Supporting information

# Efficient polymer solar cells based on a new quinoxaline derivative with fluorinated phenyl side chain

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### 1. TGA measurement



Fig. S1 TGA curve of PBDTT-DTFPQx at a scan rate of 20 °C/min under nitrogen

atmosphere.

#### 2. DSC measurement



Fig. S2 DSC curves of polymers with a heating rate of 10  $^{\circ}$ C min<sup>-1</sup> under N<sub>2</sub>

atmosphere.

## 3. DFT calculation



Fig. S3 The calculated HOMO and LUMO levels of non fluorinated PBDTDT(Qx-3)-

T and fluorinated PBDTT-DTFPQx by Gaussian at the B3LYP/6-31G\* level.

4. Photovoltaic properties of polymer-based PSCs at different conditions



**Fig. S4** *J-V* curves of the PBDTT-DTFPQx/PC<sub>71</sub>BM-based PSCs with different blend ratios (*w/w*) under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

Table S1 Photovoltaic properties of the PBDTT-DTFPQx/PC71BM-based PSCs with

| D/A Ratio | $J_{\rm sc}$ / mA cm <sup>-2</sup> | $V_{\rm oc}/{ m V}$ | FF/ % | PCE <sub>max</sub> (PCE <sub>ave</sub> <sup>a</sup> )/ % |
|-----------|------------------------------------|---------------------|-------|----------------------------------------------------------|
| 1/3       | 8.2                                | 0.79                | 70    | 4.5 (4.3)                                                |
| 1/4       | 10.1                               | 0.87                | 65    | 5.8 (5.6)                                                |
| 1/5       | 7.5                                | 0.81                | 68    | 4.2 (4.1)                                                |

different blend ratios (w/w) under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

<sup>a)</sup> The average PCE was obtained from over 10 devices.



Fig. S5 *J-V* curves of the PBDTT-DTFPQx/PC<sub>71</sub>BM-based PSCs with different

temperature under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

Table S2 Photovoltaic properties of the PBDTT-DTFPQx/PC71BM-based PSCs with

| Temperature/ °C | $J_{\rm sc}/~{ m mA~cm^{-2}}$ | $V_{\rm oc}/~{ m V}$ | FF/ % | PCE <sub>max</sub> (PCE <sub>ave</sub> <sup>a</sup> )/ % |
|-----------------|-------------------------------|----------------------|-------|----------------------------------------------------------|
| 25              | 10.1                          | 0.87                 | 65    | 5.8 (5.6)                                                |
| 80              | 11.3                          | 0.86                 | 71    | 6.9 (6.6)                                                |
| 110             | 10.4                          | 0.89                 | 65    | 6.0 (5.8)                                                |

different temperature under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

<sup>a)</sup> The average PCE was obtained from over 10 devices.



**Fig. S6** *J-V* curves of the PBDTT-DTFPQx/PC<sub>71</sub>BM-based PSCs with different DIO additive concentrations under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

Table S3 Photovoltaic properties of the PBDTT-DTFPQx/PC71BM-based PSCs with

| DIO additive concentrations | $J_{\rm sc}/~{\rm mA~cm^{-2}}$ | $V_{ m oc}/~{ m V}$ | FF/ % | PCE <sub>max</sub> (PCE <sub>ave</sub> <sup>a</sup> )/ % |
|-----------------------------|--------------------------------|---------------------|-------|----------------------------------------------------------|
| 0.0%                        | 11.3                           | 0.86                | 71    | 6.9 (6.6)                                                |
| 0.5%                        | 11.7                           | 0.86                | 71    | 7.1 (6.8)                                                |
| 1.0%                        | 11.4                           | 0.87                | 73    | 7.2 (7.0)                                                |
| 2.0%                        | 11.1                           | 0.87                | 58    | 5.6 (5.5)                                                |

different DIO additive concentrations under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

<sup>a)</sup> The average PCE was obtained from over 10 devices.



**Fig. S7** *J-V* curves of the PBDTT-DTFPQx/PC<sub>71</sub>BM-based PSCs with different spincoating rates under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

Table S4 Photovoltaic properties of the PBDTT-DTFPQx/PC71BM-based PSCs with

| spin-coating<br>rates/ rpm | $J_{\rm sc}/~{ m mA~cm^{-2}}$ | $V_{\rm oc}/~{ m V}$ | FF/ % | PCE <sub>max</sub> (PCE <sub>ave</sub> <sup>a</sup> )/ % |
|----------------------------|-------------------------------|----------------------|-------|----------------------------------------------------------|
| 2000                       | 11.3                          | 0.86                 | 71    | 7.0 (6.7)                                                |
| 2250                       | 11.4                          | 0.87                 | 73    | 7.2 (7.0)                                                |
| 2500                       | 11.5                          | 0.86                 | 72    | 7.1 (6.9)                                                |

different spin-coating rates under illumination of AM 1.5G, 100 mW/cm<sup>2</sup>.

<sup>a)</sup> The average PCE was obtained from over 10 devices.

# 5. <sup>1</sup>HNMR, <sup>13</sup>C NMR and MS data of monomer and <sup>1</sup>H NMR data of polymer

## <sup>1</sup>H NMR plot of **DTFPQx-Br<sub>2</sub>**



<sup>13</sup>C NMR plot of **DTFPQx-Br<sub>2</sub>** 





MALDI-TOF plot of DTFPQx-Br<sub>2</sub>



<sup>1</sup>H NMR plot of **PBDTT-DTFPQx** 

