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Electronic Supplementary Information

for

Low-bandgap polymer electron acceptor based on double B←N bridged bipyridine (BNBP) and diketopyrrolopyrrole (DPP) units for all-polymer solar cells

Xiaojing Long,[a,b] Ning Wang,[a,b] Zicheng Ding,[a] Chuandong Dou,*[a] Jun Liu*[a] and Lixiang Wang[a]

[a]*State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, People's Republic of China.*
[b]*University of Chinese Academy of Sciences, Beijing 100864, People's Republic of China.*
**Email: chuandong.dou@ciac.ac.cn; liujun@ciac.ac.cn.*

Contents

1. Thermal property

The thermal property of **P-BNBP-DPP** was studied by thermogravimetric analysis (TGA). TGA analysis shows that it has good thermal stability with decomposition temperature at 5% weight loss of 400 °C under N_2.

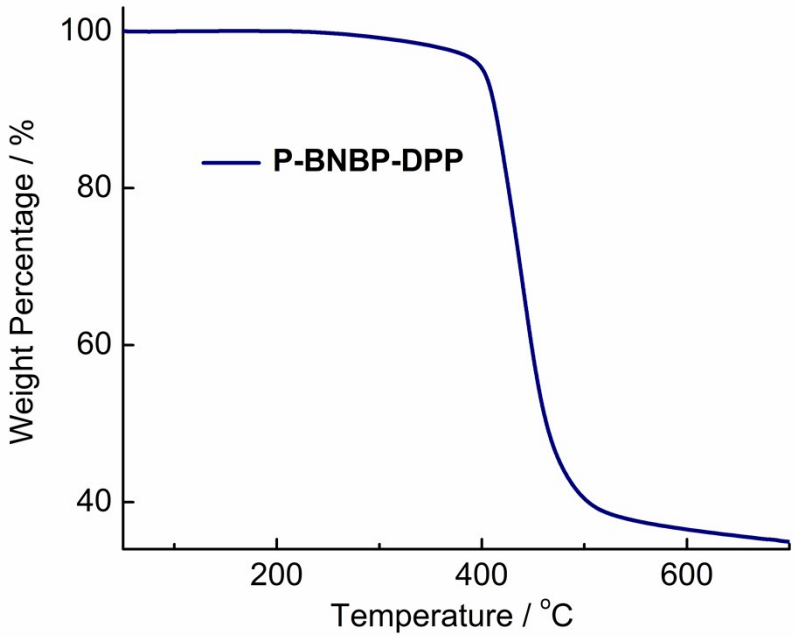

Figure S1. TGA curve of **P-BNBP-DPP**.

2. Charge transporting properties

The electron/hole mobilities of the films were measured using the space-charge-limited current (SCLC) method. The electron-only and hole-only device structures for **P-BNBP-DPP** are ITO/PEIE/Active layer/Ca/Al and ITO/PEDOT:PSS/Active layer/MoO_3/Ag, respectively. The electron-only device structure for **P-BNBP-T** is ITO/ZnO/Active layer/LiF/Al. The current-voltage curves in the range of 0–10 V were recorded using a computer-controlled Keithley 2400 source meter, and the results were fitted to a space-charge limited function:

$$J = \frac{9}{8}\varepsilon_r\varepsilon_0\mu\frac{V^2}{L^3}\exp\left(0.89\beta\frac{\sqrt{V}}{\sqrt{L}}\right)$$

where J is the current density, ε_0 is the permittivity of free space, ε_r is the relative permittivity of 2.3 for **P-BNBP-DPP** and **P-BNBP-T**, μ is the zero-field mobility, V is the potential across the device ($V = V_{applied}–V_{bias}–V_{series}$), L is the thickness of active layer, and β is the field-activation factor. The series and contact resistance (V_{series}) of the device (10–15 Ω) were measured using blank devices of ITO/PEIE/Ca/Al or ITO/PEDOT:PSS/MoO_3/Ag or ITO/ZnO/LiF/Al.

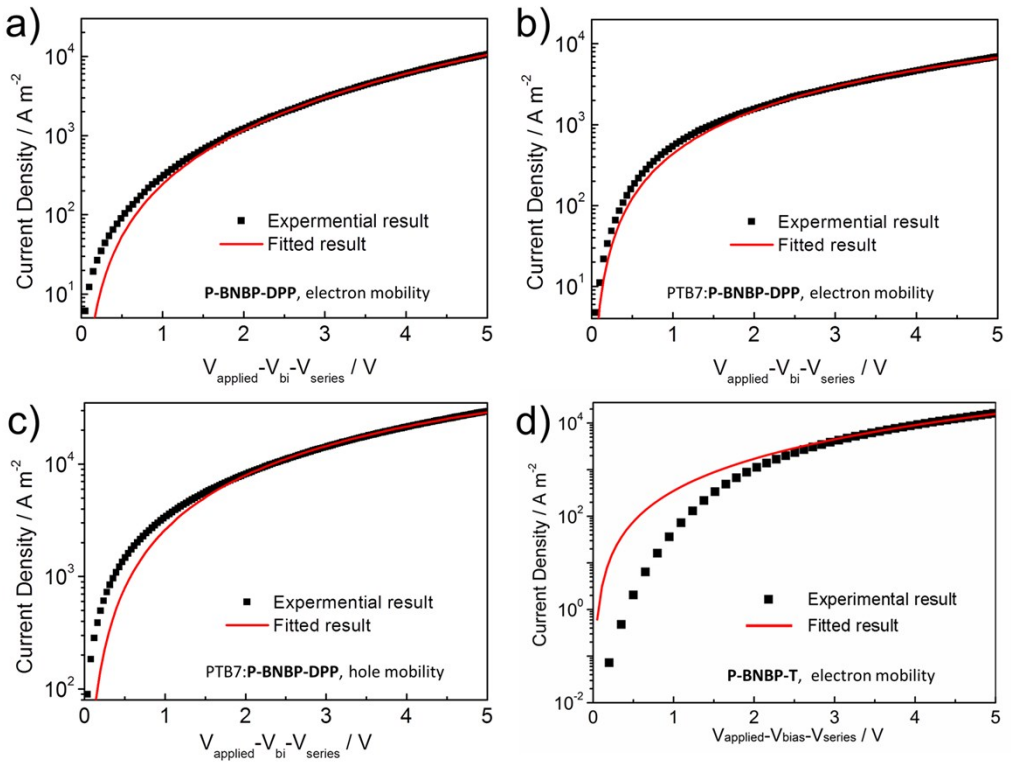

Figure S2. Space-charge-limited current (SCLC) fittings of the devices based on the prime films and the blend films.

3. All-polymer solar cell device performance

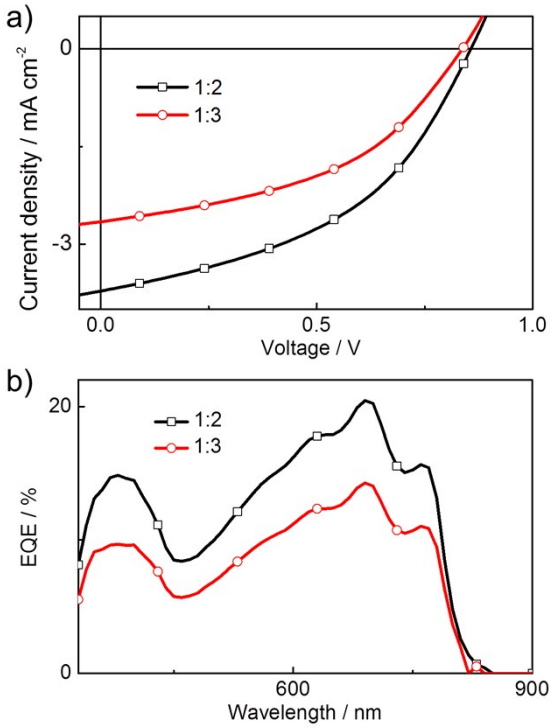

Figure S3. a) The *J–V* curves and b) the EQE curves of the all-PSC devices based on the PTB7:**P-BNBP-DPP** blends with various donor:acceptor weight ratios.

Table S1. Summary of the PTB7:**P-BNBP-DPP** all-PSC device performance.

D:A (*w*:*w*)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	$PCE_{max/ave}$[a] (%)
1:3	0.81	2.81	0.40	0.93 (0.82)
1:2	0.86	3.72	0.44	1.43 (1.29)
1:1	0.86	5.48	0.45	2.11 (2.01)
2:1	0.88	7.54	0.41	2.69 (2.58)
3:1	0.88	5.43	0.42	2.0 (1.89)

[a]The average PCE value is calculated from six devices.

4. Reference

Gaussian 09 (Revision A.02), 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, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian, Inc*., Wallingford CT, 2009.

5. ^{1}H NMR spectrum

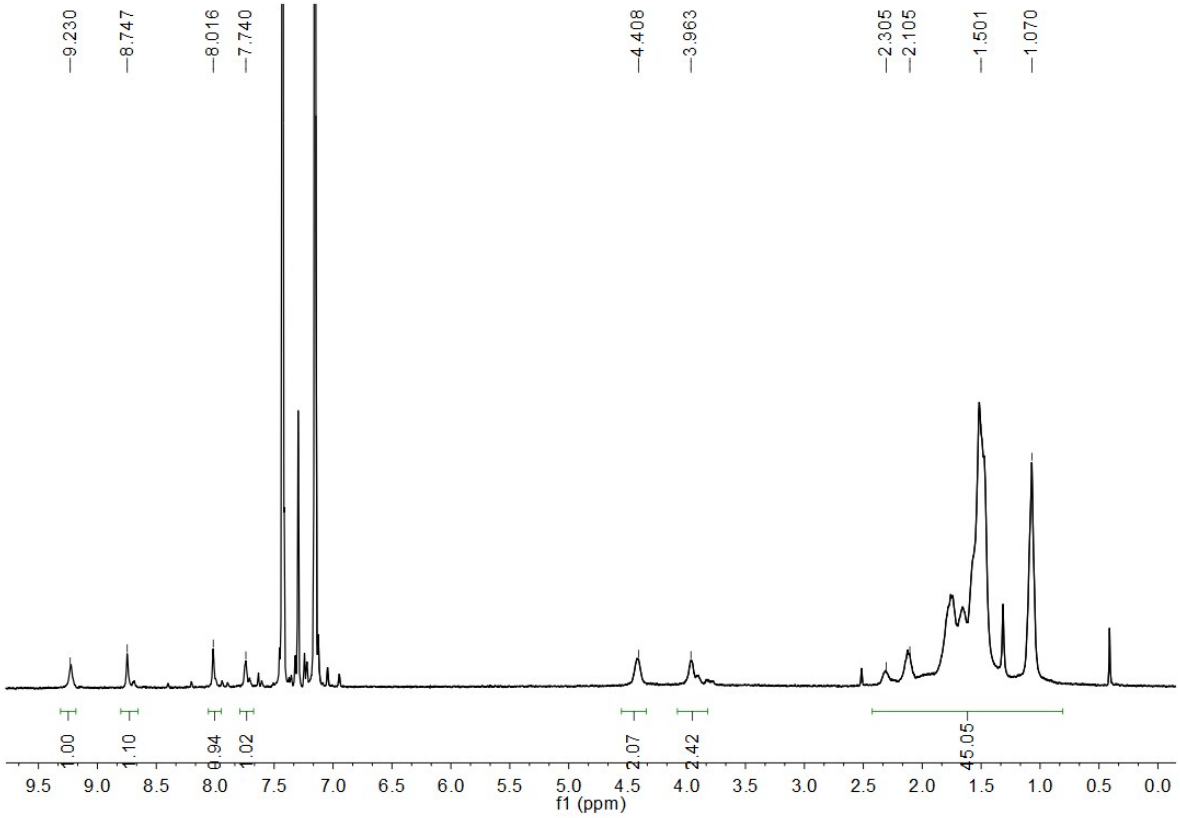

Figure S4. ^{1}H NMR spectrum of **P-BNBP-DPP**.