

Supporting Information

Toward Reliable and Accurate Evaluation of Polymer Solar Cells Based on Low Band Gap Polymers

Long Ye,^{a,d} Chengyue Zhou^b, Haifeng Meng^{*c}, Heng-Hsin Wu^c, Chi-Ching Lin^c, Hua-Hsien Liao^c, Shaoqing Zhang^a, Jianhui Hou^{*a}

^aState Key Laboratory of Polymer Physics and Chemistry, Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China

^bEnli Technology Co. Ltd., Kaohsiung 821, Taiwan

^cNational Institute of Metrology, Beijing 100029, China

^dUniversity of Chinese Academy of Sciences, Beijing 100049, China

*Corresponding author.

Prof. Jianhui Hou, E-mail address: hjhzlz@iccas.ac.cn, Tel: +86-010-82615900.

Dr. Haifeng Meng, E-mail: menghf@nim.ac.cn

S1. Device fabrication details

The PSCs were prepared on glass substrates with tin-doped indium oxide (ITO, 15 Ω/sq) patterned on the surface. We cleaned ITO substrates in sequential ultrasonic baths using detergent, water, acetone, and 2-propanol, followed by 15 min UV-ozone treatment. Then, an aqueous solution of PEDOT:PSS (Clevios P VP AI 4083) was spin-cast at 4000 rpm onto the substrates for ~35 nm thin film and baked at 150 °C for 15 min. Immediately after baking the substrates, the samples were then transferred into a dry nitrogen glovebox (<5 ppm O₂) for active layer deposition. The polymer/PC₇₁BM blend solutions were stirred for 6 hours. The solution details of active layers are listed in the **Table S1**. For instance, PBDTTT-C-T and PC₇₁BM at a 1:1.5 weight ratio in a 10 mg/ml *o*-dichlorobenzene (DCB) solution was spin-coated at 800 rpm for 90 s, and 3% vol 1,8-diiodooctane (DIO) was added into the blend solution for morphology modulation. PSBTBT and PC₇₁BM at a 1:1 weight ratio in a 10 mg/ml chlorobenzene (CB) solution was spin-coated at 1000 rpm for 60 s, and then the active layer was subsequently annealed at 140 °C for 5 min. Prior to evaporating metal cathodes, the blend films with processing additives were treated with 60 uL methanol to remove the residual DIO.^[1] The device fabrication was completed by thermal evaporation of a 20 nm thick Ca

and a 80 nm thick Al layer as cathode under vacuum at a base pressure of 2×10^{-4} Pa. Following electrode deposition, samples underwent *J-V* testing.

Table S1. The fabrication details of PSCs based on various photovoltaic polymers.

Polymer	Concentration of Polymer [mg/ml]	D/A ratio	Solvent	Thickness [nm]	Ref.
PBDTTT-C-T:PC ₇₁ BM	10	1:1.5	DCB/DIO (97/3)	95 nm	[1]
P3HT:PC ₇₁ BM	17	1:1	DCB	180 nm	[2]
PTB7-Th:PC ₇₁ BM	10	1:1.5	DCB/DIO (97/3)	100 nm	[3]
PBDTBDD:PC ₇₁ BM	10	1:1	DCB/DIO (97/3)	85 nm	[4]
PBTTDPP-T:PC ₇₁ BM	6	1:2	CB/DIO (99.5/0.5)	100 nm	[5]
PDPP3T:PC ₇₁ BM	5	1:2	DCB/CF/DIO (76/19/5)	110 nm	[6]
PBDTTPD:PC ₇₁ BM	20	1:1	CF/DIO (97/3)	105 nm	[7]
PBDD4T:PC ₇₁ BM	10	1.5:1	DCB/DIO (97/3)	75 nm	[8]
PSBTBT:PC ₇₁ BM	10	1:1	CB	80 nm	[9]

S2. Absorption spectrum of different photovoltaic polymers

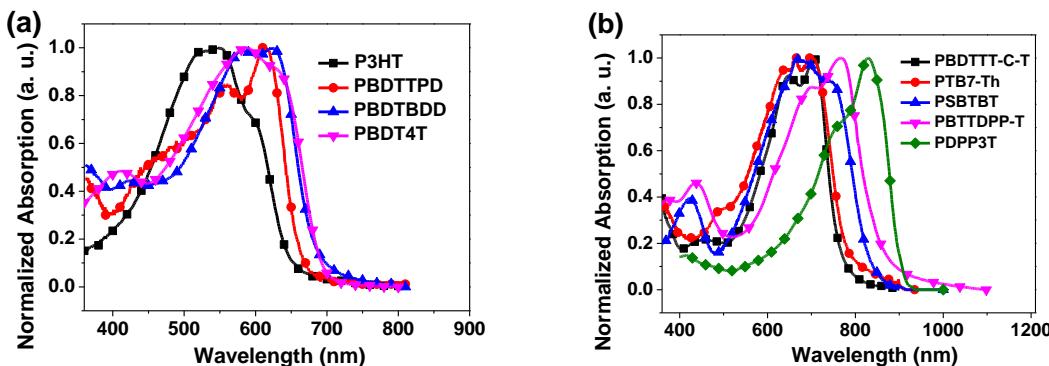


Fig. S1. Absorption spectrum of different photovoltaic polymers: (a) P3HT, PBDTTPD, PBDTBDD, and PBDD4T; (b) PTB7-Th, PBDTTT-C-T, PSBTBT, PDPP3T, and PBTTDPP-T.

References

- [1]. L. Ye, Y. Jing, X. Guo, H. Sun, S. Zhang, M. Zhang, L. Huo and J. Hou, *J. Phys. Chem. C*, 2013, **117**, 14920-14928.
- [2]. G. Li, V. Shrotriya, J. S. Huang, Y. Yao, T. Moriarty, K. Emery and Y. Yang, *Nat. Mater.*, 2005, **4**, 864-868.
- [3]. S. Zhang, L. Ye, W. Zhao, D. Liu, H. Yao and J. Hou, *Macromolecules*, 2014, **47**, 4653-4659.

- [4]. D. P. Qian, L. Ye, M. J. Zhang, Y. R. Liang, L. J. Li, Y. Huang, X. Guo, S. Q. Zhang, Z. A. Tan and J. H. Hou, *Macromolecules*, 2012, **45**, 9611-9617.
- [5]. S. Zhang, L. Ye, Q. Wang, Z. Li, X. Guo, L. Huo, H. Fan and J. Hou, *J. Phys. Chem. C*, 2013, **117**, 9550-9557.
- [6]. L. Ye, S. Q. Zhang, W. Ma, B. H. Fan, X. Guo, Y. Huang, H. Ade and J. H. Hou, *Adv. Mater.*, 2012, **24**, 6335-6341.
- [7]. J. Warnan, A. El Labban, C. Cabanetos, E. T. Hoke, P. K. Shukla, C. Risko, J.-L. Br édas, M. D. McGehee and P. M. Beaujuge, *Chem. Mater.*, 2014, **26**, 2299-2306.
- [8]. D. Qian, W. Ma, Z. Li, X. Guo, S. Zhang, L. Ye, H. Ade, Z. a. Tan and J. Hou, *J. Am. Chem. Soc.*, 2013, **135**, 8464-8467.
- [9]. J. Hou, H.-Y. Chen, S. Zhang, G. Li and Y. Yang, *J. Am. Chem. Soc.*, 2008, **130**, 16144-16145.