# Supporting information

## Design of Benzodithiophene-Diketopyrrolopyrrole Based Donor-Acceptor Copolymers for Efficient Organic Field Effect Transistors and Polymer Solar Cells

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### Hole Mobility Measure (SCLC)[1]

Hole-only devices were fabricated to measure the hole mobility using the space charge limited current (SCLC) method with a device structure of ITO/PEDOT/Active layer/$MoO_3$/Al. The mobility was determined by fitting the dark current to the model of a single carrier SCLC, described by the equation:

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

where $J$ is the current density, $\mu_h$ is the mobility under zero field, $\varepsilon_0$ is the permittivity of free space, $\varepsilon_r$ is the material relative permittivity, $d$ is the active layer thickness, and $V$ is the effective voltage. The effective voltage can be obtained by subtracting the built-in voltage ($V_{bi}$) and the voltage drop ($V_s$) from the substrate's series resistance from the applied voltage ($V_{appl}$), $V=V_{appl} - V_{bi}$. The hole-mobility can be calculated from the slope of the $J_{1/2} \sim V$ curves.

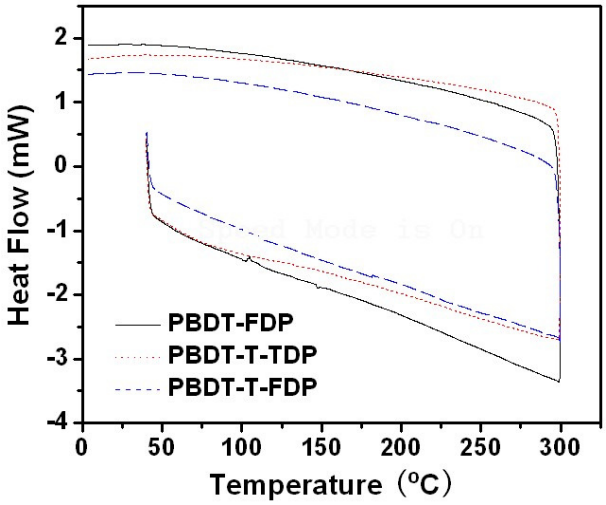


**Figure S1** DSC curves of copolymers at a scanning rate of 10 °C/min under nitrogen

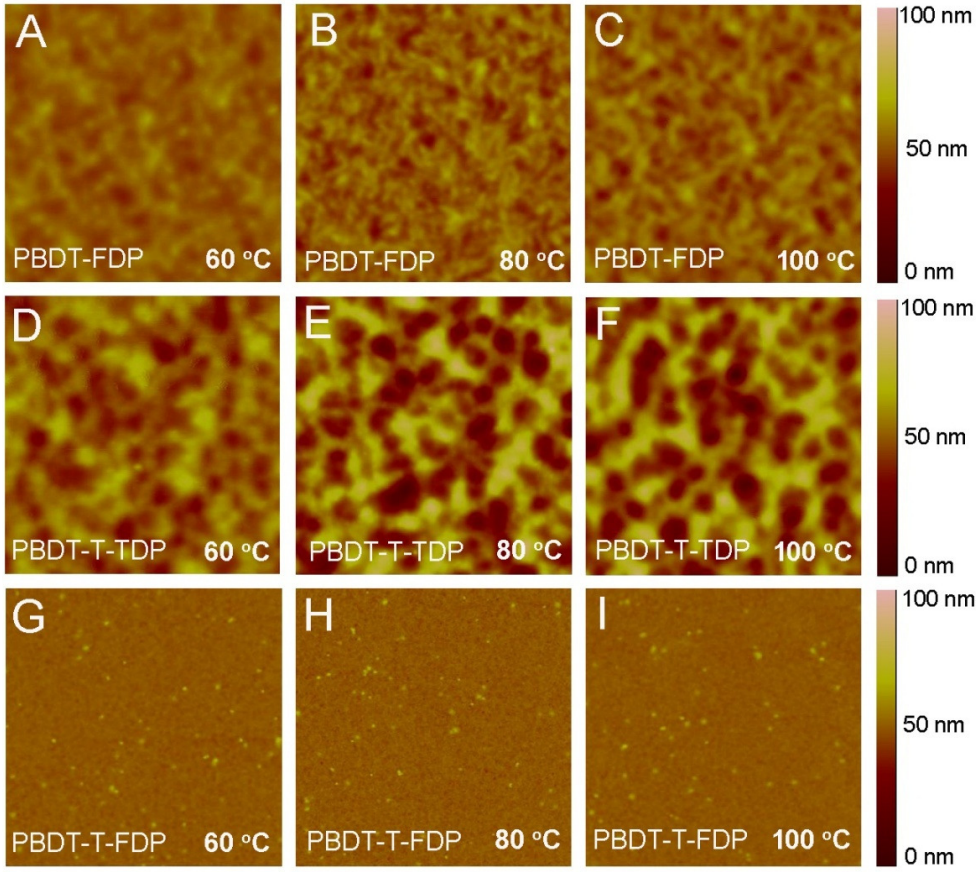


**Figure S2** AFM tapping-mode images (heights) of copolymers spin-cast from CF on OTS-treated Si-$SiO_2$ substrates under different annealing temperatures.

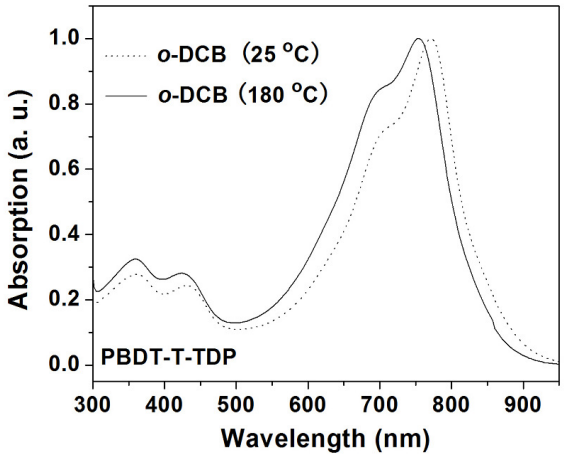


**Figure.S3** Normalized UV–vis. absorption spectra of PBDT-T-TDP in *o*-DCB at room temperature or 180 °C. The high temperature solution spectra of the polymer shows a 15nm blue-shift compared to the room temperature spectra, indicating a breakup of aggregates.

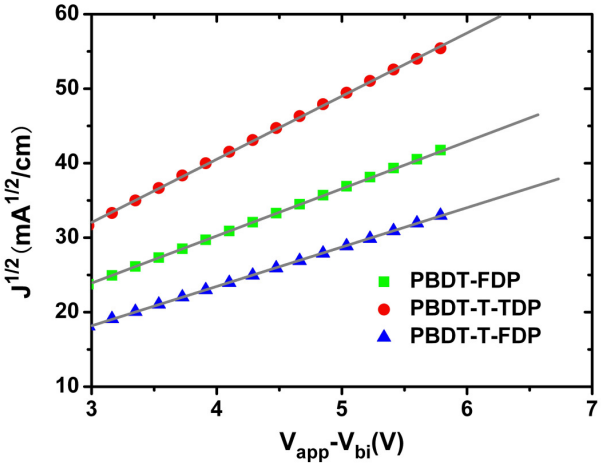


**Figure S4** $J^{1/2}-V$ characteristics of Polymer/$PC_{71}BM$ hole-only devices

**Table S1.**Summary of field effect mobilities, on/off ratios ($I_{on}/I_{off}$) and threshold voltages (V) for the copolymers

| Polymer | Annealing Temperature °C | Mobility $cm^2V^{-1}s^{-1}$ Avg(Max) | Threshold Voltage V Avg(Min) | $Log(I_{on}/I_{off})$ |
|---|---|---|---|---|
| **PBDT-FDP** | RT | 0.022(0.026) | -2.3(-0.4) | 5-9 |
| | 60 | 0.018(0.023) | -2.9(-2.5) | 7 |
| | 80 | 0.023(0.054) | -1.7(-1.7) | 6-9 |
| | 100 | 0.010(0.018) | -10.2(-2.6) | 6-8 |
| | 140 | 0.016(0.017) | -6.6(-6.0) | 6-7 |
| | 180 | 0.026(0.028) | -11.55(-7.9) | 8 |
| **PBDT-T-TDP** | RT | 0.003(0.003) | 1.2(0.5) | 5-7 |
| | 60 | 0.008(0.011) | -0.3(-1.8) | 6-7 |
| | 80 | 0.055(0.106) | 0.3(-0.1) | 6-8 |
| | 100 | 0.016(0.021) | -1.8(2.0) | 6-7 |
| | 140 | 0.029 (0.034) | -4.6(-4.4) | 7-8 |
| | 180 | 0.025(0.027) | -4.3(-3.5) | 6-8 |
| **PBDT-T-FDP** | RT | 0.052(0.065) | -0.4(-0.3) | 7-8 |
| | 60 | 0.089(0.111) | -2.3(-0.7) | 8 |
| | 80 | 0.063(0.158) | -4.4(-2.3) | 7-9 |
| | 100 | 0.060(0.086) | -5.8(-2.7) | 8-10 |
| | 140 | 0.062(0.067) | -4.6(-3.6) | 3-8 |
| | 180 | 0.053(0.062) | -4.8(-4.5) | 6-8 |

**Table S2.** Effect of solvents on the performance of devices using $PC_{61}BM$

| Polymer | Solvent | Donor:$PC_{61}BM$ | $J_{sc}$ (mA $cm^{-2}$) | $V_{oc}$ (V) | *FF* (%) | *PCE* (%) |
|---|---|---|---|---|---|---|
| **PBDT-FDP** | *o*-DCB | 1:2 | 4.47 | 0.72 | 59 | 1.90 |
| **PBDT-FDP** | *o*-DCB, 2% DIO | 1:2 | 7.58 | 0.73 | 60 | 3.32 |
| **PBDT-FDP** | CF, | 1:2 | 1.93 | 0.74 | 55 | 0.79 |
| **PBDT-FDP** | CF, 2% DIO | 1:2 | 7.87 | 0.73 | 56 | 3.24 |
| **PBDT-T-TDP** | *o*-DCB | 1:2 | 8.19 | 0.68 | 51 | 2.85 |
| **PBDT-T-TDP** | *o*-DCB, 2% DIO | 1:2 | 8.41 | 0.65 | 52 | 2.84 |
| **PBDT-T-TDP** | CF, | 1:2 | 6.37 | 0.66 | 41 | 1.71 |
| **PBDT-T-TDP** | CF, 2% DIO | 1:2 | 8.86 | 0.65 | 42 | 2.42 |
| **PBDT-T-FDP** | *o*-DCB | 1:2 | 8.80 | 0.77 | 52 | 3.50 |
| **PBDT-T-FDP** | *o*-DCB, 2% DIO | 1:2 | 6.98 | 0.73 | 59 | 3.03 |
| **PBDT-T-FDP** | CF, | 1:2 | 9.95 | 0.76 | 49 | 3.74 |
| **PBDT-T-FDP** | CF, 2% DIO | 1:2 | 10.80 | 0.78 | 51 | 4.25 |

**Table S3.** Effect of solvents on the performance of devices using $PC_{71}BM$

| Polymer | Solvent | Donor:$PC_{71}BM$ mg/mL | RPM | $J_{sc}$ (mA $cm^{-2}$) | $V_{oc}$ (V) | *FF* (%) | *PCE* (%) |
|---|---|---|---|---|---|---|---|
| **PBDT-FDP** | *o*-DCB | 5:10 | 800 | 4.97 | 0.73 | 61 | 2.22 |
| **PBDT-FDP** | *o*-DCB, 2% DIO | 5:10 | 800 | 7.71 | 0.71 | 62 | **3.42** |
| **PBDT-FDP** | *o*-DCB /CF=1/1, 2% DIO | 5:10 | 800 | 8.30 | 0.70 | 51 | 2.97 |
| **PBDT-T-TDP** | *o*-DCB | 5:10 | 1500 | 6.91 | 0.67 | 57 | 2.66 |
| **PBDT-T-TDP** | *o*-DCB, 2% DIO | 5:10 | 1500 | 7.39 | 0.66 | 60 | 2.92 |
| **PBDT-T-TDP** | *o*-DCB /CF=1/1, 2% DIO | 5:10 | 1500 | 9.80 | 0.68 | 59 | **3.91** |
| **PBDT-T-FDP** | CF | 5:10 | 1500 | 5.34 | 0.73 | 34 | 1.31 |
| **PBDT-T-FDP** | CF, 2% DIO | 5:10 | 1500 | 11.76 | 0.76 | 59 | 5.15 |
| **PBDT-T-FDP** | *o*-DCB/CF=1/1, 2% DIO | 5:10 | 1200 | 12.55 | 0.73 | 60 | **5.54** |

**Table S4.** The hole mobility of Polymers/$PC_{71}BM$ blend films measured by SCLC method

| Polymer | Thickness (nm) | Mobility ($cm^2V^{-1}s^{-1}$) |
|---|---|---|
| **PBDT-FDP** | 95 | $1.37*10^{-4}$ |
| **PBDT-T-TDP** | 80 | $1.27*10^{-4}$ |
| **PBDT-T-FDP** | 90 | $7.10*10^{-5}$ |

1. M. Wang, X. Hu, P. Liu, W. Li, X. Gong, F. Huang, Y. Cao, *J. Am. Chem. Soc.* **2011**, 133, 9638.