Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting information

14.7% all-small- molecule organic solar cells enabled with a Fullerene derivative incorporation

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1. Experimental section

1.1. Materials source

BTR-Cl was prepared methods of our reported literature [1]. All reagents and solvents of material preparation, unless otherwise specified, were purchased from Energy Chemical, Tansoole, Suna Tech, Aldrich, Sinopharm Chemical Reagent (OurChem) and JiangSu GE-Chem Biotech., Ltd. All materials of device fabrication were purchased from commercial suppliers: ITO (Youxuan Tech.), PEDOT:PSS (Clevios PVP AI. 4083 (Heraeus)), Y6 (Derthon Ltd.), Phen-NaDPO (One Material Ltd.), Chloroform (Sinopharm Chemical Reagent Co., Ltd.), Isopropyl alcohol (Chongqing Chuandong Chemical Co., Ltd.) and Ag (ZNXC Ltd.). And all reagents and solvents are used directly without further purification.

1.2. Thin-film characterizations

Ultraviolet−visible light (UV-vis) absorption spectra were recorded on a Perkin Elmer Lambda 365 spectrophotometer. Topographic images of the films were obtained on a Bruker atomic force microscopy (AFM) with the type of dimension edge with Scan Asyst^{TM} in the tapping mode using an etched silicon cantilever at a nominal load of ~2nN, and the scanning rate for a 10 μm×10 μm image size was 1.5 Hz.

1.3. Device fabrication and testing

ITO coated glass substrates were cleaned with detergent water, deionized water, acetone and isopropyl alcohol in an ultrasonic bath sequentially for 30 min, and further treated with UV exposure for 30 min in a UV-ozone chamber. A thin layer (ca. 30 nm) of PEDOT:PSS was first spin-coated on the substrates with 4000 rpm and baked at 120 °C for 10 min under ambient conditions. The substrates were then transferred into a nitrogen-filled glove box. The optimized concentration was 18 mg·mL^{-1} chloroform solution with BTR-Cl:Y6:ICBA ratio of 1.8:1:0.15 (w/w). After spin coating, the blend films were treated with chloroform solvent for 30 s and annealed at 120 °C for 5 mins. The active layer thickness was around 120 nm. Then Phen-NaDPO as the electron transporting layer was spin-coated on the active layer by 2000 rpm from isopropyl alcohol solution. Finally, 100 nm of Ag electrodes evaporated at 0.5 Å/s during the former 100 Å period and then evaporated at 2 Å s^{-1}, pressure of less than 2×10^{-4} Pa.

The current density–voltage (*J–V*) curves of OSCs were tested in air atmosphere by a Keithley 2400 source meter and an AAA grade solar simulator (Sirius-SS150A-D, Zolix Ltd.) along with AM 1.5 G spectra whose intensity was corrected by a certified standard silicon solar cell (Certificate No.: GXtc2017-1280, NIM) at 1000 $W \cdot m^{-2}$. The J-V curves are measured in the forward direction from 0.2 to 1.2 V. The external quantum efficiency (EQE) was measured by a certified incident photon to electron conversion (IPCE) equipment (QE-R) from Enli Technology Co., Ltd.

1.4. Carrier mobility measurement

The carrier mobility (hole and electron mobility) of photoactive active layer was obtained by fitting the dark current of hole/electron-only diodes to the space-charge-limited current (SCLC) model. Hole-only diode configuration: Glass/ITO/PEDOT:PSS/active layer/MoO_3/Ag; here, V_{bi}=0 V (flat band pattern formed by PEDOT:PSS-MoO_3). Electron-only diode configuration: Glass/ITO/ZnO/phen-NaDPO/active layer/phen-NaDPO/Ag; here, V_{bi}=0.5V was used following the protocol reported.[1] The active layer thickness was determined by a Tencor surface profilometer. The electric-field dependent SCLC mobility was estimated using the following equation [2] :

$$J(V) = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_0 exp\left(0.89\beta\sqrt{\frac{V - V_{bi}}{L}}\right)\frac{(V - V_{bi})^2}{L^3}$$

1.5. TPC and TPV measurements

Transient photocurrent (TPC) measurements were tested under the short-circuit condition to explore the time-dependent extraction of photo generated charge carriers. The 10 ns light plus laser was selected as the light source. The devices are otherwise kept in the dark between pulses in order to avoid any influence of pulse frequency on the current responses. Transient photovoltage (TPV) were tested under the open-circuit condition to explore the photovoltage decay. The subsequent voltage decay is then recorded to directly monitor non-geminate charge carrier recombination. The photovoltage decay kinetics of all devices follow a mono-exponential decay: $\delta V = Aexp(-t/\tau)$ where t is the time, and τ is the charge carrier lifetime.

2. Supplementary data

Table S1. Photovoltaic performances of ASM OSCs with different ratio of ICBM.

Active layer	V_{OC} [mV]	J_{SC} [mA cm^{-2}]	FF [%]	PCE [%]	[a)]$PCE_{Ave.}$[%]
BTR-Cl:Y6	834.2	23.24	69.34	13.4	13.2
BTR-Cl:Y6:ICBA (2%)	838.9	23.39	71.87	14.2	14.0
BTR-Cl:Y6:ICBA (5%)	843.0	23.55	73.88	14.7	14.5
BTR-Cl:Y6:ICBA (7%)	851.1	23.36	69.89	13.9	13.6
BTR-Cl:Y6:ICBA (10%)	863.4	23.27	65.84	13.2	12.9
BTR-Cl:ICBA	924.6	14.06	38.83	5.0	4.6

[a)] The average PCE values were obtained from 15 devices.

Fig. S1. (a, b) The electron and hole mobility fitting curves of control device; (c, d) the electron and hole mobility fitting curves of optimized device.

References

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