Supporting Information

Improvement of Open-Circuit Voltage and Photovoltaic Properties of

2D-Conjugated Polymers by Alkylthio Substitution

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Figure S1. LUMO and HOMO levels for the polymer repeat unit. Calculations were carried out by DFT/B3LYP/6-31G (d, p) level on the polymers with a chain length of 2. Methyl groups were used to replace alkyl substituents here to simplify the calculations.



Figure S2. X-ray diffraction pattern of PBDTT-S-TT:PC₇0BM (1:1.5, w/w) blend films processed without or with DIO additive.



Figure S3. The topography (left) and the corresponding phase (right) images $(3 \times 3 \ \mu m)$ of PBDTT-S-TT:PC₇₀BM (1:1.5, w/w) blend films processed without (a, b) or with (c, d) DIO additive.