

Supporting Information

for

Non-Fullerene Acceptors Containing Fluoranthene-Fused Imide for Solution-Processed Inverted Organic Solar Cells

Yan Zhou, Ya-Zhong Dai, Yu-Qing Zheng, Xiao-Ye Wang, Jie-Yu Wang, and Jian Pei**

Beijing National Laboratory for Molecular Sciences, the Key Laboratory of
Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College
of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

E-mail: jianpei@pku.edu.cn, jieyuwang@pku.edu.cn

General Methods: ^1H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz using CDCl_3 as solvent. Absorption spectra were recorded on PerkinElmer Lambda 750 UV-Vis Spectrometer. PL spectra and quantum efficiency were carried out on integration sphere equipped Horiba Jobin-Yvon FluoroMax-4 Luminescence Spectrometer. AFM experiments were carried out with a Nanoscope IIIa microscope (Multimode, Digital Instruments) under ambient conditions. MS experiments were performed on a high resolution electrospray ionization mass spectrometer (ESI-HRMS). Elemental analyses were carried out on a German Vario EL III elemental analyzer. Cyclic voltammetry was performed using BASI Epsilon workstation and measurements were carried out in acetonitrile (for the thin film) or dichloromethane (for the solution) containing 0.1 M *n*-Bu₄NPF₆ as a supporting electrolyte. Glassy carbon electrode was used as a working electrode and a platinum sheet as a counter electrode. All potentials were recorded versus Ag/AgCl as a reference electrode. The scan rate was 50 mV s⁻¹. The X-ray diffraction data were obtained at beamline BL14B1 of the Shanghai Synchrotron Radiation Facility (SSRF) at a wavelength of 1.2398 Å. BL14B1 is a beamline based on bending magnet and a Si (111) double crystal monochromator was employed to monochromatize the beam. The size of the focus spot is about 0.5 mm and the end station is equipped with a Huber 5021 diffractometer. NaI scintillation detector was used for data collection. X-ray photoelectron spectra were carried out on Axis Ultra Imaging Photoelectron Spectrometer.

Device fabrication: Glass coated with patterned indium-doped tin oxide (ITO) with the square resistance of 13 Ω cm⁻² was purchased from Tianjin Glass Factory. Before device fabrication, the glass underwent a wet-cleaning course in an ultrasonic bath sequentially in acetone, detergent, deionized water and isopropanol. After dried in the vacuum oven under 80 °C for 10 mins and 15 mins oxygen plasma treatment, ZnO sol-gel was spin-coated onto the ITO surface at the speed of 4000 rpm for 18 s. The 30 nm thickness of ZnO layer was formed and baked at 140 °C for 1 h in air. All the active layers were spin-coated in a sealed spin-coater with 1300 rpm for 15 s in the

glove box. The wet films were put into a covered petry dish and allowed to dry overnight. The dried films were annealed in the glove box at 100 °C for 15 mins and tranfered to the vacuum for metal deposition. The thickness of the active layer was 140-150 nm measured by the surface profiler. The 15 nm thick MoO₃ layer followed by 100 nm thick Ag layer was thermal deposited under the pressure of 4×10^{-4} Pa. The device active area is 15 mm². All the devices were encapsulated in the glove box and tested under ambient condition. The PCE was tested under AM 1.5G irradiation with the intensity of 100 mW cm⁻² (Newport Solar Simulator 94021A) calibrated by a NREL certified standard silicon cell (4 cm²). *J-V* curves were recorded with a Keithley 2636A semiconductor analyzer. IPCE test were carried out under monochromic illumination (Newport 74125 monochromator equipped with 66984 ARC lamp) and the calibration of the incident light intensity was performed with a calibrated silicon photodiode.

Th-CN and ***p*-CH₃OPh-CN** were prepared following the previous literature.^[15]

Ph-CN: ¹H NMR (400 MHz, CDCl₃, δ): 8.05-8.07 (d, *J* = 7.7 Hz, 1H), 7.74-7.77 (d, *J* = 7.2 Hz, 1H) 7.74 (m, 7H), 7.50-7.57 (m, 5H), 7.91-7.93 (d, *J* = 7.2 Hz, 1H), 7.85-7.87 (d, *J* = 7.7 Hz, 1H), 3.51-3.54 (d, *J* = 7.7 Hz, 2H), 1.57-1.59 (m, 2H), 1.21-1.25 (m, 10H), 0.83-0.87 (t, *J* = 7.8 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz, δ): 167.2, 143.5, 141.5, 139.2, 136.4, 135.8, 135.3, 134.9, 134.8, 134.3, 132.7, 130.5, 129.7, 129.1, 129.00, 128.97, 128.8, 128.61, 128.55, 126.7, 125.8, 123.9, 117.1, 110.0, 38.2, 31.8, 29.1, 29.1, 28.5, 27.0, 22.6, 14.1. HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₃₉H₃₃N₂O₂, 561.2536; Found, 561.2537. Anal. calcd for: C₃₉H₃₂N₂O₂: C, 83.54; H, 5.75; N, 5.00; Found: C, 83.45; H, 5.80; N, 4.98.

***o*-CH₃Ph-CN:** ¹H NMR (400 MHz, CDCl₃, δ): 8.07-8.08 (d, *J* = 7.6 Hz, 1H), 7.75-7.77 (d, *J* = 7.2 Hz, 1H), 7.38-7.57 (m, 9H), 6.78-6.80 (d, *J* = 7.2 Hz, 1H), 6.72-6.74 (d, *J* = 7.7 Hz, 1H), 3.52-3.55 (d, *J* = 7.2 Hz, 2H), 2.17 (s, 6H) 1.59-1.71 (m, 2H), 1.21-1.25 (m, 10H), 0.83-0.87 (t, *J* = 7.8 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz, δ): 167.2, 143.6, 141.5, 139.3, 135.8, 135.8, 135.7, 135.7, 135.6, 135.4, 134.9, 134.6, 134.5, 134.4, 132.6, 130.8, 130.6, 130.6, 130.5, 130.0, 129.2, 129.2, 129.1, 129.0, 128.4, 128.4, 126.6, 126.6, 126.6, 126.2, 125.8, 123.4, 117.1, 110.0, 38.2, 31.7, 29.2, 29.1, 28.5, 27.0, 22.6, 20.0, 19.9, 14.1. HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₄₁H₃₈N₂O₂, 589.2849; Found, 589.2849. Anal. calcd for: C₄₁H₃₇N₂O₂: C, 83.64; H, 6.16; N, 4.76; Found: C, 83.32; H, 6.17; N, 4.72.

***α*-Nath-CN:** ¹H NMR (400 MHz, CDCl₃, δ): 8.15-8.17 (d, *J* = 7.6 Hz, 2H), 8.04-8.07 (m, 2H), 7.70-7.77 (m, 4H), 7.52-7.62 (m, 5H), 7.28-7.40 (m, 3H), 6.46-6.48 (m, 1H), 6.39-6.41(m, 1H), 3.40-3.44 (d, *J* = 7.2 Hz, 2H), 1.45-1.55 (m, 2H), 1.11-1.27 (m, 10H), 0.80-0.83 (t, *J* = 7.8 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz, δ): 166.9, 144.4, 142.4, 138.9, 135.0, 134.7, 134.4, 134.0, 133.7, 132.7, 132.6, 132.6, 132.5, 132.5, 131.5, 131.5, 131.2, 130.6, 130.2, 129.5, 129.4, 128.9, 126.9, 126.8, 126.8, 126.7, 126.5, 126.5, 126.5, 125.8, 124.9, 124.9, 123.8, 117.0, 110.0, 38.2, 31.7, 29.1, 29.0, 28.4, 26.9, 22.6, 14.1. HRMS (ESI) *m/z*: [M + H]⁺ calcd for C₄₇H₃₇N₂O₂, 661.2863;

Found, 668.2850. Anal. Calcd. for: $C_{47}H_{36}N_2O_2$: C, 85.43; H, 5.49; N, 4.24; Found: C, 85.20; H, 5.33, N, 4.25.

β -Nath-CN: 1H NMR (400 MHz, $CDCl_3$, δ): 8.12-8.15 (d, $J = 8.4$ Hz, 2H), 8.01-8.08 (m, 5H), 7.92-7.95 (m, 2H), 7.56-7.70 (m, 7H), 7.38-7.42 (dd, $J_1 = 8.0$ Hz, $J_2 = 7.6$ Hz, 1H), 6.90-6.91 (d, $J = 7.2$ Hz, 1H), 6.84-6.86 (d, $J = 7.6$ Hz, 1H), 3.49-3.53 (d, $J = 8.0$ Hz, 2H), 1.53-1.62 (m, 2H), 1.13-1.27 (m, 10H), 0.80-0.84 (t, $J = 7.8$ Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, δ): 167.2, 143.7, 141.6, 139.2, 136.5, 135.8, 135.3, 134.4, 133.5, 133.4, 133.4, 132.7, 132.3, 132.2, 130.6, 130.0, 129.1, 129.0, 128.8, 128.7, 128.5, 128.2, 128.0, 128.0, 126.9, 126.9, 126.8, 126.7, 126.7, 126.5, 126.4, 125.9, 124.0, 117.0, 110.1, 38.2, 31.7, 29.1, 29.1, 28.5, 27.0, 22.6, 14.1. HRMS (ESI) m/z : $[M + H]^+$ Calcd for $C_{47}H_{37}N_2O_2$, 661.2860; Found, 668.6850. Anal. calcd for: $C_{47}H_{36}N_2O_2$: C, 85.43; H, 5.49; N, 4.24; Found: C, 85.02; H, 5.33, N, 4.26.

Table S1. The XPS data of the surface elements of different active layers.

Counts/a. u.	Th-CN	Ph-CN	<i>o</i> -CH ₃ Ph-CN	<i>p</i> -CH ₃ OPh-CN	α -Naph-CN	β -Naph-CN	P3HT
C _{1s}	122815	110727	103096	113876	107875	112642	96100
S _{2p}	18921	15743	14575	16639	15801	16123	13854
S _{2p} /C _{1s}	0.154	0.142	0.141	0.146	0.146	0.143	0.144

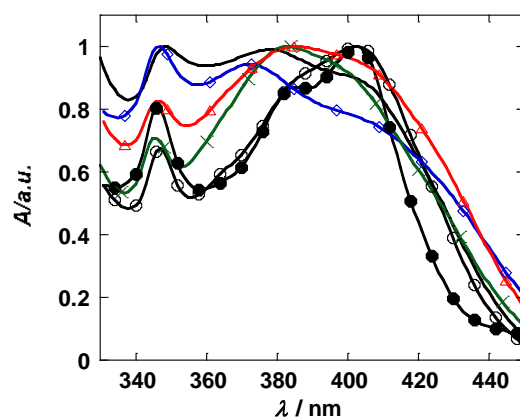


Fig. S1 The absorption spectra of the acceptors films on ZnO substrates. **Th-CN** (solid line), **Ph-CN** (empty circles), ***o*-CH₃Ph-CN** (solid circles), ***p*-CH₃OPh-CN** (empty squares), **α -Naph-CN** (cross), and **β -Naph-CN** (empty triangles).

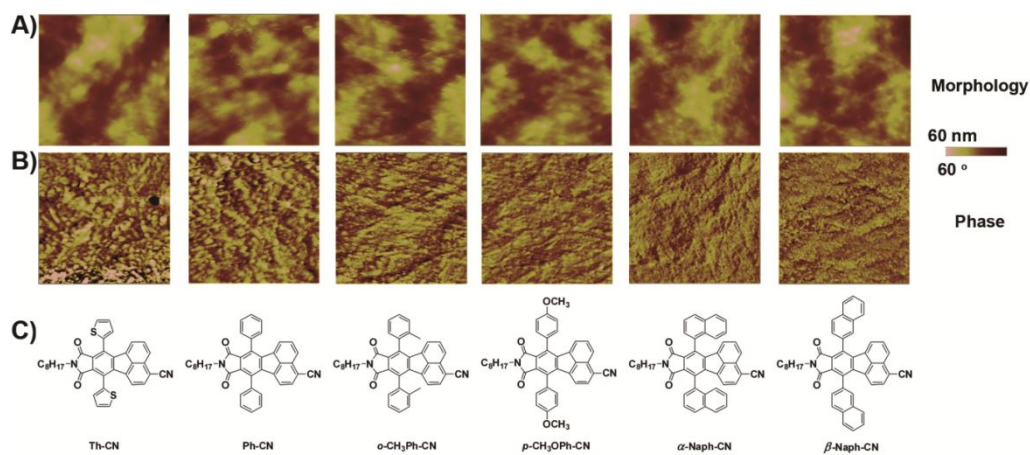


Fig. S2 The morphology and phase images of the active layers with the weight ratio of P3HT/acceptor as 1/1.

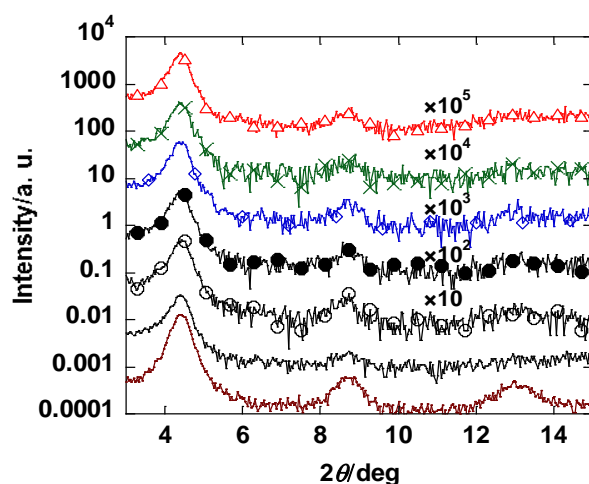


Fig. S3 Linear diffraction data in the face-on direction of different active films on ZnO substrates. The weight ratio of donor/acceptor was 1/1 for all the active films. Acceptors IDs from top to bottom were β -Naph-CN, α -Naph-CN, *p*-CH₃OPh-CN, *o*-CH₃Ph-CN, Ph-CN, Th-CN, and P3HT.

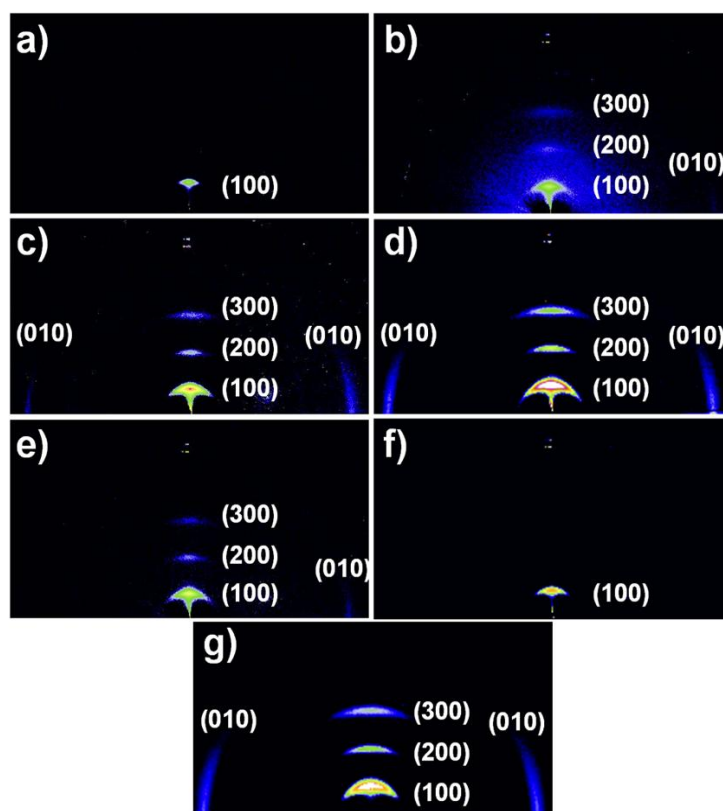


Fig. S4 The GIXRD diffraction patterns of the active layers of the blends with the weight ratio of P3HT/acceptors as 1/1 and the pure P3HT film. a) Th-CN, b) Ph-CN, c) *o*-CH₃Ph-CN, d) *p*-CH₃OPh-CN, e) α -Naph-CN, f) β -Naph-CN, and g) P3HT.