Supplementary Materials

Effect of Dihydronaphthyl-based C60 Bisadduct as Third Component Materials on the Photovoltaic Performance and Charge Carrier Recombination of Binary PBDB-T:ITIC Polymer Solar Cells

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2. Experimental details

ITIC and PBDB-T were purchased from Solarmer Materials and Luminescence Technology Co respectively; chlorobenzene (CB, anhydrous, 99%) was purchased from Sigma-Aldrich Co. MoO_3, and Ag were purchased from Alfa Aesar Co. The ZnO nanoparticles were synthesized following the Pacholski method [1]. The 40 mg blend of PBDB-T and acceptor materials (1:1, wt%) were dissolved in 2 ml chlorobenzene solution and add 2 wt% 1,8-diiodooctane (DIO) of chlorobenzene solution. The blend PBDB-T:acceptor solution were stirred at 40 ˚C for 5 hours.

The indium tin oxide (ITO) glasses (sheet resistance is ~12 Ω / W) were pre-cleaned by ultrasonic bath and UV ozone treat in a plasma asher (100 W, 20 min). A thin layer (20 nm) of ZnO was spin-coated onto the ITO glass and baked at 150 ^{O}C for 20 min in air. A blend solution of PBDB-T:NCBA:ITIC (10 mg mL^{-1} for PBDB-T, 10 mg mL^{-1} for alloy acceptor materials) was spin-coated on the ZnO layer to form an photoactive layer and annealing treatment were carried out in a N_2-filled glove box. A MoO_3 (ca.25 nm) and Ag electrode (ca. 150 nm) were evaporated under vacuum (ca. 10^{-5} Pa) through a shadow mask to define the active area of the devices (3×3 mm^2). The current density versus voltage (*J–V*) characteristics of PSCs were performed in a glove box with a computer-controlled Keithley 236 Source Measure Unit under illumination at 100 mW cm^{-2} using an AM1.5 G solar simulator. The external quantum efficiency (*EQE*) spectrum was measured with the Stanford Research Systems model SR830 DSP lock-in amplifier coupled with a WDG3 monochromator and a 500 W xenon lamp.

The charge carrier mobility in the photoactive layers may be optimized by partial ITIC replacement by NCBA. The space-charge-limited-current (SCLC) method is used to evaluate the charge carrier mobility dependent on NCBA concentration. Hole-only and electron-only SCLC devices were thus fabricated with structures of ITO/PEDOT:PSS/PBDB-T:NCBA:ITIC/MoO_3/Au and Al/PBDB-T:NCBA:ITIC/Al, respectively. The charge carrier mobilities were calculated using the equation [2, 3]

$$J = \frac{9}{8}\varepsilon_r\varepsilon_0\mu\frac{V^2}{d^3},$$

where J is the current density, μ the charge carrier mobility, ε_0 and ε_r the permittivity of free space and relative permittivity of the material (ε_r was assumed to be 3), respectively, and V and L are, respectively, the SCLC effective voltage and the distance between the anode and cathode.

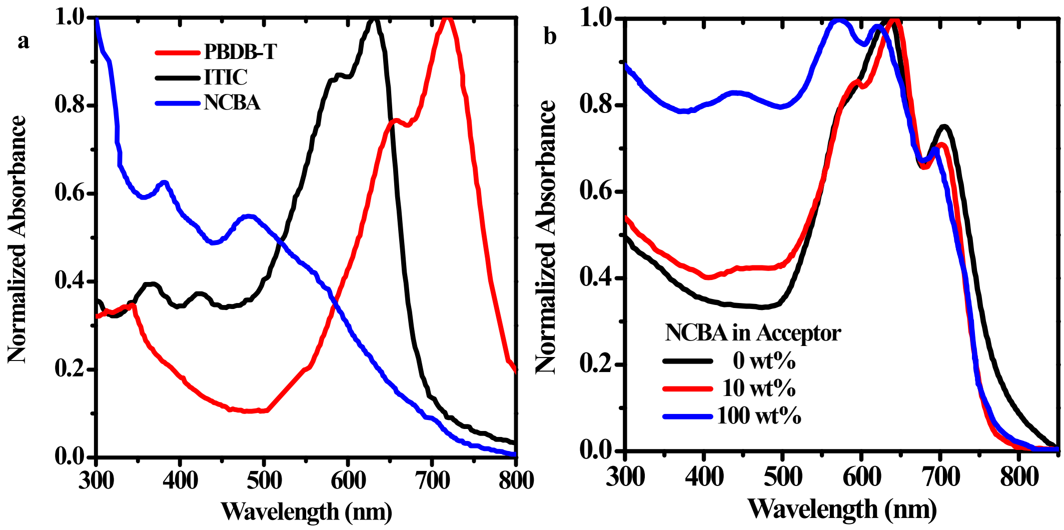

Figure S1. (a) Normalized absorption spectra of neat PBDB-T, NCBA and ITIC layer. (b) Absorption spectra of binary layer of PBDB-T:ITIC and PBDB-T:NCBA and ternary blend layer of PBDB-T:NCBA: ITIC (1:0.1:0.9).

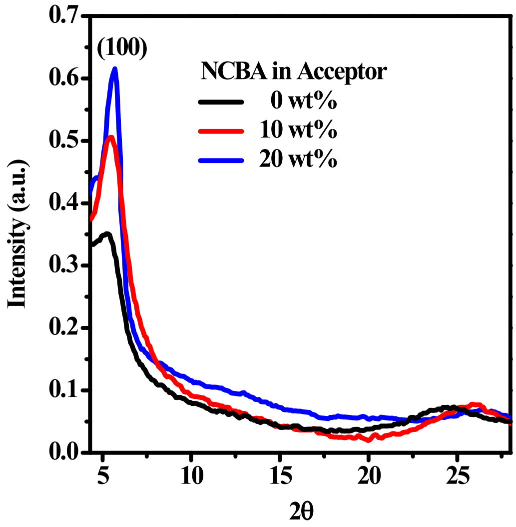

Figure S2. XRD curve of ternary blend layer with different NCBA concentration.

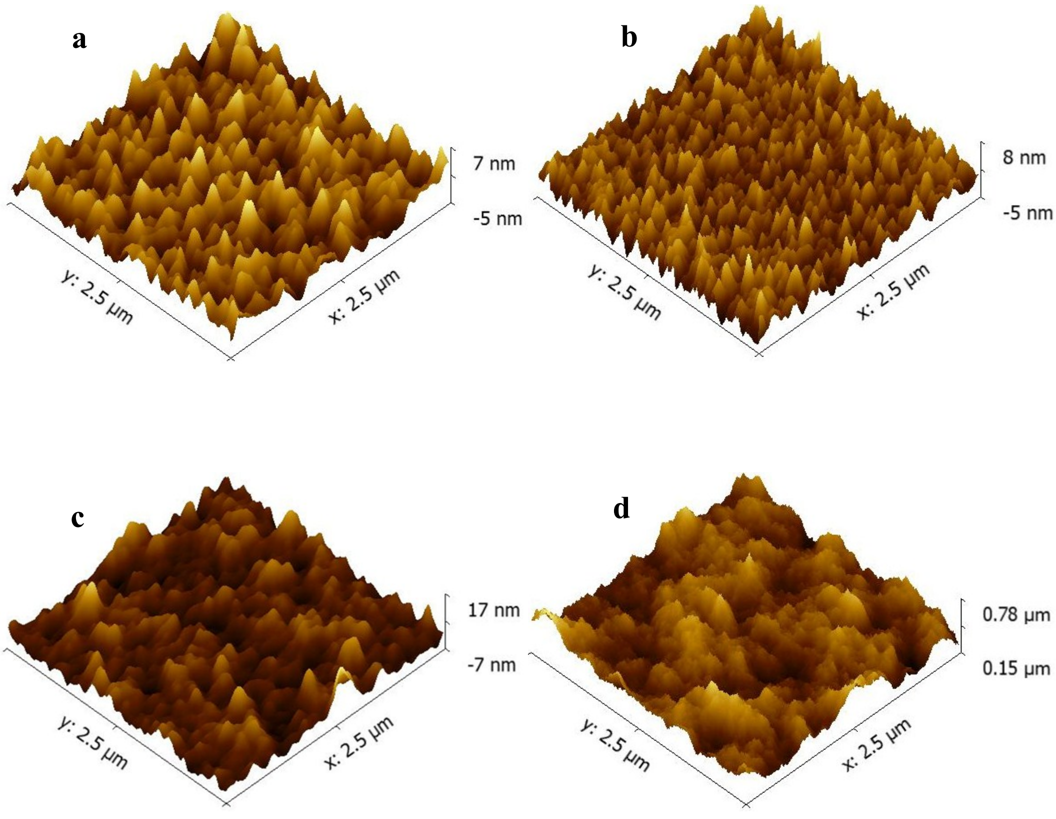

Figure S3. 3D view AFM image of binary PBDB-T:ITIC, ternary PBDB-T:NCBA:ITIC thin films with 10 wt% and 20 wt% NCBA concentration and binary PBDB-T:NCBA thin films corresponding to figure a-d respectively.

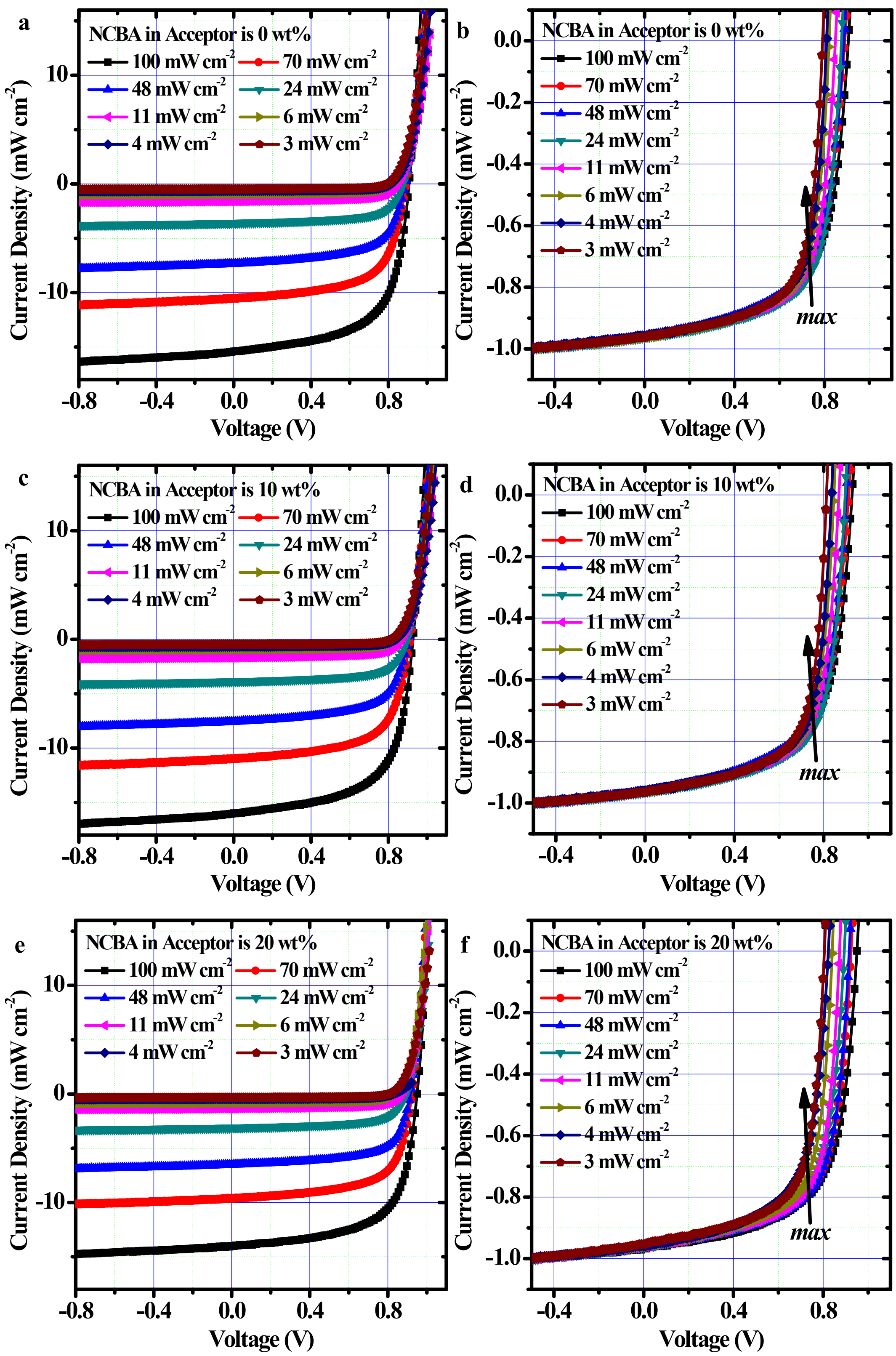

Figure S4. (a, c and e) Current-voltage characteristics of the binary PBDB-T:ITIC and ternary PBDB-T:NCBA:ITIC (1:0.1:0.9) and PBDB-T:NCBA:ITIC (1:0.2:0.8)-based PSCs as a function of incident light intensity; (b, d and f) charge collection probability:

photocurrents measured for the various intensities in a have been normalized with the photocurrent at -0.5 V.

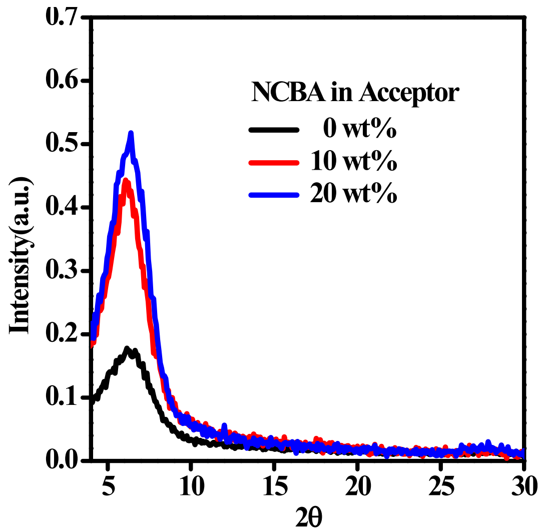

Figure S5. XRD curve of ternary blend thin films with different NCBA concentration under 10 h and 90 ^{O}C of thermal annealing treatment.

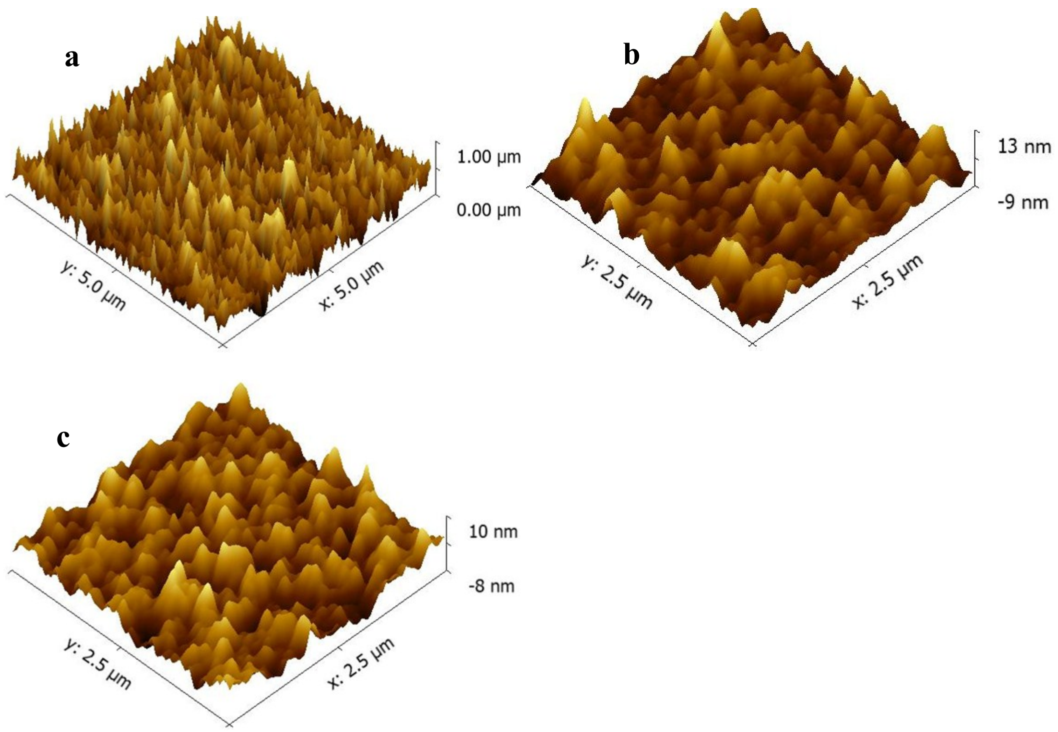

Figure S6. 3D view AFM image of binary PBDB-T:ITIC, ternary PBDB-T:NCBA:ITIC (1:0.1:0.9) and PBDB-T:NCBA:ITIC (1:0.2:0.8) thin films under 10 h and 90 ^{O}C of thermal annealing treatment corresponding to figure a-c respectively.

Reference:

1. S. B. Dkhil, D. Duché, M. Gaceur, A. K. Thakur, F. B. Aboura, L. Escoubas, J.-J. Simon, A. Guerrero, J. Bisquert, G. Garcia-Belmonte, Q. Bao, M. Fahlman, C. Videlot-Ackermann, O. Margeat and J. Ackermann, *Advanced Energy Materials*, 2014, n/a-n/a.
2. H.-W. Li, Z. Guan, Y. Cheng, T. Lui, Q. Yang, C.-S. Lee, S. Chen and S.-W. Tsang, *Advanced Electronic Materials*, 2016, **2**, 1600200-1600209.
3. V. Narasimhan, D. Jiang and S.-Y. Park, *Applied Energy*, 2016, **162**, 450-459.