Supplementary data

Efficient Solution Processed Bulk-Heterojunction Solar Cells Based a Donor-Acceptor Oligothiophene

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Hole mobility measurement

Hole mobility was measured according to a similar method described in the literature, using a diode configuration of ITO/PEDOT:PSS/DCN7T/Al by taking current-voltage current in the range of 0-6 V and fitting the results to a space charge limited form, where the SCLC is described by

$$J = 9\varepsilon_0 \varepsilon_r \mu_h V^2 / 8L^3$$

where *J* is the current density, *L* is the film thickness of active layer, μ_h is the hole mobility, ε_r is the relative dielectric constant of the transport medium, ε_0 is the permittivity of free space (8.85 × 10⁻¹² F/m), *V* is the internal voltage in the device and $V = V_{appl} - V_r - V_{bi}$, where V_{appl} is the applied voltage to the device, V_r is the voltage drop due to contact resistance and series resistance across the electrodes, and V_{bi} is the built-in voltage due to the relative work function difference of the two electrodes. The V_{bi} can be determined from the transition between the Ohmic region and the SCLC region and was found to be about 1.2 V.

Device fabrication

The photovoltaic device was fabricated by use of a common process. The ITO-coated glass substrates were cleaned by ultrasonic treatment in detergent, deionized water, isopropyl alcohol, and acetone under ultrasonication for 20 minutes each and subsequently dried in oven for 12 hours. A thin layer of PEDOT:PSS (Baytron PH 500) was spin-coated (4000 rpm, ca. 40nm thick) onto ITO surface. After being baked at 120 °C for 20 min, the active layer was then spin-cast from a varied weight-to-weight (1:1, 1:1.4, 1:1.8, w/w) mixture of DCN7T (8 mg mL⁻¹) and PCBM solution in chloroform at 500 rpm for 3 sec. and at 1300 rpm. for 9 sec on the ITO/PEDOT:PSS substrate without further special treatments. The active layer thickness was measured as ca. 110nm using a profilometer (Dektak 6M Stylus Profiler). After the film was transferred into a nitrogen filled glove box (< 0.1 ppm O² & H₂O), 1 nm LiF layer and 70nm Al layer were deposited in sequence on the active layer. The effective area of each cell is ~ 9 mm².

Current-Voltage measurement

All current–voltage (*J-V*) characteristics of the photovoltaic devices were measured in air using a Keithley SMU 2400 unit. A Xenon lamp with a filter (broadpasss GRB-3, Beijing Changtuo Scientific limited company) to simulate AM1.5G conditions was used as the excitation source with a power of 100 mW cm⁻² white light illumination from the ITO side. Light source illumination intensity was measured using a calibrated broadband optical power meter (FZ-A, wave length range 400-1000 nm, Photoelectric Instrument Co, Beijing Normal University, China). The fabrication and measurement are conducted in air at room temperature. The calculation of the power conversion efficiency, η , has been performed using the following equation:

$$\eta = V_{oc} J_{sc} FF/P_{in}$$

where V_{oc} , J_{sc} , FF, and P_{in} are the open circuit voltage, the short circuit current density, the fill factor and the incident light power, respectively. The fill factor FF is determined according to $FF = (V_m J_m)/(V_{oc} J_{sc})$, where V_m and J_m are the voltage and the current density in the maximum power point of the J-V curve in the fourth quadrant.

Supplementary Figures

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Fig. S1. Fluorescence emission spectra of DCN7T(0.16 mg ml⁻¹)/PCBM with different blend ratios (w/w) in CHCl3 ($\lambda_{ex} = 467$ nm).



Fig. S2. AFM topography image($5\mu m \times 5\mu m$) of film cast from chloroform solution of DCN7T (3D image)



Fig. S3. AFM topography image (5 μ m × 5 μ m) of film cast from chloroform solution of the blend of DCN7T/PCBM with the ratio of 1:1 (w/w) (3D image).



Fig. S4. AFM topography image (5 μ m × 5 μ m) of film cast from chloroform solution of the blend of DCN7T/PCBM with the ratio of 1:1.4 (w/w) (3D image).



Fig. S5. AFM topography image (5 μ m × 5 μ m) of film cast from chloroform solution of the blend of DCN7T/PCBM with the ratio of 1:1.8 (w/w) (3D image).



Fig. S6. AFM phase images (5 μ m × 5 μ m) of films cast from chloroform solutions of the blend of DCN7T/PCBM with the following ratios (w/w): (a) 1:0, (b) 1:1, (c) 1:1.4, and (d) 1:1.8.