Supporting Information

Perylene Diimides: a Thickness-Insensitive Cathode Interlayer for High Performance Polymer Solar Cells

Zhi-Guo Zhang, Boyuan Qi, Zhiwen Jin, Dan Chi, Zhe Qi, Yongfang Li and Jizheng Wang**

Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190 (China)
E-mail: jizheng@iccas.ac.cn (J. Wang) and liyf@iccas.ac.cn (Y. Li)

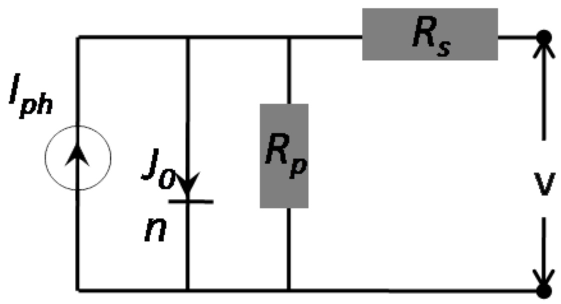


Figure S1. Equivalent circuit of the solar cell.

The current density-voltage characteristic of an organic photovoltaic device can be described with conventional (Si) p-n solar cells, so the following simplified expression can be derived for the open-circuit voltage V_{OC}:

$$V_{OC} \approx \frac{nKT}{q} \ln \left(\frac{J_{SC}}{J_0}\right) \quad (1)$$

where J_{SC} is the short-circuit current density under illumination, J_0 is the reverse bias saturation current density, q is the elementary charge, K is Boltzmann's constant, T is temperature (T is 300 K here.), KT is thermal energy, and n is the ideality factor of the diode, in which n is a key factor to reflect whether the semiconductor device is good or not.

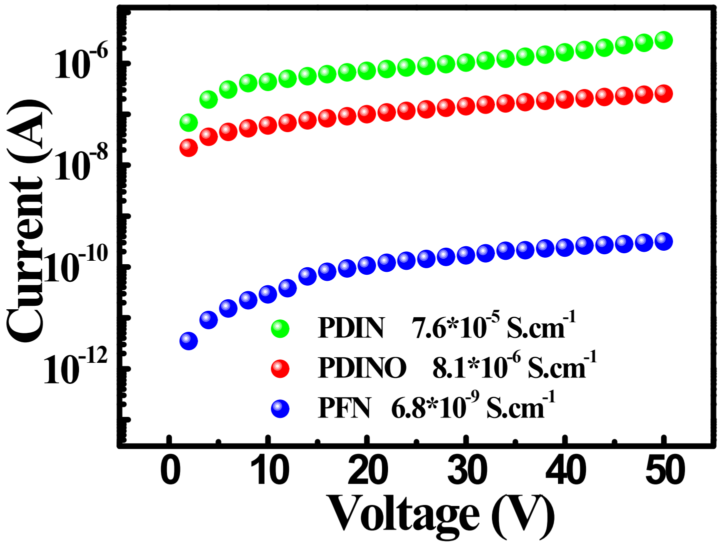


Figure S2. The measurements of the conductivities.

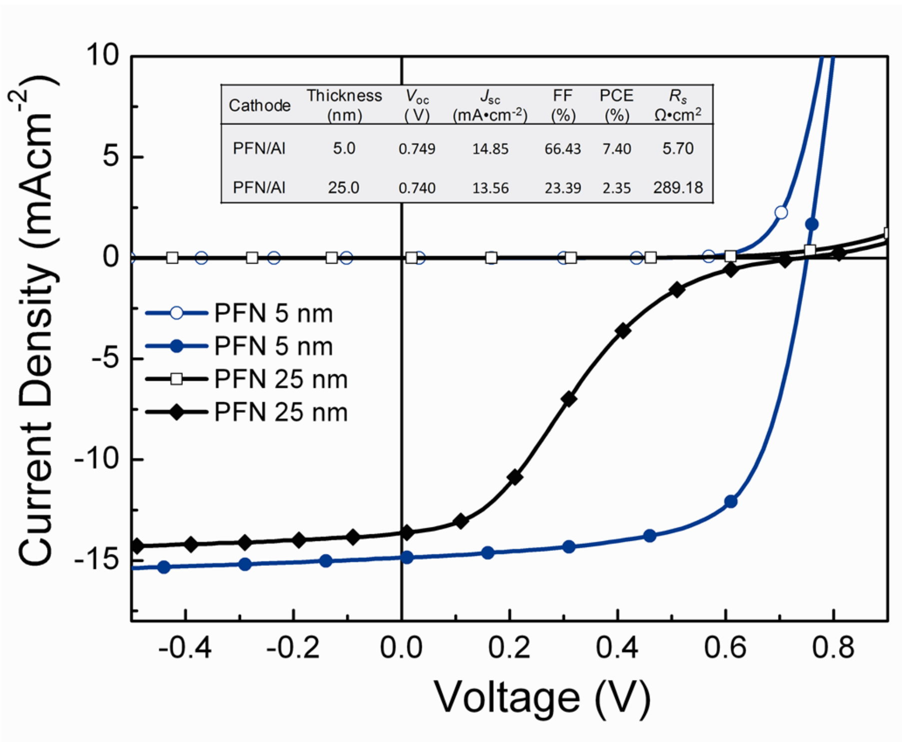


Figure S3. J-V curves of the PSCs based on PTB7/$PC_{70}BM$ with PFN cathode interlayer under the illumination of AM1.5G, 100 mW/cm^2.

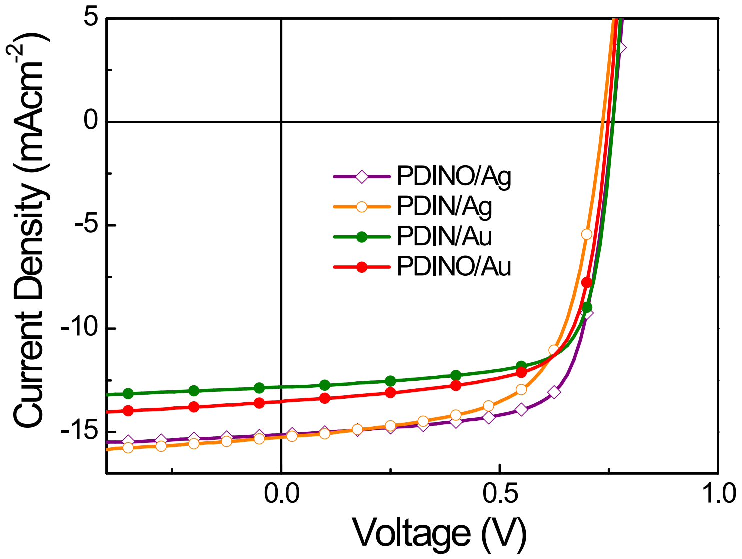


Figure S4. J-V curves of the PSCs based on PTB7/$PC_{70}BM$ with PDIN (14 nm) or PDINO (10 nm) cathode interlayer and different metal top electrodes under the illumination of AM1.5G, 100 mW/cm^2.

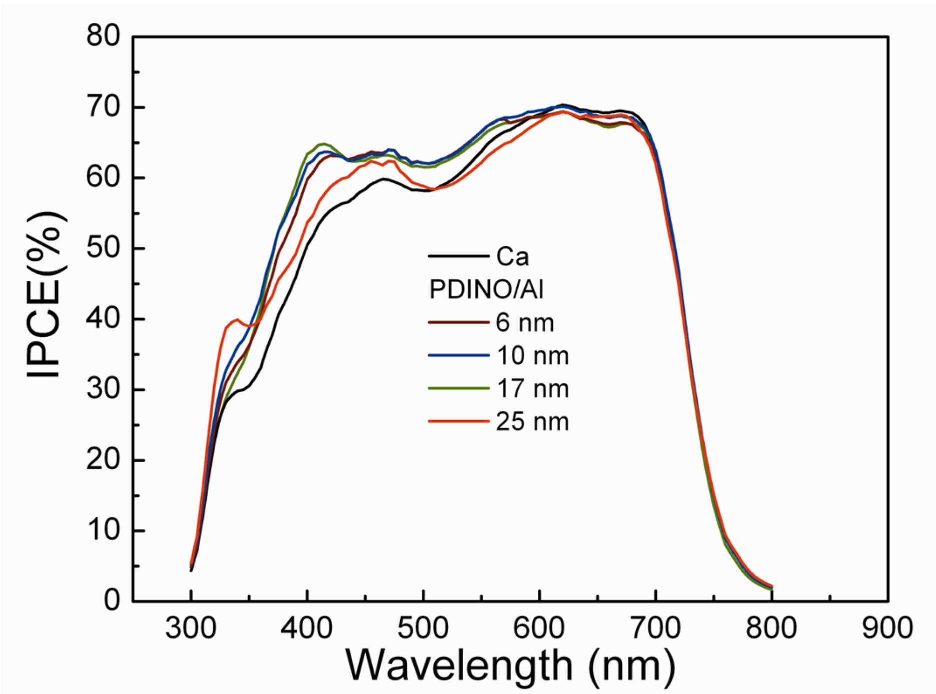


Figure S5. The IPCE spectra of the PSCs based on PTB7/$PC_{70}BM$ with PDINO cathode interlayerwith different interlayer thickness along with that of the device with Ca/Al cathode.

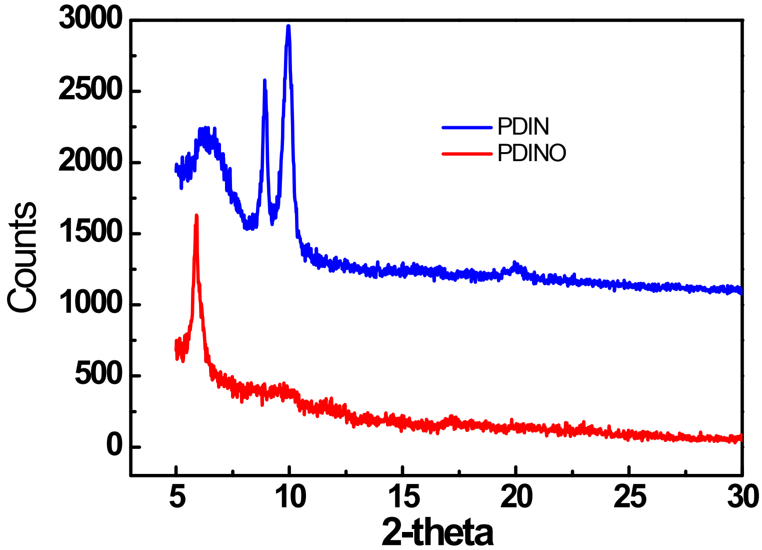


Figure S6. X-ray diffraction patterns of the polymer films drop-cast onto a silicon substrate.

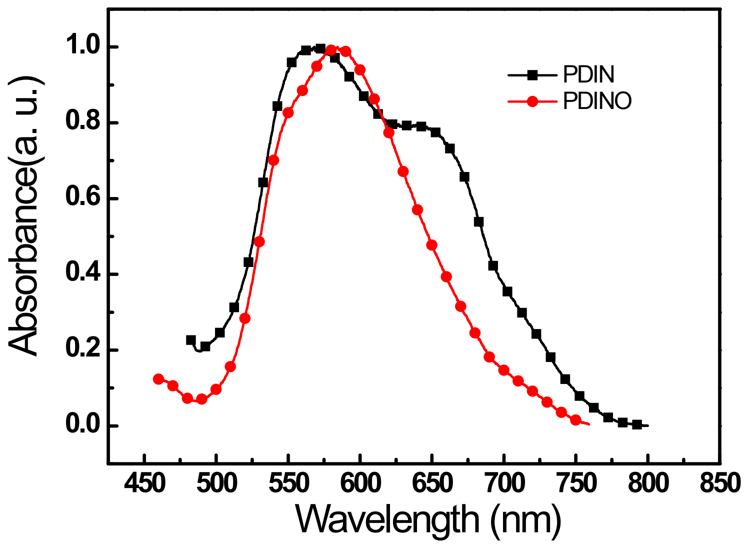


Figure S7. PL spectrum of PDINO/PDIN in the solid state.

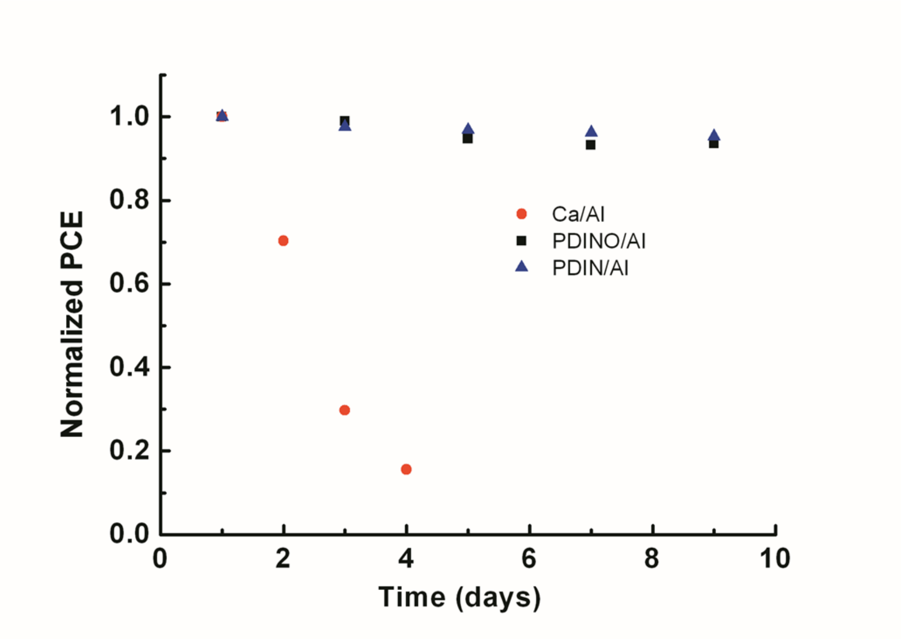


Figure S8. Normalized PCEs under ambient condition for PTB7/$PC_{70}BM$ based devices.

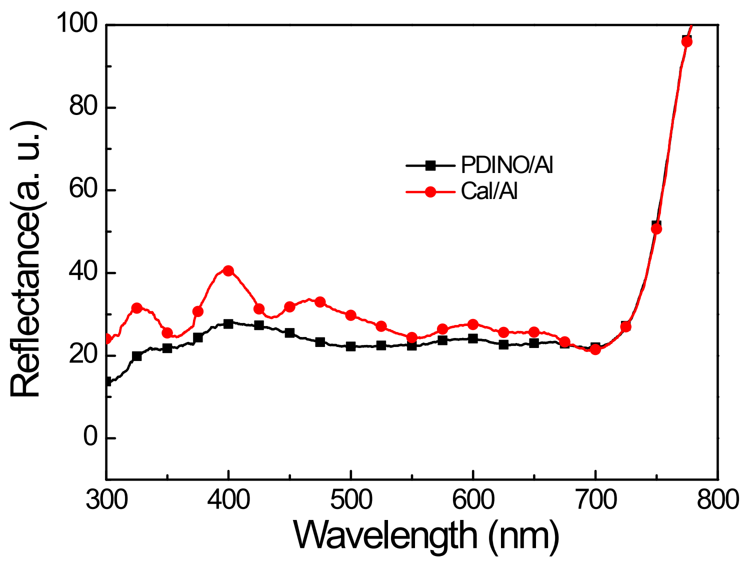


Figure S9. The reflectance spectra of the conventional Ca/Al and the PDINO/Al PTB7-Th: $PC_{70}BM$ PSCs.

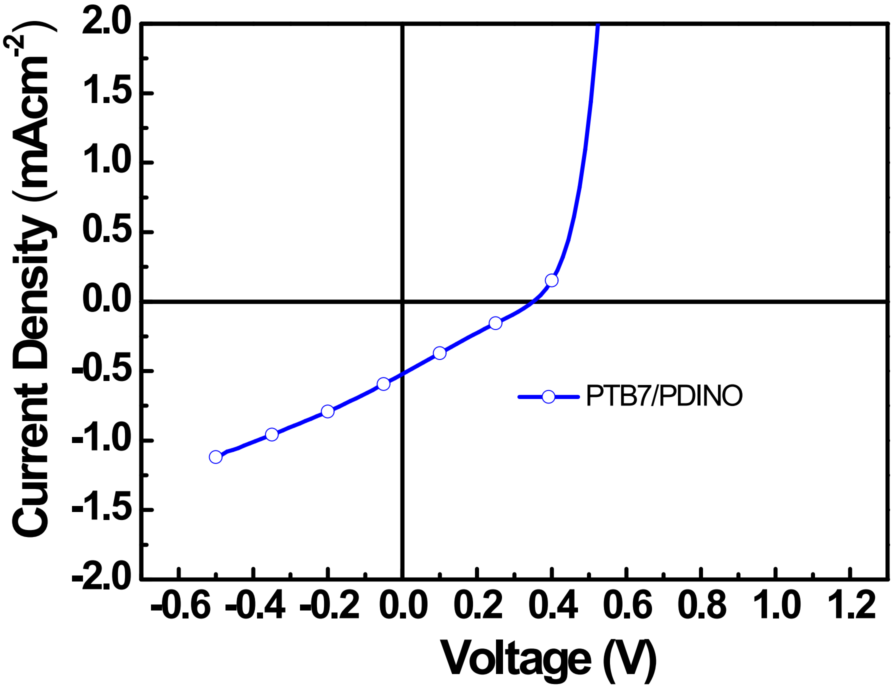
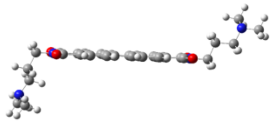
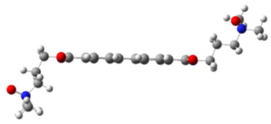
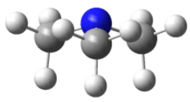
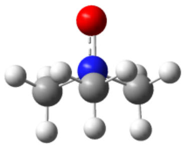


Figure S10. *J*-*V* curves of the PSCs based on PTB7/PDINO bilayer device with Al as cathode under the illumination of AM1.5G, 100 mW/cm^2.

Table S1.The Optimized geometry and the dipole moments obtained from DFT calculations on PDINO, PDIN, trimenthylamine and trimethylamine oxide at B3LYP/6-31G* level.[1]

Chemical Name	Optimized geometry	Dipole moment
PDIN		**1.0757**
PDINO		**7.2693**
Trimethylamine		**0.5806**
Trimethylamine Oxide		**4.3739**

For the two PDIs, they bear the same alkyl chains at the both side. Due to lower energy difference of the alkyl chain orientations, they are stochastic distribution in the solid films. So their symmetric orientation in solid film for a given molecule can't be guaranteed. Thus, dipole moment could be generated in case of an asymmetric orientation.

Reference

[1]. Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.