Electronic Supplementary Information for:

A Planar Electron Acceptor for Efficient Polymer Solar Cells

Yao Wu,[§a] Huitao Bai,[§b] Zaiyu Wang,[c] Pei Cheng,[bd] Siya Zhu,[a] Yifan Wang,[bd] Wei Ma[c] and Xiaowei Zhan*[a]

[a]*Department of Materials Science and Engineering, College of Engineering, Key Laboratory of Polymer Chemistry and Physics of Ministry of Education, Peking University, Beijing, 100871, P. R. China. E-mail: xwzhan@pku.edu.cn*

[b]*Beijing National Laboratory for Molecular Sciences, Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100871, P. R. China*

[c] *State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049, P. R. China*

[d]*University of Chinese Academy of Sciences, Beijing, 100049, P. R. China*

Materials. Unless stated otherwise, all the solvents and chemical reagents used were obtained commercially and were used without further purification. Toluene was distilled from sodium benzophenone under nitrogen prior to use. Compound **1** was synthesized according to a literature procedure.[1] Compounds **2** were purchased from LumTec Inc.

Characterization. The ^{1}H- and ^{13}C-NMR spectra were measured using a Bruker AVANCE 400 MHz spectrometer employing tetramethylsilane (TMS; δ = 0 ppm) as an internal standard. Elemental analysis was carried out using a Flash EA 1112 elemental analyzer. Mass spectra were measured using a Bruker Daltonics Biflex III MALDI-TOF Analyzer in the MALDI mode. Solution (chloroform) and thin film (on a quartz substrate) UV-vis absorption spectra were recorded using a Jasco V-570 spectrophotometer. Electrochemical measurements were carried out under nitrogen in a deoxygenated solution of tetra-n-butylammonium hexafluorophosphate (0.1 M) in acetonitrile using a potential scan rate of 100 mV s^{-1} employing a computer-controlled Zahner IM6e electrochemical workstation, a glassy-carbon working electrode coated with the IDT-2BR film, a platinum-wire auxiliary electrode, and an Ag/AgCl electrode as a reference electrode. The potentials were referenced to a ferrocenium/ferrocene ($FeCp_2^{0/+}$) couple using ferrocene as an external standard. Thermogravimetric analysis (TGA) measurements were performed using a Shimadzu thermogravimetric analyzer (Model DTG-60) under flowing nitrogen gas at a heating rate of 10 °C min^{-1}. The nanoscale morphology of the blended films was observed

using a Veeco Nanoscope V atomic force microscope (AFM) in the tapping mode. The transmission electron microscopy (TEM) characterization was carried out using a JEM-2200FS. The samples for the TEM measurements were prepared as follows: The active-layer films were spin-casted on ITO/PEDOT:PSS substrates, and the ITO glass with the active layers were submerged in deionized water (10 min) to make the active layers float onto the air–water interface. Then the floated films were picked up on unsupported 200 mesh copper grids for the TEM measurement.

Computational Details. Density functional theory calculations were performed with the Gaussian 09 program,[2] using the B3LYP functional[3] and 6-311G* basis sets.[4] Geometry optimization was performed with no symmetry constraints in gas phase without solvent effects. Vibration frequency calculation was performed and no imaginary frequencies were found.

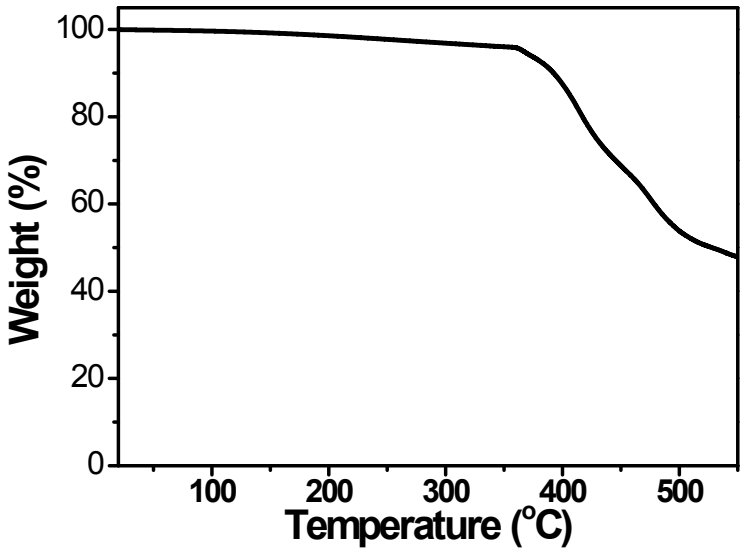

Fig. S1 TGA curve of IDT-2BR.

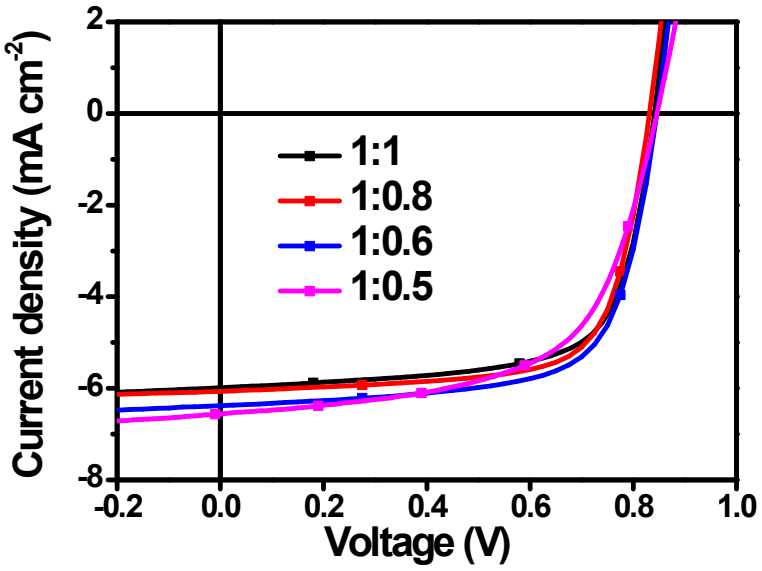

Fig. S2 The *J–V* curves of the devices based on P3HT: IDT-2BR with different donor/acceptor ratios under the illumination of AM 1.5G, 100 mW cm^{-2}.

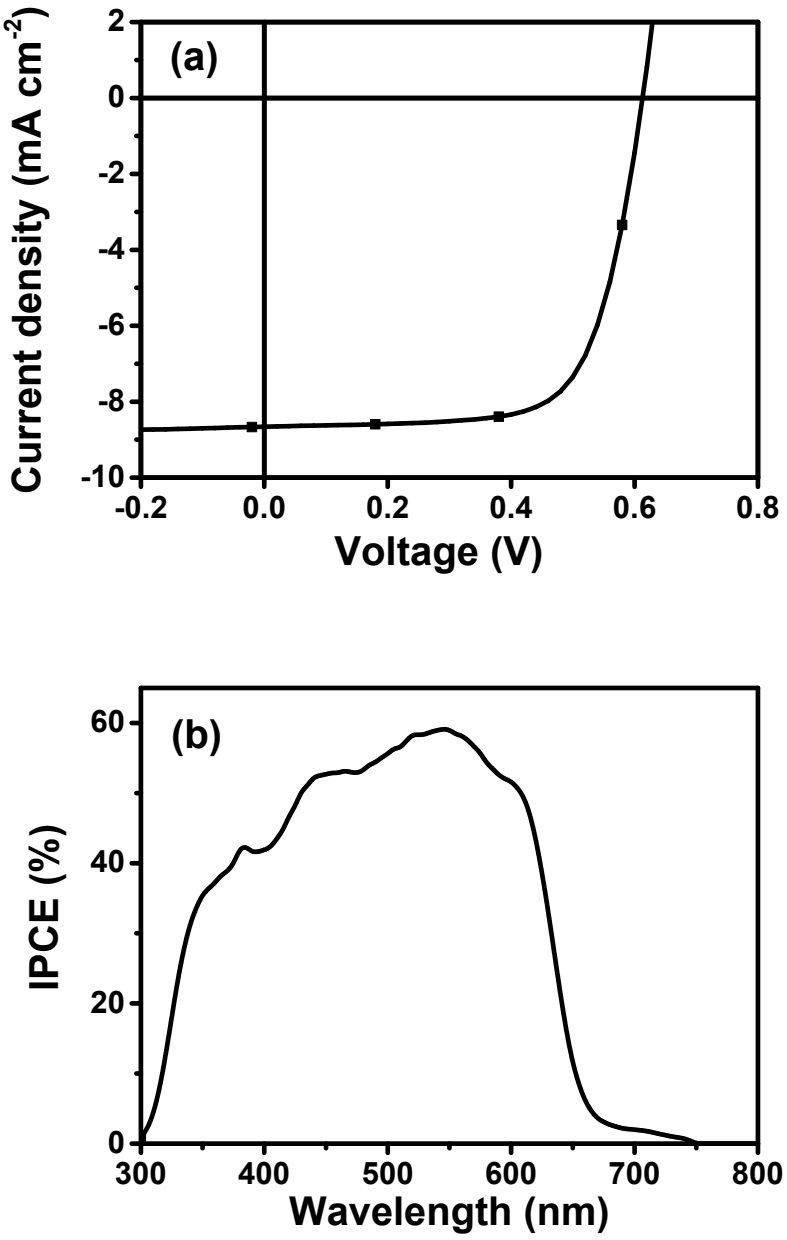

Fig. S3 (a) The *J–V* curve under the illumination of AM 1.5G, 100 mW cm^{-2} and (b) IPCE curve of the device based on P3HT: $PC_{61}BM$ (1:1, w/w) after thermal annealing at 140 °C for 10 min.

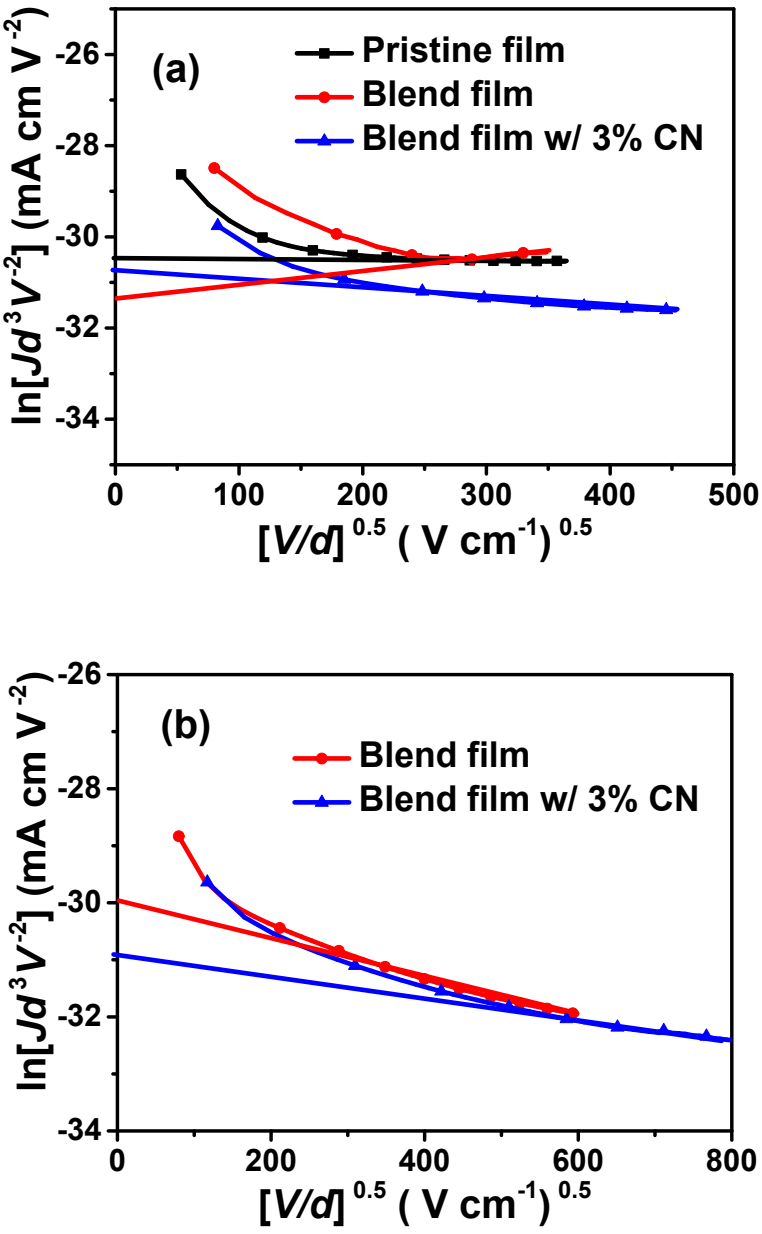

Fig. S4 *J-V* characteristics for (a) electron-only and (b) hole-only devices based on IDT-2BR pristine and blended (P3HT: IDT-2BR = 1: 0.6, w/w) films.

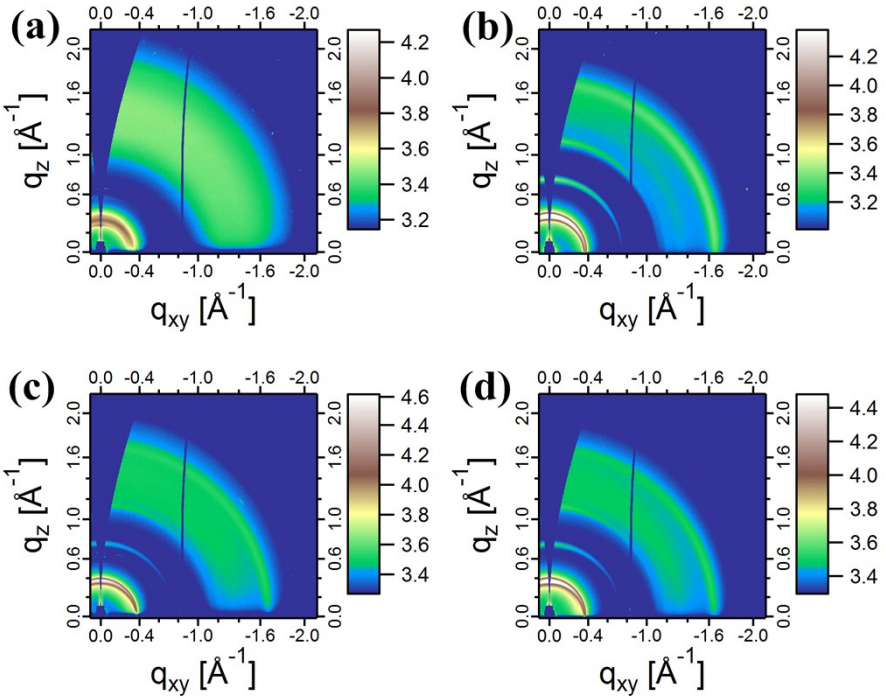

Fig. S5 Two-dimensional GIWAXS patterns of (a) IDT-2BR, (b) P3HT pristine and P3HT: IDT-2BR (1: 0.6, w/w) blended films (c) without CN and (d) with 3% CN on SiO_2/Si substrate.

Table S1 Photovoltaic performance of the OSCs based on P3HT: IDT-2BR blends (1: 0.6, w/w) with 3% CN with various active layer thicknesses

thickness (nm)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE_{max} (PCE_{ave}) (%)
60	0.85	8.48	68.0	4.91 (4.82)
80	0.84	8.91	68.1	5.12 (5.04)
110	0.84	8.70	67.7	4.95 (4.88)
140	0.83	8.55	67.8	4.83 (4.74)
180	0.83	8.49	66.9	4.72 (4.61)
220	0.83	8.39	65.9	4.60 (4.50)

Table S2 SCLC data of hole-only and electron-only devices based on IDT-2BR neat film, P3HT: IDT-2BR (1: 0.6, w/w) blended film, and P3HT: $PC_{61}BM$ (1:1, w/w) blended film

film	CN (%)	μ_h (cm^2 V^{-1} s^{-1})	μ_e (cm^2 V^{-1} s^{-1})	μ_h/μ_e
IDT-2BR	/	/	3.4×10^{-4}	/
P3HT: IDT-2BR	/	6.1×10^{-4}	1.5×10^{-4}	4.1
P3HT: IDT-2BR	3	2.0×10^{-4}	2.6×10^{-4}	0.77
P3HT: $PC_{61}BM$	/	1.4×10^{-5}	3.8×10^{-4}	0.04

References

1 Y. C. Chen, C. Y. Yu, Y. L. Fan, L. I. Hung, C. P. Chen, C. Ting, *Chem. Commun.,* 2010, **46**, 6503.

2 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.01, Gaussian, Inc., Wallingford CT, 2009.

3 (a) C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B.,* 1988, ***37***, 785; (b) A. D. Becke, *J. Chem. Phys.,* 1993, ***98***, 5648.

4 (a) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople*, J. Chem. Phys*., 1980, ***72***, 650; (b) A. D. McLean and G. S. Chandler, *J. Chem. Phys.,* 1980, **72**, 5639.