Electronic Supplementary Information for:

A simple perylene diimide derivative with the highly twisted geometry as electron acceptor for efficient organic solar cells

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Instrument

^{1}H NMR spectra were obtained on a Bruker Advance III 400 (400 MHz) nuclear magnetic resonance (NMR) spectroscope. UV-vis absorption spectra were recorded on a Shimadzu UV-2450 spectrophotometer. MALDI-TOF MS spectra were measured on a Walters Maldi Q-TOF Premier mass spectrometry. Elemental analysis was conducted on a Flash EA 1112 elemental analyzer. Thermogravimetric analysis (TGA) was carried out on a WCT-2 thermal balance under protection of nitrogen at a heating rate of 10 ^{o}C/min. Differential scanning calorimetry (DSC) was recorded on a Pekin-Elmer Pyris 1 differential scanning calorimeter. Cyclic voltammetry (CV) was done on a CHI600A electrochemical workstation with Pt disk, Pt plate, and standard calomel electrode (SCE) as working electrode, counter electrode, and reference electrode, respectively, in a 0.1 mol/L tetrabutylammoniumhexafluorophosphate (Bu_4NPF_6) CH_2Cl_2 solution. The CV curves were recorded versus the potential of SCE, which was calibrated by the ferrocene-ferrocenium (Fc/Fc^+) redox couple (4.8 eV below the vacuum level). Topographic images of the films were obtained on a VeecoMultiMode atomic force microscopy (AFM) in the tapping mode using an etched silicon cantilever at a nominal load of ~2 nN, and the scanning rate for a 10 μm×10 μm image size was 1.5 Hz.

Materials

All reagents and solvents, unless otherwise specified, were purchased from

Aladdin, Aldrich and J&K Scientific Ltd. and were used without further purification. **Br-PDI** and **3Bpin-B** were synthesized according to reported procedure.[1,2]

DFT calculation

Geometry optimizations were carried out by the density functional theory (DFT) method at the B3LYP/6-31G level. All the calculations were performed using Gaussian 03 program. All 7-tridecane substituents were replaced with methyl groups in calculations.

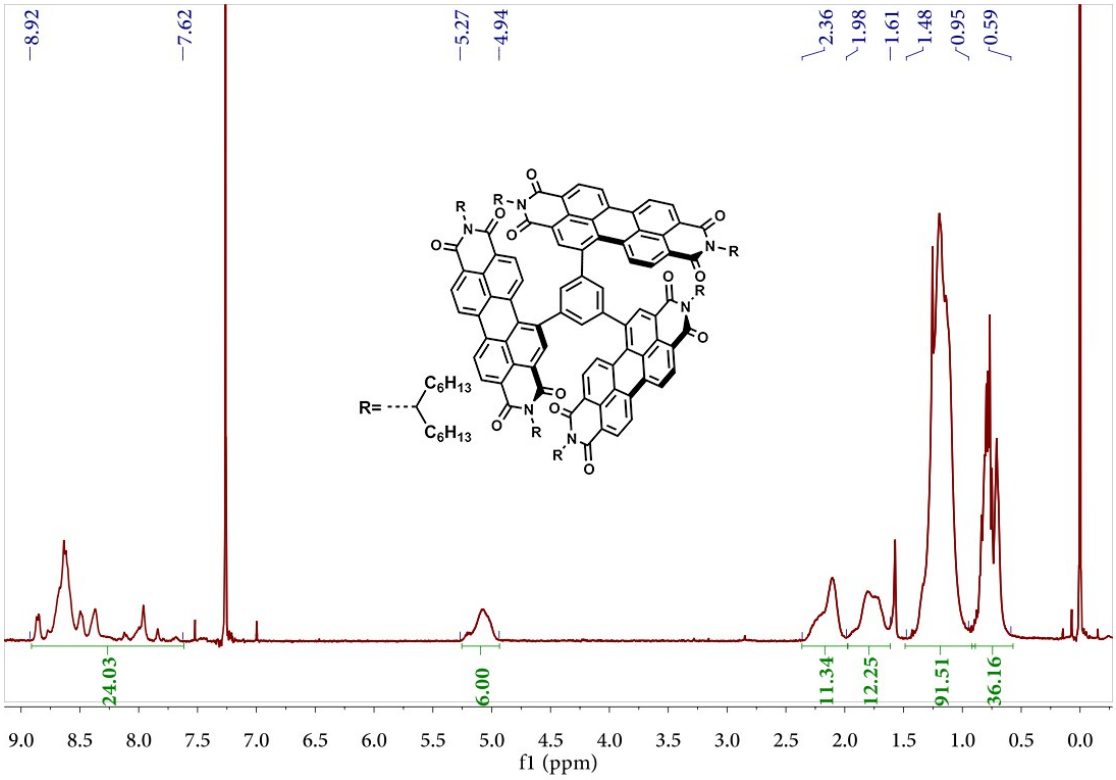

Fig. S1 ^{1}H NMR spectrum of $B(PDI)_3$ solution in $CDCl_3$.

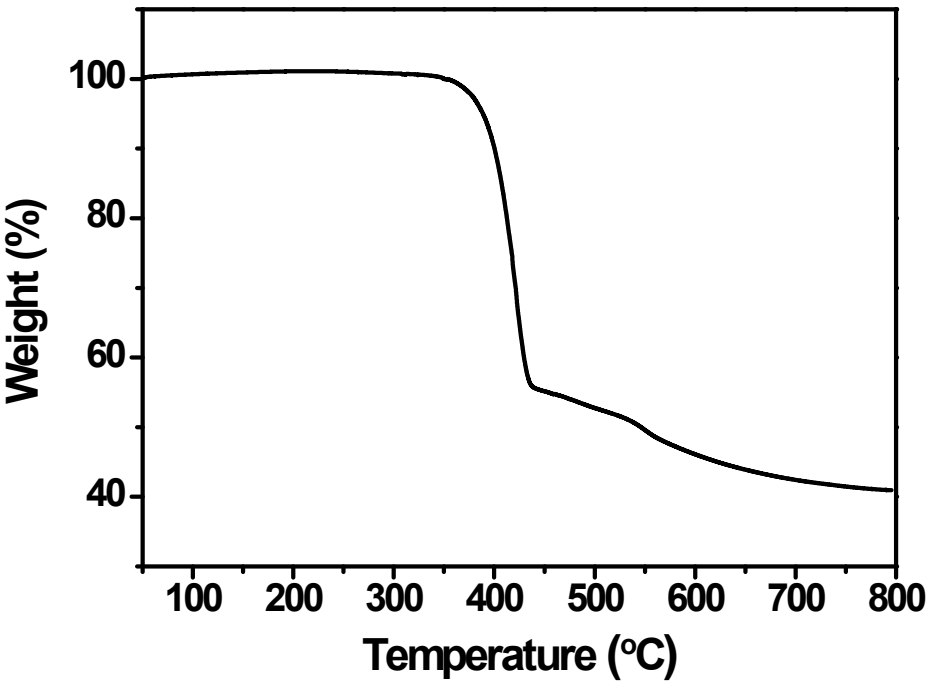

Fig. S2 TGA curve of $B(PDI)_3$.

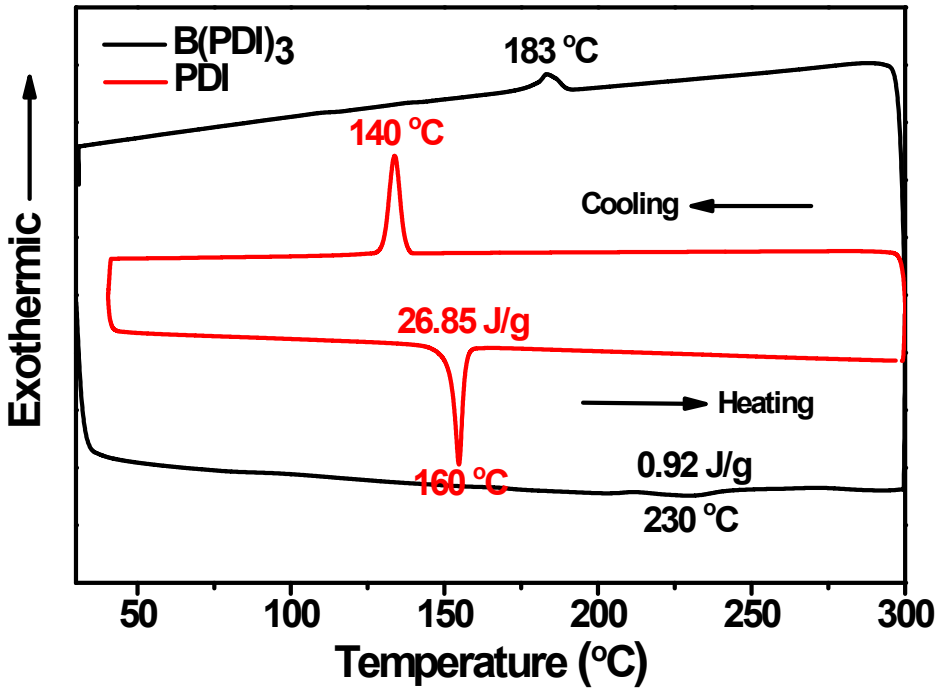

Fig. S3 DSC curves of $B(PDI)_3$ and PDI.

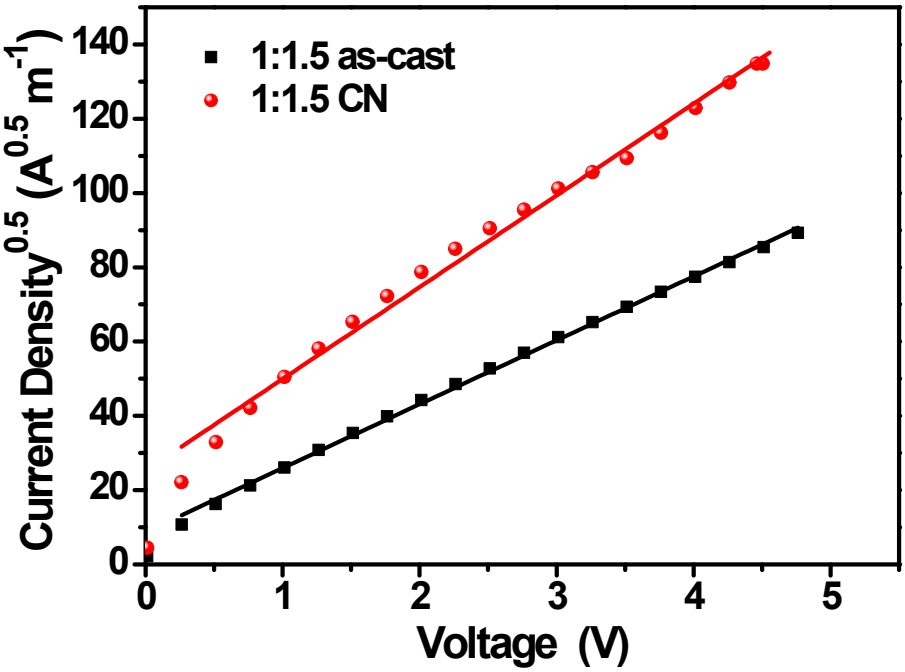

Fig. S4 $J^{0.5}$-V curves of the hole-only devices based on PTB7-Th:B(PDI)$_3$ films.

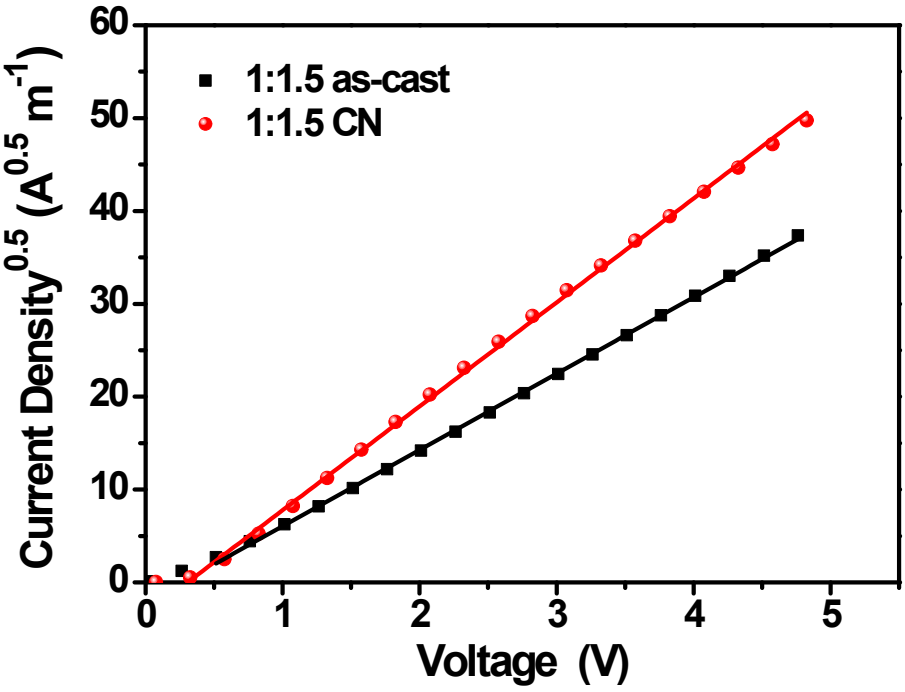

Fig. S5 $J^{0.5}$-V curves of the electron-only devices based on PTB7-Th:B(PDI)$_3$ films.

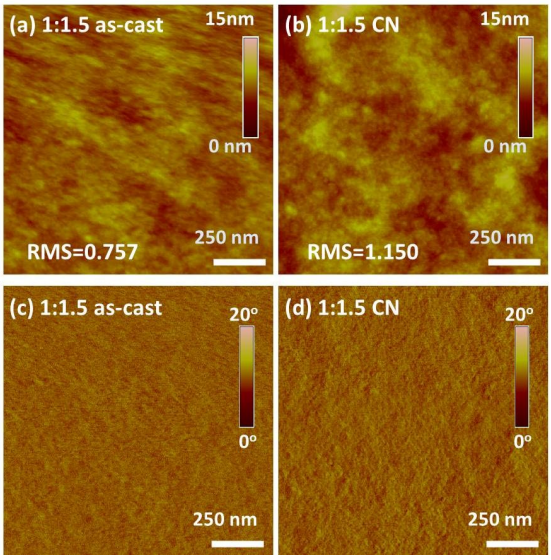

Fig. S6 AFM height images (a, b) and phase images (c, d) of 1:1.5 as-cast (a, c) and 1:1.5 CN (b, d) films.

References

1. J. Lee, R. Singh, D. H. Sin, H. G. Kim, K. C. Song and K. Cho, *Adv. Mater.*, 2016, **28**, 69-76.
2. B. Bao, L. Yuwen, X. Zhan and L. Wang, *J. Polym. Sci. Pol. Chem.*, 2010, **48**, 3431-3439.