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Supplementary Information

Solution-processed boron subphthalocyanine derivatives as acceptors for organic bulk-heterojunction solar cells

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Fig. S1 shows the cyclic voltammetry of compound **1** and **2**. The square wave derived potentials for the HOMO and LUMO values are given in the main text.

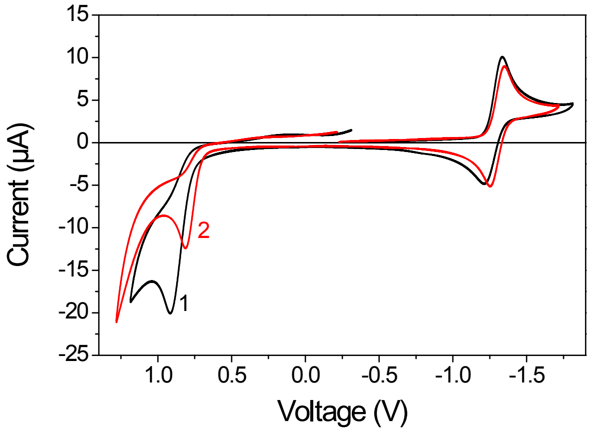

Fig. S1 Cyclic voltammetry of compound **1** and **2**.

Fig. S2 shows the spatial distribution of the HOMO and LUMO of compounds **1** and **2** calculated by density functional theory (B3LYP/6-31G*), using the Spartan ’14 (64-bit) software suite.

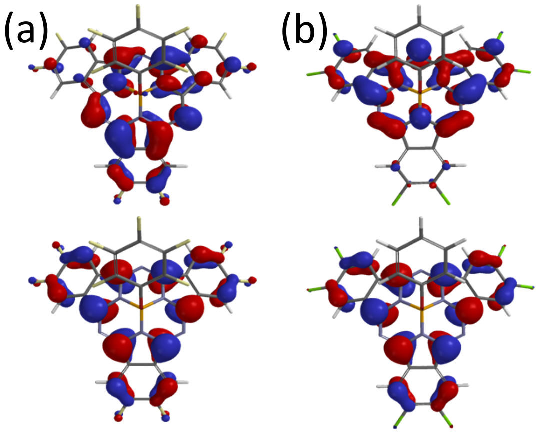

Fig. S2 DFT modelled structures of **1** (a) and **2** (b) showing LUMO (top) and HOMO (bottom) maps.

Fig. S3 shows crystalline structures as grown in spin coated films of compound **1** and an undissolved crystal.

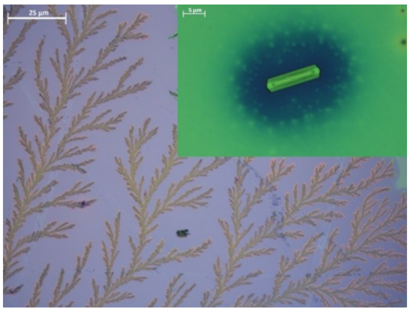

Fig. S3 Optical microscopy image showing the crystalline structures found in films spin -coated from compound **1**.

Fig. S4 shows a measurement of charge extraction by linearly increasing voltage (CELIV) on P3HT:**2**. P3HT has the advantage that it contains intrinsic charge carriers which can be extracted by a linear voltage ramp.[1] The figure shows a clear charge extraction peak from which the mobility of the blend can be determined. At a voltage ramp of 33 kV/s, the mobility of majority charge carriers amounts to 9 x 10^{-6} cm^2/Vs. This suggests a reduced mobility compared to fullerene acceptors, where the CELIV mobility is of typically 1 x 10^{-3} cm^2/Vs.[2,3]

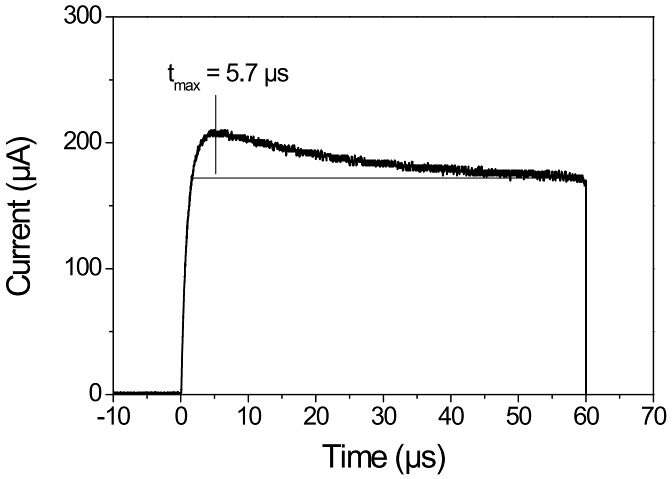

Fig. S4 Dark CELIV current transient of P3HT:2 (1:3) at a voltage ramp of 33 kV/s. The mobility of 9×10^{-6} cm2/Vs is obtained from the peak charge extraction and the film thickness of 38 nm.

Fig. S5 shows the device parameters of PTB7:**2** solar cells for various annealing conditions. The efficiency forms a clear maximum for a temperature of 160 °C and duration of 10 minutes, which agrees with the overall trend of short circuit current density (J_{SC}), open circuit voltage (V_{OC}) and fill factor (FF).

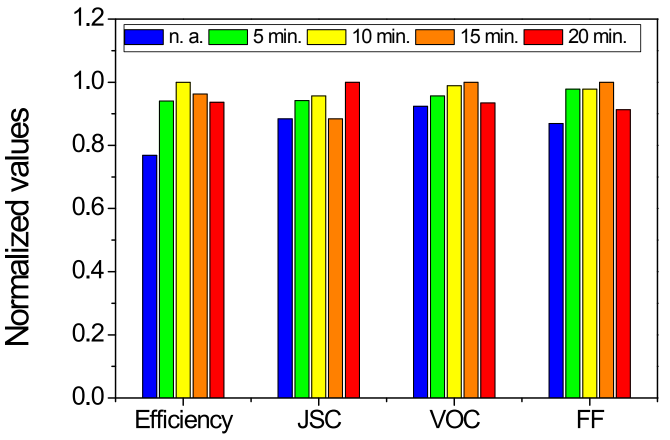

Fig. S5 Normalized device parameters of PTB7:**2** solar cells for varying annealing duration at 160 °C.

Table 1 shows the device properties of solar cells based on MEH-PPV, P3HT and PTB7. The properties shown are an average of working pixels on each substrate. For some devices configurations further device optimisation is possible.

Table 1 Summary of device properties of solar cells comprising SubPC acceptor **1** and **2**. (Tol = Toluene, DCB = 1,2-Dichlorobenzene)

Blend	Ratio	Solution	DIO	Annealing	Thickness (nm)	PCE (%)	JSC (mA/cm2)	VOC (mV)	FF (%)
MEH-PPV:**1**	1:5	13 mg/ml Tol	–	160 °C, 10 min.	89 ± 30	0.04	0.5	340	27
MEH-PPV:**2**	1:3	11 mg/ml Tol	–	160 °C, 10 min.	50 ± 14	0.42	1.60	910	29
P3HT:**1**	1:2	20 mg/ml DCB	–	120 °C, 20 min.	55 ± 4	0.15	1.67	280	32
P3HT:**2**	1:3	20 mg/ml DCB	–	120 °C, 20 min.	38 ± 3	1.09	4.31	590	43
PTB7:**1**	1:1.5	20 mg/ml DCB	2 %	160 °C, 10 min.	52 ± 11	1.88	6.0	776	40
PTB7:**2**	1:1.5	20 mg/ml DCB	1 %	160 °C, 10 min.	41 ± 4	3.51	7.8	935	48
PTB7:PC_{71}BM	1:1.5	20 mg/ml DCB	3 %	–	63 ± 4	7.10	13.3	768	70

Fig. S6 shows the collapsed JV-curves of PTB7:**1** and PTB7:**2** solar cells for varying light intensity. The curves were normalized at -0.5 V to a value of -1. The spread at short circuit can be attributed to trap-assisted recombination and the spread at open circuit to bimolecular recombination.[4,5] For PTB7:**1** stronger trap-assisted recombination is observed compared to PTB7:**2**. The normalized JV-curves of PTB7:**1** reveal a crossing point at about 0.6 V, this is an indication of strong trap-assisted recombination and can be an origin of reduced open circuit voltage.

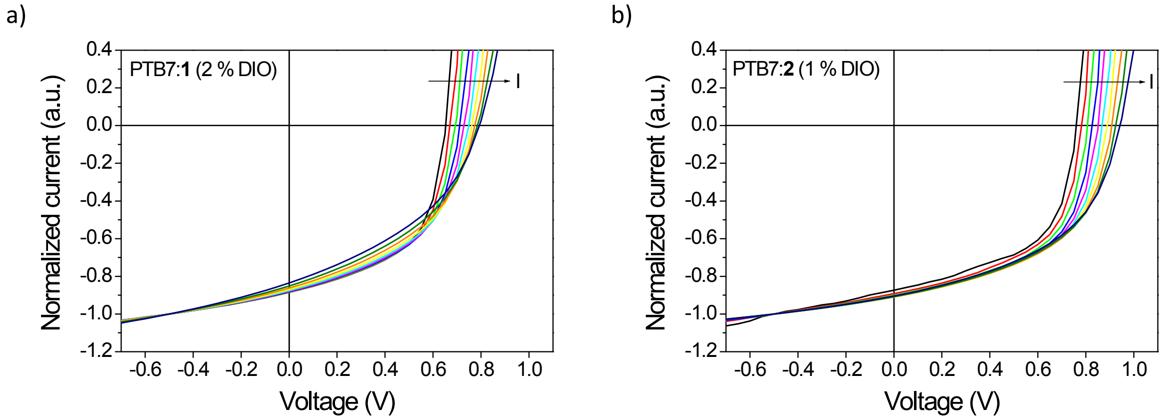

Fig. S6 a) Collapsed JV-curves of optimized devices with varying light intensity of PTB7:**1** and b) PTB7:**2**. The curves are normalized at -0.5 V.

Fig. S7 shows excitation scans of a blend of PTB7:**2** at the prominent emission peaks at 800 nm and 650 nm. The curves are in good agreement with the absorption spectra of PTB7 and compound **2** respectively. This clearly assigns the contribution from PTB7 to the 800 nm emission and compound **2** to the emission at 650 nm.

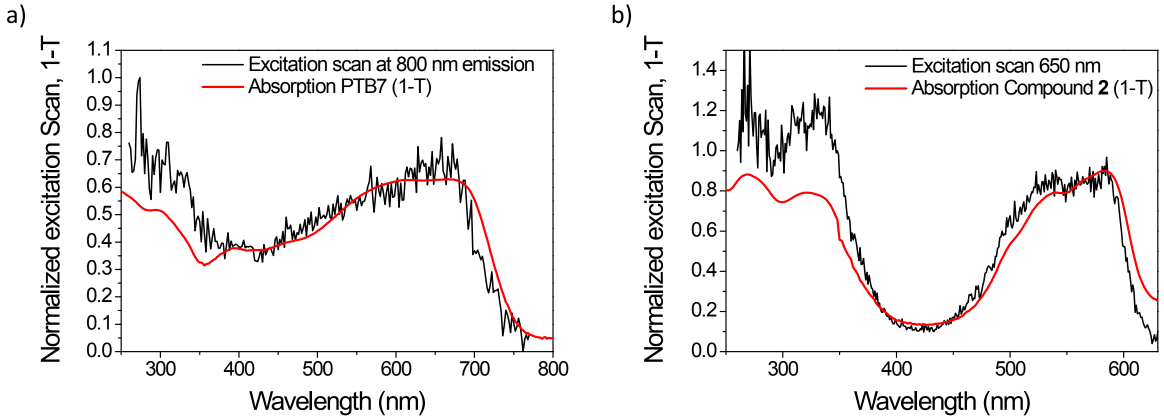

Fig. S7 a) Excitation scan of a PTB7:2 blend film with emission at 800 nm compared to an absorption spectrum of PTB7. b) Excitation scan at 650 nm emission compared to the absorption spectrum of compound **2**.

Fig. S8 shows tapping mode AFM images of PTB7:**1** and PTB7:**2**. Films of PTB7:**2** have a slightly finer intermixed layer, which can result in better exciton dissociation.

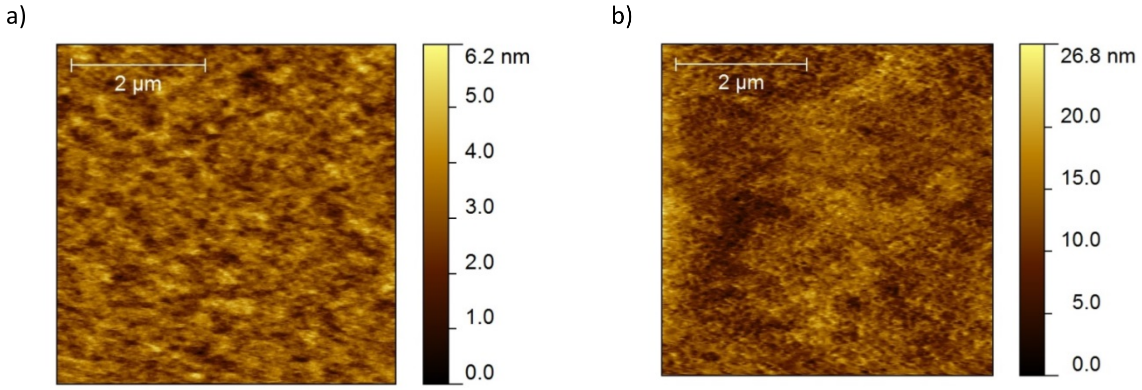

Fig. S8 a) Image of tapping mode atomic force microscopy of PTB7:**1** and b) PTB7:**2**

References

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