

Supporting Information

Planar heterojunctions for reduced non-radiative open-circuit voltage loss and enhanced stability of organic solar cells

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Methods

Organic solar cells fabrication and characterization

Devices were fabricated with the inverted structure of indium-tin-oxide (ITO)/ZnO/active layer/MoO₃/Ag. ITO substrates (sheet resistance < 15 Ω sq⁻¹) were cleaned in deionized water, acetone, and isopropanol by sonication 3 times (each time for 15 min) subsequently. The clean ITO substrate was pretreated with UV-ozone for 15 mins. The sol-gel film of ZnO interlayer was fabricated by spin-coating of precursor solution onto ITO glass substrates at 4000 rpm for 30 s, and subsequently dried at 200 °C for 30 min in air. The precursor solution was prepared by dissolving 100 mg Zn(CH₃COO)₂ · 2H₂O and 28.29 mL ethanolamine in 973 mL 2-methoxyethanol and then stirred overnight. For devices with PHJ configuration, the Y6 solution (6 mg mL⁻¹ in chloroform) was spin-coated at 2000 rpm for 30 s on the top of ZnO film in nitrogen glove box with thickness of 35 nm. After that, donor materials (Rub and DTDCTB) were deposited through thermal evaporation method under vacuum (*ca.* 10⁻⁵ Pa) on the top of Y6 film at deposition rate of 0.1 nm s⁻¹ with thickness of 35 nm. Finally, the MoO₃ (3 nm), and a top Ag electrode (100 nm) were sequentially deposited under vacuum (*ca.* 10⁻⁵ Pa). For devices with BHJ configuration, mixture of Rub:Y6 or DTDCTB:Y6 were dissolved in chloroform (1:1, w/w, totally 12 mg mL⁻¹) then spin-coated onto ZnO layer through at 2000 rpm for 30 s in nitrogen glove box. The active area of the cells was 0.040 cm².

The *J-V* curves of all devices were employed using an AAA solar simulator (XES-70S1, SAN-EI Electric Co., Ltd) under illumination (AM1.5G, 100 mW cm⁻²) and calibrated with a standard photovoltaic cell equipped with a KG5 filter (certificated by the National Institute of Metrology) and a Keithley 2450 source-measure unit. The thickness of the film was measured *via* the Bruker Dektak-

XT.

Measurements

The UV-vis absorption spectra were recorded on a UH4150 Spectrophotometer and film was fabricated with the same methods of active layers in solar cell devices. Electroluminescence quantum efficiency (EQE_{EL}) and electroluminescence (EL) measurements were performed by an integrated system (REPS, Enli Technology Co., Ltd.). Fourier-transform photocurrent spectroscopy external quantum efficiency (FTPS-EQE) were obtained on an integrated system (PECT-600, Enli Technology Co., Ltd.), where the photocurrent was amplified and modulated by a lock-in instrument. Trap density of states (tDOS) were performed on Keysight 4980A.

Stability test

For photo-stability test, OSCs were encapsulated in nitrogen atmosphere with a transparent encapsulation glass, fixed by UV-curing adhesives. Then the devices were placed under the LED with power of 100 mW cm^{-2} calibrated with an irradiatometer (OHSP-350S, Hangzhou HOPOO Light&Color technology Co., Ltd). The test temperature was the environmental temperature. The photovoltaic parameters were recorded by Keithley 2400 source meter.

Additional Figures

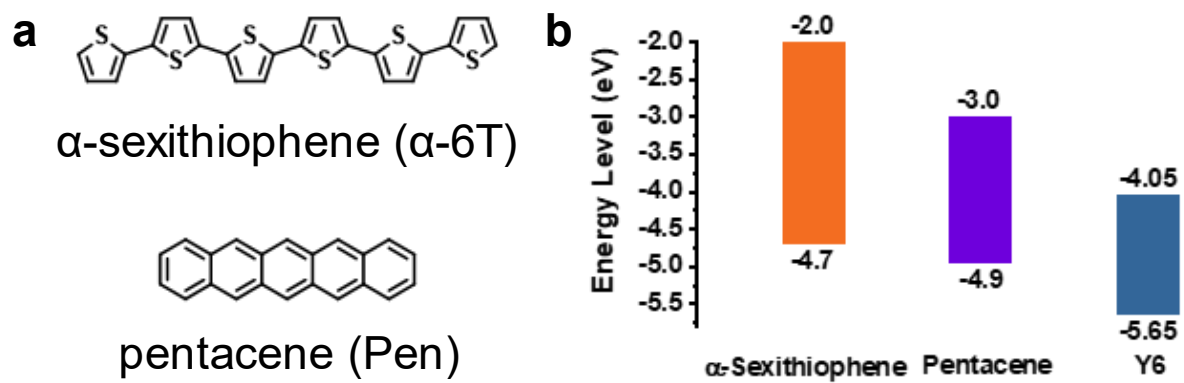


Fig. S1 (a) The chemical structures of pentacene (Pen) and α -sexithiophene (α -6T), (b) The energy level diagram of α -6T, Pen, and Y6.

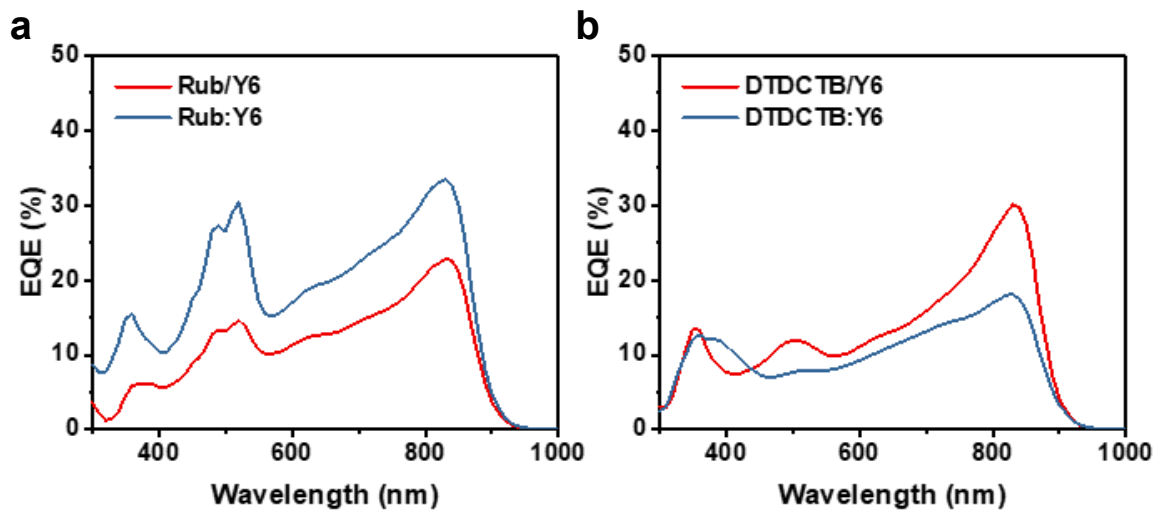


Fig. S2 The external quantum efficiency (EQE) spectra for (a) Rub and (b) DTDC TB based devices with PHJ and BHJ configurations.

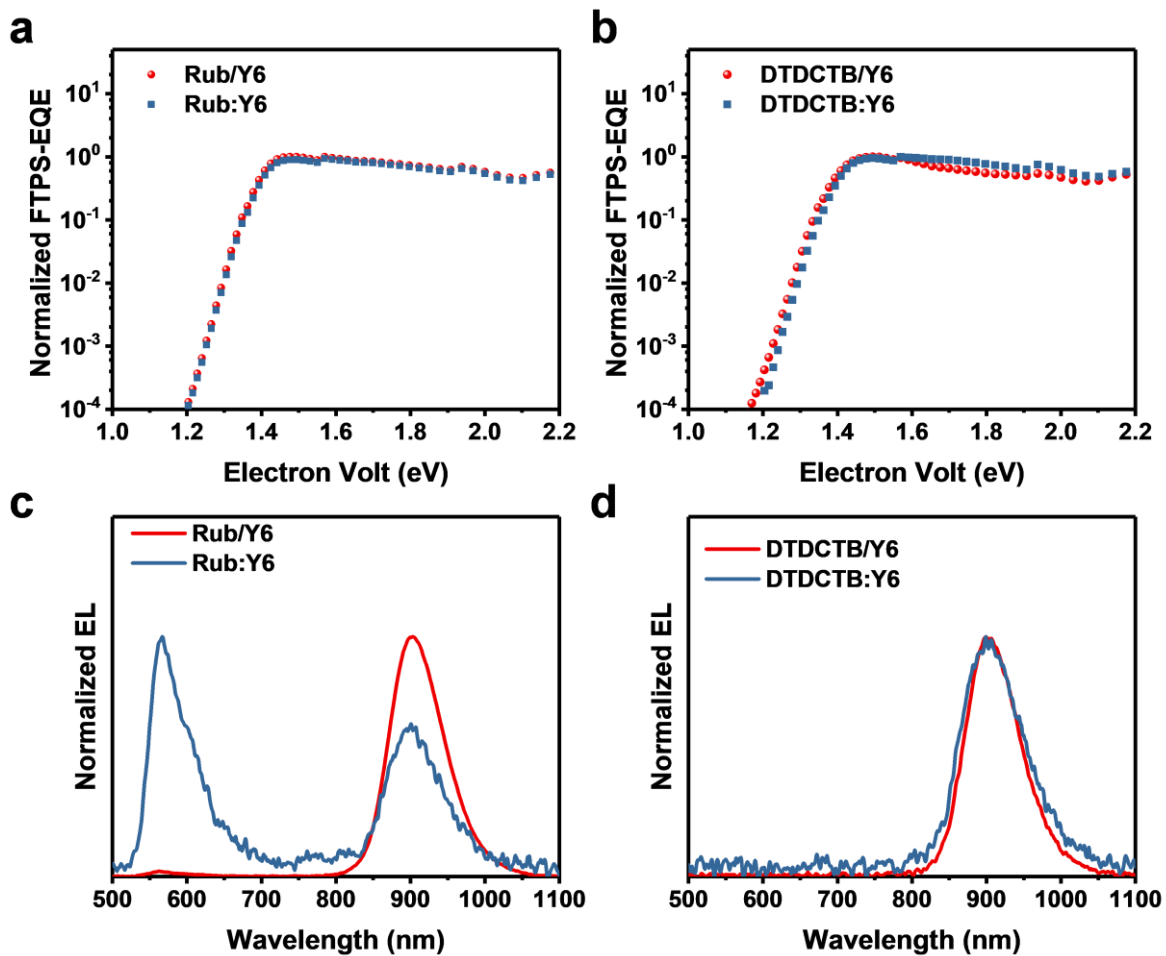


Fig. S3 FTPS-EQE of (a) Rub-based devices and (b) DTDCTB-based devices with different configurations at the absorption onset. Normalized EL spectra of (c) Rub-based devices and (d) DTDCTB-based devices with different configurations.

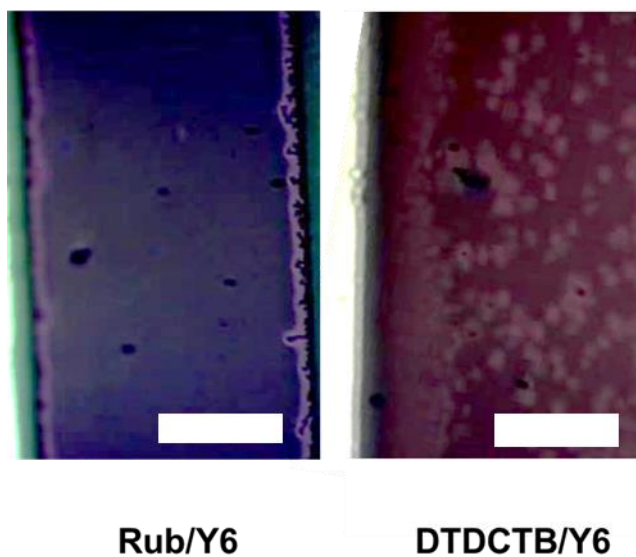


Fig. S4 The photographs of the PHJ devices based on Rub and DTDCTB after 200 hours irradiation.

Scale bar: 1 mm.