Impact of dithienyl or thienothiophene units on the optoelectronic and photovoltaic properties of benzo[1,2,5]thiadiazole based donor-acceptor copolymers for organic solar cell devices.


Electronic Supporting Information for:

Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2014
**Table S1**: OPV device optimisation data, with the current-voltage characteristics of best performing solar cells in each set highlighted in red. 

- Polymer:PC_{71}BM wt%. 
- Annealing time 30 minutes.
**Fig. S1:** 2D-GIWAXS images of X-ray scatter from 1:4 wt% copolymer:PC<sub>71</sub>BM blend thin-films. (a) PCDT2BT-8:PC<sub>71</sub>BM (b) PCDTTBT-8:PC<sub>71</sub>BM (c) PFDT2BT-8:PC<sub>71</sub>BM and (d) PFDTTBT-8:PC<sub>71</sub>BM.
**Fig. S2:** Out-of-plane GIWAXS patterns from neat copolymer thin-films. Here, the region of zero scattering intensity at low q corresponds to the position of the beam-stop.
Fig S3: Tapping-mode AFM height scans (left column) and phase scans (right column) of the surface of each copolymer:PC\textsubscript{71}BM (1:4 wt\%) blend thin-film. (a), (b) PCDT2BT-8:PC\textsubscript{71}BM, (c), (d) PCDTTBT-8:PC\textsubscript{71}BM, (e), (f) PFDT2BT-8:PC\textsubscript{71}BM, (g), (h) PFDTTBT-8:PC\textsubscript{71}BM. Calculated RMS roughness values are 0.32 nm for (a), 0.24 nm for (c), 0.22 nm for (e) and 0.25 nm for (g).
Fig S4: Steady-state PL spectra for each material investigated in this study. Blend films prepared according to the same composition ratio as OPV devices (1:4 wt % copolymer :PC$_{71}$BM). All spectra have been corrected for film absorption at the excitation wavelength (550 nm).
Fig S5: Average output and transfer characteristics for copolymer-based OFETS. (a), (b) PCDT2BT-8:PC$_7$BM, (c), (d) PCDTTBT-8:PC$_7$BM, (e), (f) PFDT2BT-8:PC$_7$BM, (g), (h) PFDTTBT-8:PC$_7$BM.
The field effect mobility of conjugated polymers can show non-negligible gate voltage dependence, a feature that is directly inherited from the effect of the applied gate field on the carrier traps DOS in the conduction channel [1]. Consequently, the OFET saturation transfer characteristic are more appropriately described by the following equation,

\[
\mu = \left( \frac{\partial I_D}{\partial V_{GS}} \right)^2 \frac{2L}{WC}.
\]

To avoid propagation of measurement uncertainty due to the numerical calculation of the derivative in the formula above, we devised an algorithm (FACT) that automatically partitions the transfer characteristic into ten-point data sets. From these, we extrapolate the linear fit for each set and return the respective gate-voltage dependent mobility if the condition \(R^2 > 0.999\) is satisfied. Over the region of validity of Eq 1, i.e. for \(V_{GS} >> V_{th}\) and \(V_{DS} \geq (V_{GS}-V_{th})\), the mobility is monotonically increasing with the gate voltage, a behaviour that can be explained by a relative high density of traps in close proximity to the dielectric/semiconductor interface.

[1] Organic field effect Transistors, Zhenan Bao(ed) and Jason Locklin(ed); CRC Press- Taylor & Francis Group, 2007