

Electronic Supplementary Information (ESI)

A Highly Crystalline Non-fused Ring Small Molecule Acceptor As Third Component Significantly To Enhance the Efficiency of All- Polymer Solar Cells

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1. Materials and Instruments.

The nonfused ring small molecule receptor DFTQA-2FIC was prepared according to the reaction steps described in the reference. All reagents and chemicals were purchased commercially and used directly without further purification unless otherwise stated. Unless otherwise stated, all reactions were carried out under inert atmosphere using standard Schlenk-line techniques. UV-vis absorption spectra of polymer solutions and films were recorded on a Shimadzu HP-453 UV spectrophotometer. The external quantum efficiency (EQE) spectra of solar cells were recorded by a QE-R3011 measurement system (Enli Technology, Inc.). AFM measurements were obtained by using a Dimension Icon AFM (Bruker) in a tapping mode ($5 \times 5 \mu\text{m}^2$). The electron and hole mobility were measured by using the method of space-charge limited current (SCLC) for electron-only devices with the structure of ITO/ZnO/active layer/PNDIT-F3N/Ag and hole-only devices with the structure of ITO/PEDOT:PSS/active layer/MoO₃/Ag. The charge carrier mobility was determined by fitting the dark current to the model of a single carrier SCLC according to the equation: $J = 9\varepsilon_0\varepsilon_r\mu V^2/8d^3$, where J is the current density, d is the film thickness of the active layer, μ is the charge carrier mobility, ε_r is the relative dielectric constant of the transport medium, and ε_0 is the permittivity of free space. $V = V_{\text{app}} - V_{\text{bi}}$, where V_{app} is the applied voltage, V_{bi} is the offset voltage. The carrier mobility can be calculated from the slope of the $J^{1/2} \sim V$ curves.

2. Fabrication of organic solar cells

Solar cells were fabricated in a conventional device configuration of ITO/PEDOT:PSS(40 nm)/PBDB-T: N2200 or PBDB-T:N2200: DFTQA-2FIC/PFN-Br

(5 nm)/Ag(100 nm). The ITO substrates were first scrubbed by detergent and then solicited with deionized water, acetone and isopropanol subsequently, and dried overnight in an oven. The glass substrates were treated by UV-Ozone for 30 min before used. PEDOT:PSS (Heraeus Clevios P VP AI 4083) was spin-cast onto the ITO substrates at 4000 rpm for 30 s, and then dried at 150 °C for 15 min in air. The donor:acceptors blends (1.0:10 weight ratio) were dissolved in chloroform (the total concentration of blend solutions was 16 mg mL⁻¹), the mixture was stirred on a 50°C stirring heating table for 60 min at room temperature for 6 h in a nitrogen-filled glove box. The blend solution was spin-cast at 3250 rpm for 30 s. A thin PFN-Br layer was coated on the active layer, followed by the deposition of Ag (100 nm) (evaporated under 5×10⁻⁵ Pa through a shadow mask). The optimal active layer thickness measured by a Bruker Dektak XT stylus profilometer was about 105 nm. The current density-voltage (*J-V*) curves of all encapsulated devices were measured using a Keithley 2400 Source Meter in air under AM 1.5G (100 mW cm⁻²) using a Newport solar simulator. The light intensity was calibrated using a standard Si diode (with KG5 filter, purchased from PV Measurement to bring spectral mismatch to unity). Optical microscope (Olympus BX51) was used to define the device area (6.0 mm²). EQEs were measured using an Enlitech QE-S EQE system equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

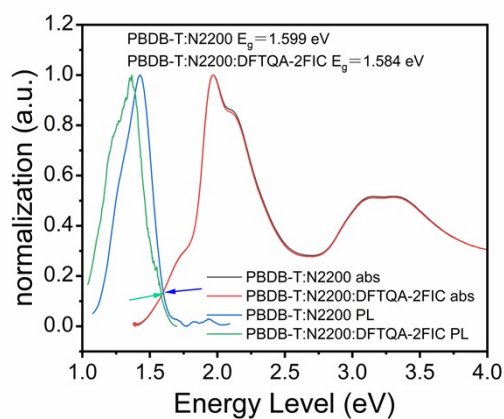


Fig.S1. E_g is determined at the intersection between absorbance and emission.

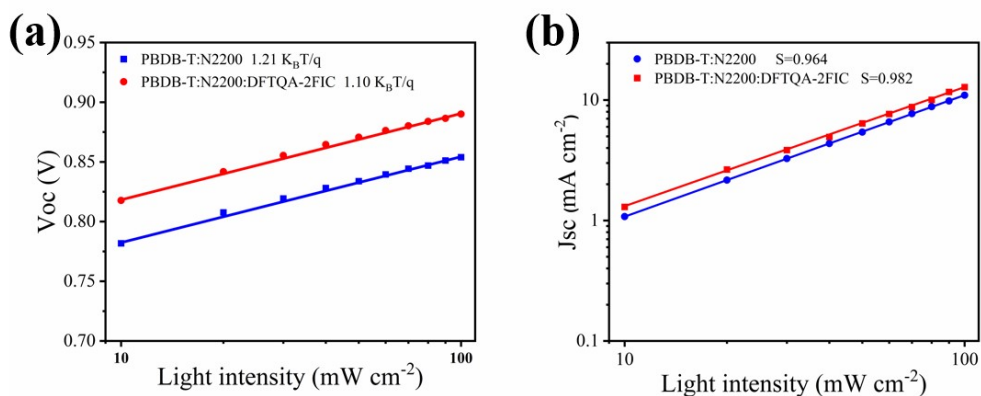


Fig.S2. (a) J_{SC} -Plight and (b) V_{OC} -Plight fitting lines.

Table S1. Photovoltaic parameters of the PSCs.

D:A1:A2	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
2:1:0%	0.86	10.98	68.32	6.45
2:1:2%	0.89	12.81	70.77	8.07
2:1:5%	0.89	11.87	72.99	7.68
2:1:8%	0.88	11.99	69.69	7.33

^aD:A1:A2=PBDB-T:N2200:DFTQA-2FIC. ^b Max PCE are obtained from 15 devices.