Supporting Information

Phthalimide end-capped thienoisindigo and diketopyrrolopyrrole as non-fullerene molecular acceptors for organic solar cells

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1. $^1$H and $^{13}$C NMR spectra of TII-Pht$_2$ and DPP-Pht$_2$ in CDCl$_3$

2. FTIR spectra of TII-Pht$_2$ and DPP-Pht$_2$

3. HRMS of TII-Pht$_2$ and DPP-Pht$_2$

4. Solar cells fabrication

5. Space charge limited current (SCLC) measurements

6. References
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#### Substrat cleaning

Indium-tin oxide coated glass slides of 24×25×1.1 mm with a sheet resistance of RS = 7 Ω/sq were purchased from Praezisions Glas & Optik GmbH. The ITO layer was patterned via a 37% hydrochloric acid solution and zinc powder etching. The substrates were then washed with a diluted Deconex® 12 PA-x solution (2% in water) and scrubbed using dishwashing soap before being cleaned by a series of ultrasonic treatments for 15 min in acetone, ethanol and isopropanol. Once dried under a steam of nitrogen, a UV-ozone plasma treatment (UV/Ozone ProCleaner Plus, Bioforce Nanosciences) was performed for 15 min.

#### Inverted structure

Zinc acetate dihydrate (196 mg ; 1eq) and ethanol amine (54 μL ; 1eq) were added into 6 mL of absolute ethanol. The solution was stirred at 45°C for 2 hours and was used without any further purification. This ZnO solution was then spun-cast onto the patterned ITO surface described above at 700 rpm for 60 s before being baked at 180°C for 15 min. Then, blends of molecular acceptor TII-Pht	extsubscript{2} or DPP-Pht	extsubscript{2} and P3HT were spun-cast onto the ZnO layer. Finally, devices were completed by the successive deposition of molybdenum trioxide (7 nm) and silver (70 nm) at a pressure of 1.5 x 10⁻⁶ Torr through a shadow mask defining six cells of 27 mm² each (13.5 mm x 2 mm).

#### Device characterization

J-V curves were recorded in the dark and under illumination using a Keithley 236 source-measure unit and a home-made acquisition program. The light source is an AM1.5 Solar Constant 575 PV simulator (Steuernagel Lichttecknik, equipped with a metal halogen lamp). The light intensity was measured by a broad-band power meter (13PEM001, Melles Griot). EQE were measured under ambient atmosphere using a halogen lamp (Osram) with an Action Spectra Pro 150 monochromator, a lock-in amplifier (Perkin-Elmer 7225) and a S2281 photodiode (Hamamatsu). Atomic Force Microscopy (AFM) experiments were performed using the Nano-Observer microscope from CSInstrument. The topographic images were obtained in tapping mode. Images were processed using Gwyddion SPM data analysis software.
5. Space charge limited current (SCLC) measurements

A solution of neat molecular acceptor TII-Pht$_2$ or DPP-Pht$_2$ (20 mg/mL) in chloroform was spun cast at different spin-rates on the above described ITO substrates to provide organic layers of various thicknesses which have been measured using a Dektak 3M profilometer. Lithium fluoride (1 nm) and aluminum anodes (100 nm) were thermally and successively evaporated under a vacuum of $1.5 \times 10^{-5}$ Torr, through a shadow mask defining actives area of 12.60 mm$^2$, 3.10 mm$^2$ and 0.78 mm$^2$ per substrates. Electrons mobilities $\mu_e$ were evaluated using the Mott-Gurney law, $J_{\text{SCLC}} = (9/8)\varepsilon_0\varepsilon_r\mu_e(V^2/d^3)$ where $\varepsilon_r$ is the static dielectric constant of the medium ($\varepsilon_r = 3$) and $d$, the thickness of the active layer.$^2$ J-V characteristics of both compounds are plotted in Figure 2.

![Figure2](image.png)

**Figure2.** J–V characteristics of electron only devices: DPP-Pht$_2$ (red circles, $d = 105\text{nm}$) and TII-Pht$_2$ (black square, $d = 110 \text{nm}$)

6. References
