Electronic Supplementary Information (ESI)

High performance polymer solar cell with a polar fullerene derivative as the cathode buffer layer

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1. Cyclic voltammetry (CV) measurement

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CV measurements of CPTA and PC₇₁BM: This measurement was taken in tetrahydrofuran (THF) solution. The LUMO level was calculated from the onset of reduction potential (assuming ferrocene/ferrocenium energy level is 4.8 eV below vacuum level). The ¹⁵ measured level of Fc/Fc⁺ was 0.52 V against Ag/Ag⁺. From the reduction curves, we could find that the onset reduction potential (versus Fc/Fc⁺) was 0.86 eV and 1.11 eV for CPTA and PC₇₁BM, respectively.



Fig. S1 Cyclic voltammograms of PC₇₁BM and CPTA in a tetrahydrofuran solution of 0.1mol/L Bu₄NPF₆.2. UV-Visible spectra



Fig. S2 UV-Visible spectra of PC71BM and CPTA in tetrahydrofuran solution.

5 3. Device fabrication

The ITO glass was cleaned by sequential ultrasonic treatment in detergent, deionized water, acetone and isopropanol for 15 minutes each. Then, the pre-cleaned ITO glass was moved into an ultraviolet chamber for UV-ozone treatment of 20 minutes. Next, PEDOT:PSS (Clevios PAI4083) aqueous solution was filtered through 0.45 µm PTFE filter and spin-coated at 4000rpm for 60s on the ITO substrate. Then the PEDOT coated ITO was heated on a hot plate in air at 140 °C for 10min. Next, the ITO substrate was moved into glove box

¹⁰ Then the PEDOT coated ITO was heated on a hot plate in air at 140 °C for 10min. Next, the ITO substrate was moved into glove box filled with Ar atmosphere and photoactive materials were spin-coated at 2000rpm for 120s. The PTB7, PC₇₁BM and CPTA were purchased from 1-Material Chemscitech Inc. (Canada), American Dye Source, Inc. (USA) and Sigma-aldrich, respectively and used as received. The solution consisted of 10mg PTB7 and 15mg PC₇₁BM in 1mL mixed solvent of chlorobenzene/1,8 diiodoctane (97/3 by volume). Then the substrate was put in vacuum for 20min to make the solvent volatilization. At last, the CPTA in methanol solution 15 (0.5mg/mL) was spin-coated on the photoactive films at 5000rpm for 60s to form a ~5nm film. Then, the substrate was put in vacuum

again for 25min to exclude the effect of methanol as possible as we can. Finally, 100nm Al was evaporated (deposition rate of 1.0 Å/s) on the films in vacuum chamber (10^{-6} mbar). The device area was 4 mm².

4. Device characterization

²⁰ The J-V measurement was conducted using Keithley 2440 sourcemeter controlled by computer. And the characterization was taken in glove box under a simulated AM 1.5G spectrum (100mW/cm²) with an Oriel So13A solar simulator. The EQE measurement was done using Newport quantum efficiency measurement system (ORIEL IQE 200TM) combined with a lock-in amplifier and 150 W xenon lamp. The light intensity at each wavelength was calibrated by one standard Si/Ge solar cell. Notably, the EQE was done in ambient atmosphere at room temperature.