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Supporting Information

Small molecules based N-phenyl Carbazole Substituted Diketopyrrolopyrroles as donor for solution processed bulk heterojunction organic solar cells

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Table of Contents……...……Page No.

General methods……..…S1

Fig. S1 Cyclic Voltammetry plots of **DPP5** and **DPP6**…….……S2

Table S1 Electrochemical properties of **DPP5** and **DPP6**…….……..S3

General methods

Device fabrication and characterization

Patterned indium tin oxide (ITO) coated glass substrates (8-10 Ω/cm2) were sequentially cleaned with detergent, deionized water, acetone isopropyl alcohol in ultrasonic baths, respectively. The cleaned ITO substrates were dried in a vacuum oven for 30 min. Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS, Clevios AI 4083) was spin coated onto to the ITO coated glass substrates at 3500 rpm for 30 s and then annealed at a temperature of 110° C for 10 minutes at ambient conditions. The mixers of donor (**DPP5** or **DPP6**) and $PC_{71}BM$ with different weight ratios were dissolved into chloroform at a concentration of 14 mg/mL. Then the blend solutions were spin coated onto the PEDOT:PSS/ITO substrates at 2000 rpm for 30 s to prepare the active layers and then dried for 30 minutes. For the solvent surface treatment, the binary solvent containing MeOH with small amount of CN was dropped onto the optimized active layers DPPs:$PC_{71}BM$ (1:2) surface for a 10 s wetting treatment and spinning at 3000 rpm for 30s and then dried for 40 min. The 100 nm aluminum (Al) cathode was deposited by thermal evaporation with a

shadow mask under the vacuum of $1x10^{-5}$ torr. The active area of the devices is about 20 mm^2 defined by the vertical overlap area between ITO and Al electrodes. All the measurements were done in ambient conditions with any encapsulation. The current–voltage (J–V) characteristic curves under AM 1.5G illumination at 100 mW/cm^2 and dark conditions were measured using a Keithley source meter semiconductor characterization system. The AM 1.5G illumination at 100 mW/cm^2 was provided by solar simulator. The hole-only devices with ITO/PEODT:PSS/active layer/Au were also fabricated in an analogous way, in order to measure the hole and electron mobilities. All the measurements were performed in the air without an encapsulation of the devices.

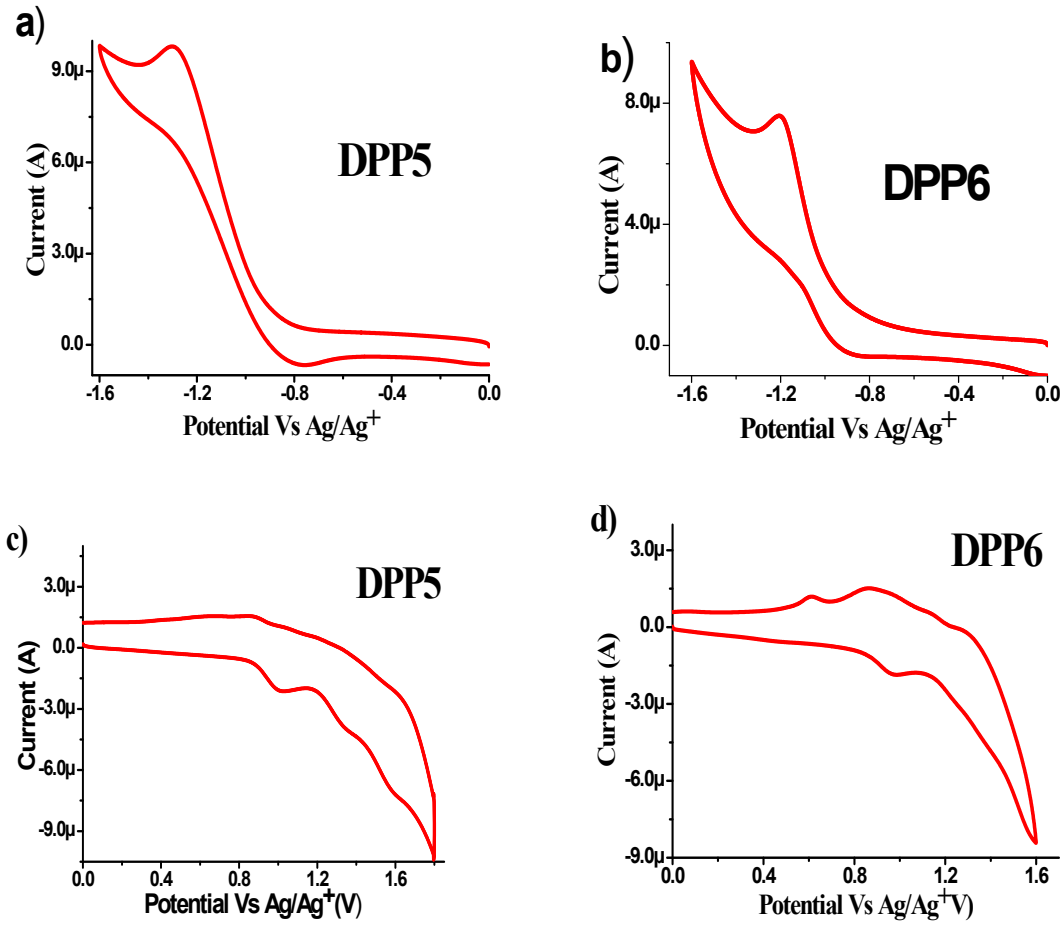

Fig. S1 Cyclic Voltammetry plots of reduction wave (a, b) and (c, d) oxidation wave of **DPP5** and **DPP6**.

Table S1 Electrochemical properties[a] of **DPP5** and **DPP6**.

Material	E^1_{Red} (V)	E^1_{Oxid} (V)	E^2_{Oxid} (V)	E_{LUMO} (eV)	E_{HOMO} (eV)
DPP5	-1.03	0.93	1.60	-3.64	-5.34
DPP6	-1.03	0.92	1.20	-3.60	-5.37

[a]The electrochemical analysis was performed in a 0.1 M solution of Bu_4NPF_6 in dichloromethane at 100 mVs^{-1} scan rate, versus Ag/Ag^+ at 25 °C.

E_{LUMO} =-(E_{red} -4.44), E_{HOMO}= (E_{oxd}+ 4.44)