6073		
4	CT_4	0.49210	1.6636		
5	CT_5	0.27703	1.7506		
6	S1(LE)	0.50957	1.7831	0.0325	
7	T1	0.74721	1.2079		
8	³ CT	0.26291	1.2332		0.0253

D18/YBTz-2

avaited state	Sr		Excitation	$\Delta F S1 (CT x)$	
exciled state			energy (eV)	ΔE SI-CI_X)	
1	¹ CT_1	0.34002	1.1280		
2	² CT_2	0.25153	1.3336		
3	³ CT_3	0.35825	1.4862		
4	⁴ CT_4	0.37896	1.5715		
5	⁵ CT_5	0.26977	1.6673		
6	S1(LE)	0.59465	1.6871	0.0198	
7	T1	0.74146	1.2087		
8	³ CT	0.41928	1.2223		0.0136

Film	$q_{ m lamina}$ (Å ⁻¹)	d_{lamina}	FWHM (Å)	CCL _{lamina}	$q_{\pi-\pi}$ (Å ⁻¹)	$d_{\pi-\pi}$ (Å)	FWHM (Å)	$\operatorname{CCL}_{\pi-\pi}$
D18:YBTz-1	0.304	20.67	0.0506	124.01	1.707	3.68	0.212	29.63
D18:YBTz-2	0.302	20.80	0.0515	122.05	1.702	3.69	0.219	28.72

Table S5. The *q* locations and π - π -stacking distances in OOP direction of GIWAXS studies

Table S6. The parameters of π - π stacking spacing (d_{π - π }) and crystal coherence lengths (CCLs) extracted from GIWAXS studies

Eilee	$q_{\pi\text{-}\pi}$	$d_{\pi\text{-}\pi}$	FWHM	$\mathrm{CCL}_{\pi\text{-}\pi}$
FIIII	(Å-1)	(Å)	(Å-1)	(Å)
L8BO	1.702	3.69	0.326	19.26
L8BO: YBTz-1 (1.2:0.15)	1.730	3.63	0.261	24.08
L8BO YBTz-2 (1.2:0.15)	1.707	3.68	0.275	22.84

	γ (mN m ⁻¹)	$\gamma_p (\text{mN m}^{-1})$	$\gamma_d (\mathrm{mN} \;\mathrm{m}^{-1})$	$CA(H_2O)$	$CA (CH_2I_2)$
D18	35.02	0.703	34.320	106.50°	56.20°
YBTz-1	42.82	0.007	42.813	92.58°	37.89°
YBTz-2	40.80	0.015	40.780	94.36°	41.97°
L8BO	40.08	0.003	40.074	92.99°	40.90°

Table S7. The parameters of surface energies and contact angles of neat films



¹H NMR spectrum of compound 3 in CDCl₃.

-10.13 448 448 448 448 448 C₁₁H₂₃ C₁₁H₂₃ онс сно C₄H₄ B 1.56 <u>-</u> 4.13 <u>-</u> Ē 29.1-0 4.27 43.91 16.18 3.17 3.13 2.00 3.33 5.5 5.0 4.5 Chemical shift (ppm) 10.0 9.5 9.0 7.5 7.0 6.5 6.0 4.0 3.5 3.0 2.5 1.5 1.0 0.0 8.5 8.0 0.5





¹H NMR spectrum of compound 5 in CDCl₃.



¹H NMR spectrum of compound 6 in CDCl₃.



¹H NMR spectrum of YBTz-2 in CDCl₃.







¹H NMR spectrum of YBTz-1 in CDCl₃.



¹³C NMR spectrum of YBTz-1 in CDCl₃