Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

AZABODIPY aggregates as a promising electroluminescent material for sustainable NIR OLED applications

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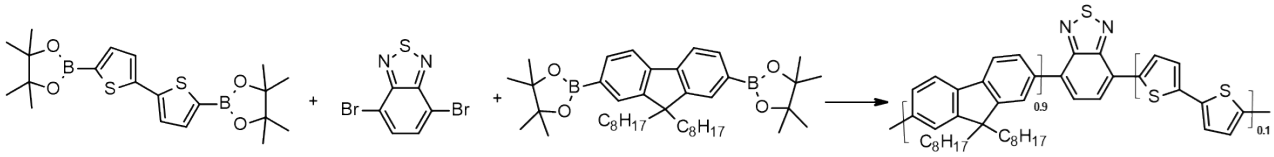

F8BT-TTBT

Scheme S1. Synthesis route of F8BT-TTBT polymer.

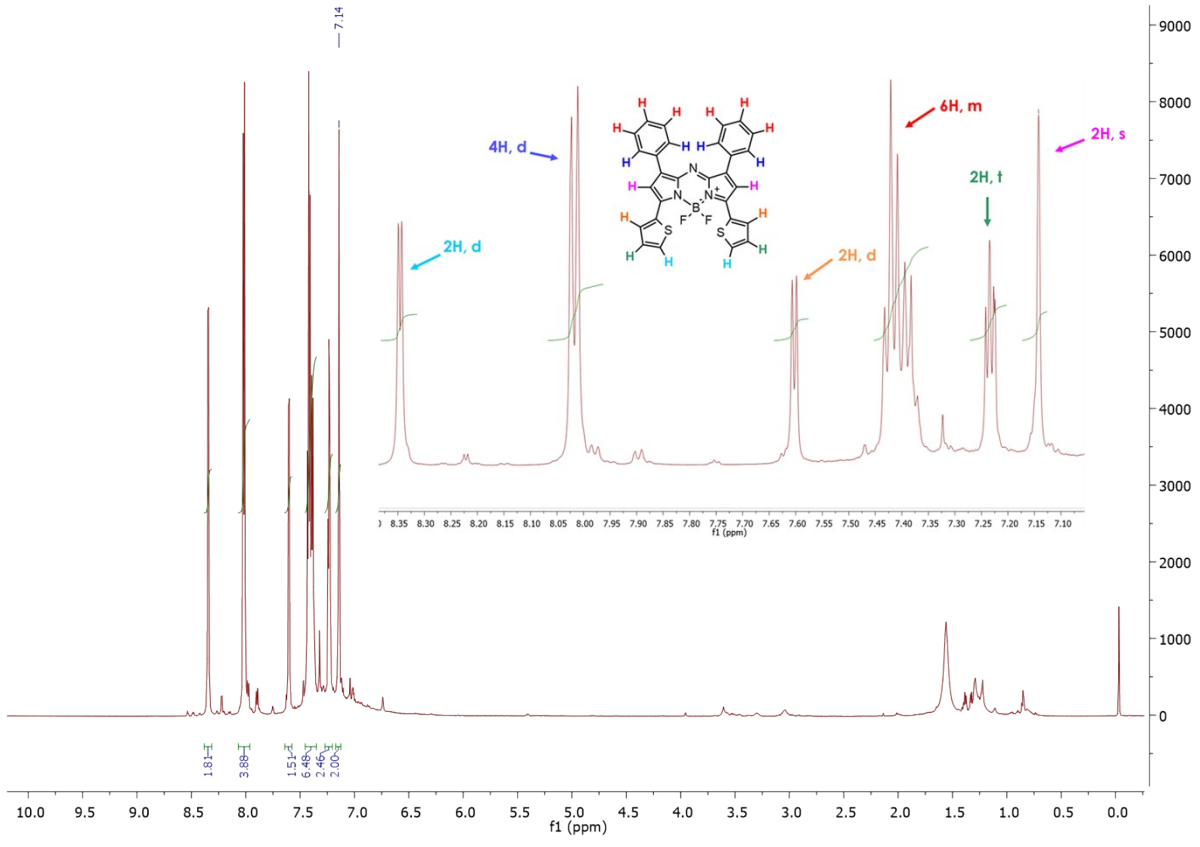

Fig. S1. ^{1}H-NMR spectrum of DTDPAB molecule.

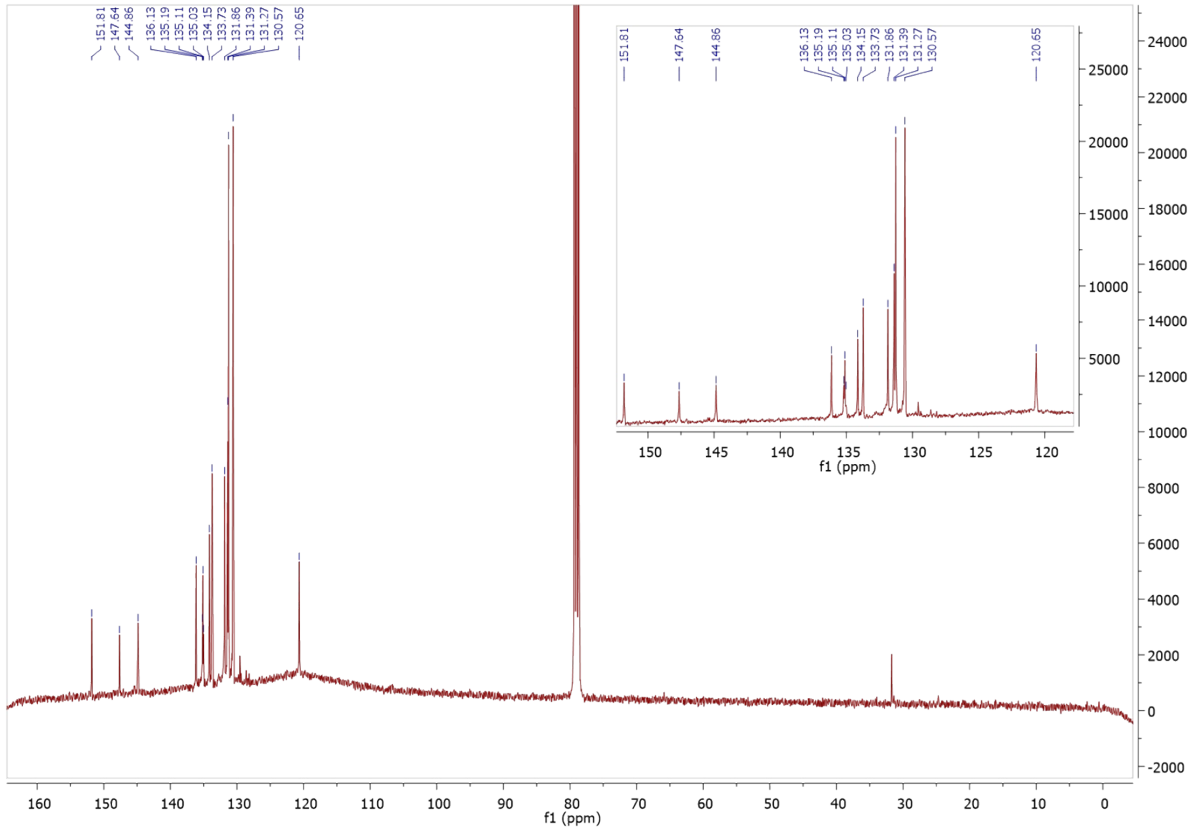

Fig. S2. ^{13}C-NMR spectrum of DTDPAB molecule.

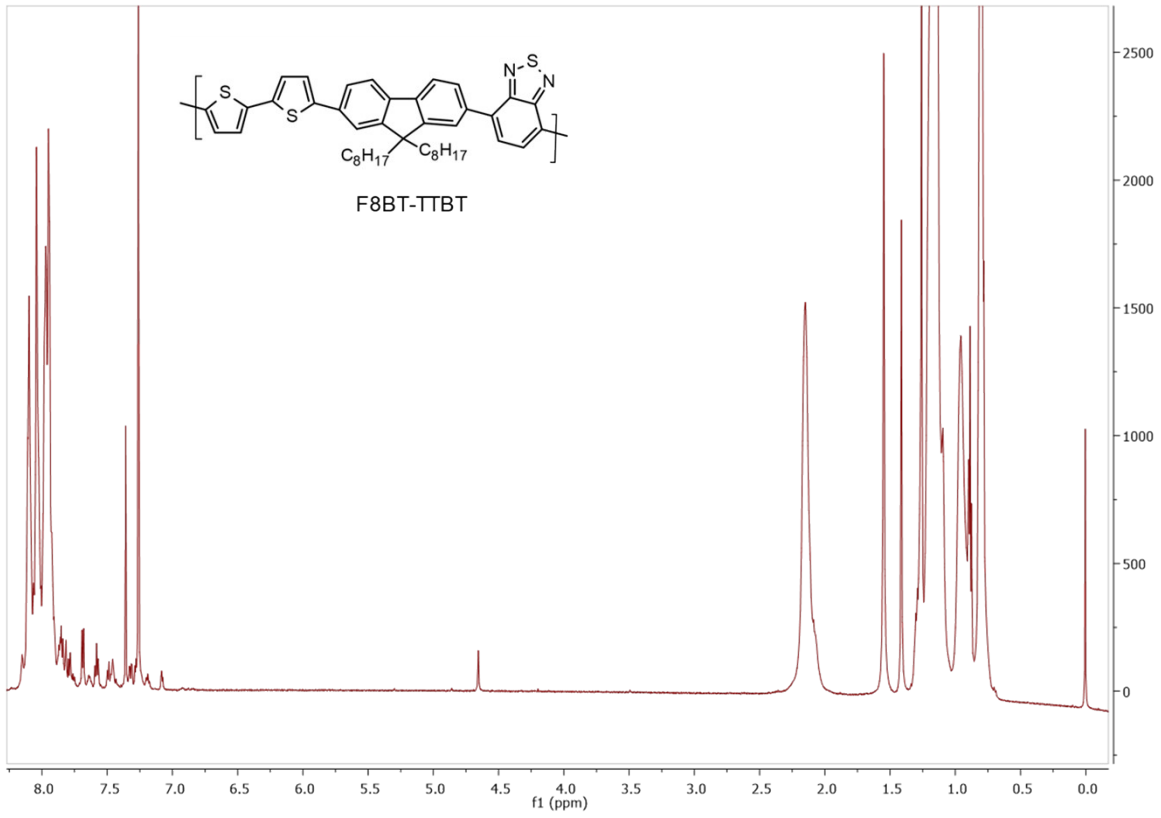

Fig. S3. ^{1}H-NMR spectrum of F8BT-TTBT polymer.

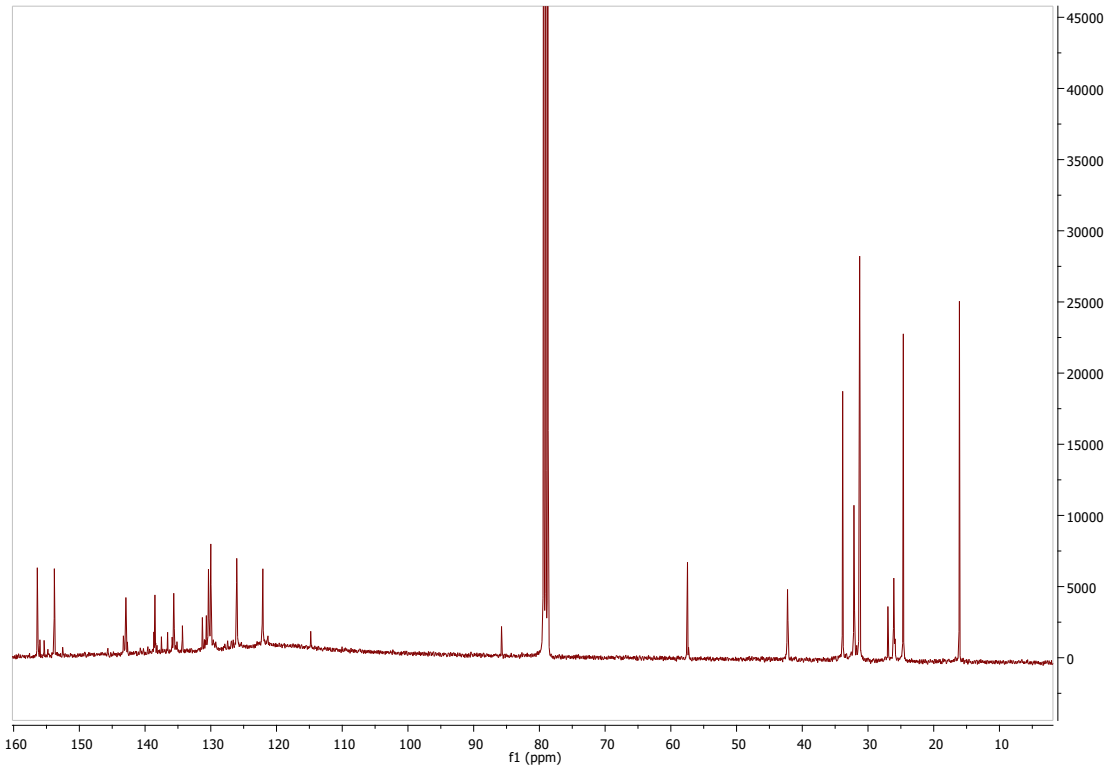

Fig. S4. ^{13}C-NMR spectrum of F8BT-TTBT polymer.

Table S1. Optical properties of DTDPAB in toluene and chloroform solutions at concentration 10^{-5}M and as a dropcasted film.

	Absorption (nm)	PLE max (nm)	PL max (nm)	PL QY (%) exc. 488nm	τ_{av} (ns) (exc. 408nm)
Toluene	721	345, 721	734	47 ± 5	3.03 (734 nm); 3.04 (820 nm)
Chloroform	720	347, 719	733	43 ± 4	3.32 (732 nm)
Casted film	777	-	930	< 0.1	$304 \cdot 10^{-3}$

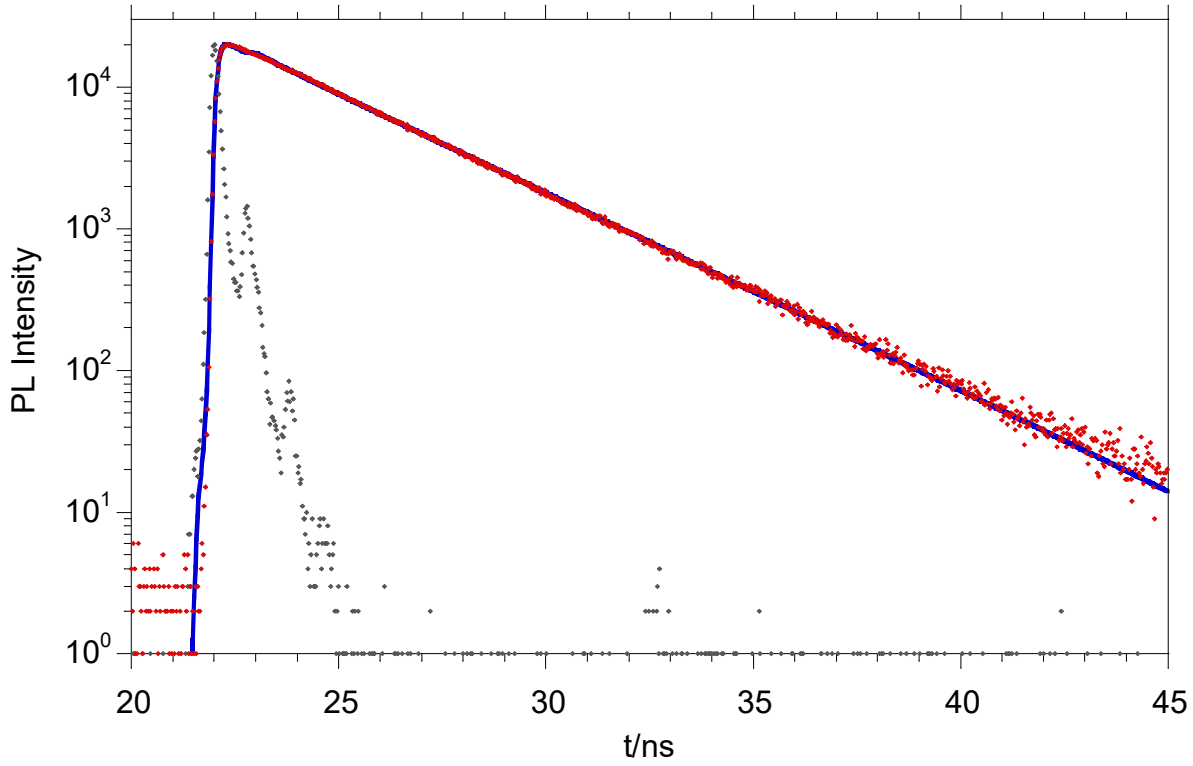

Fig. S5. PL decay of toluene solution of DTDPAB at 734nm, excited at 408nm. Bi-exponential fit (T1 = 5.374469E-10 sec, T2 = 3.122783E-09 sec, B1 = 2.489714E-02 [3.40 Rel. Ampl], B2 = 0.1217602 [96.60 Rel. Ampl], CHISQ = 2.27528.

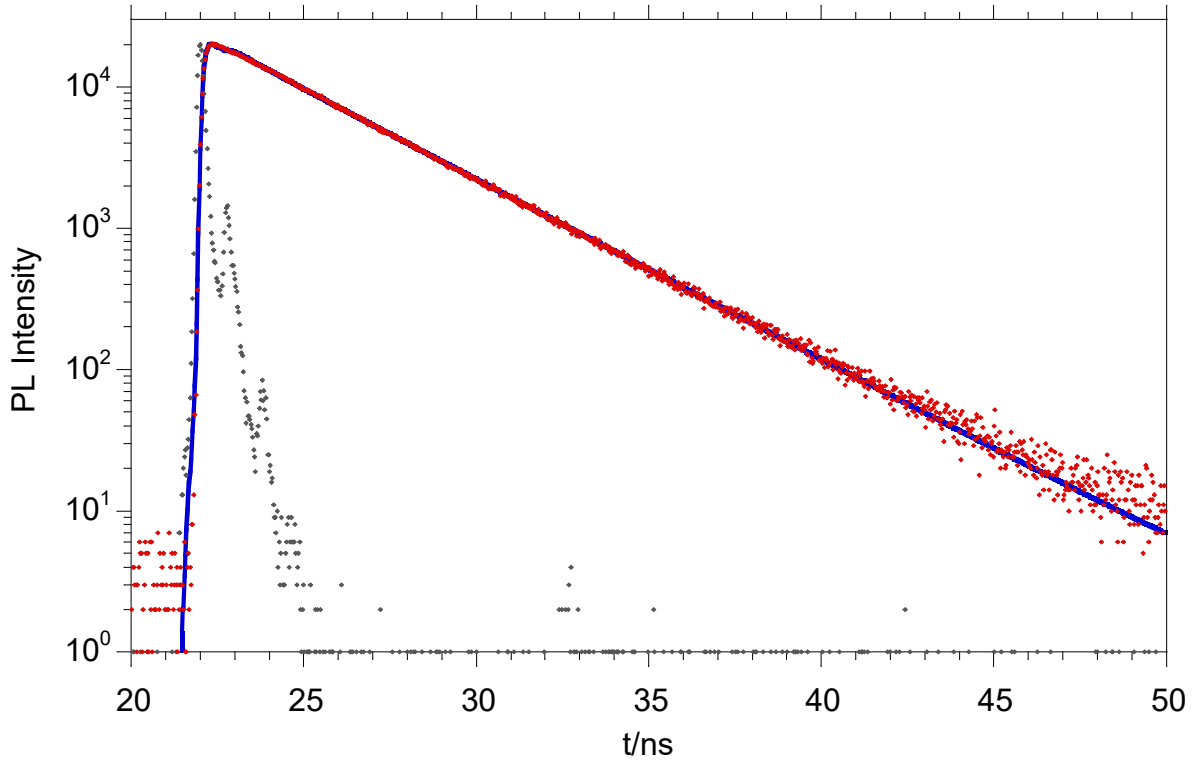

Fig. S6. PL decay of chloroform solution of DTDPAB at 732nm, excited at 408nm. Bi-exponential fit (T1 = 5.447399E-10 sec, T2 = 3.404215E-09 sec, B1 = 2.328718E-02 [2.96 Rel. Ampl], B2 = 0.1221145 [97.04 Rel. Ampl], CHISQ = 2.05874.

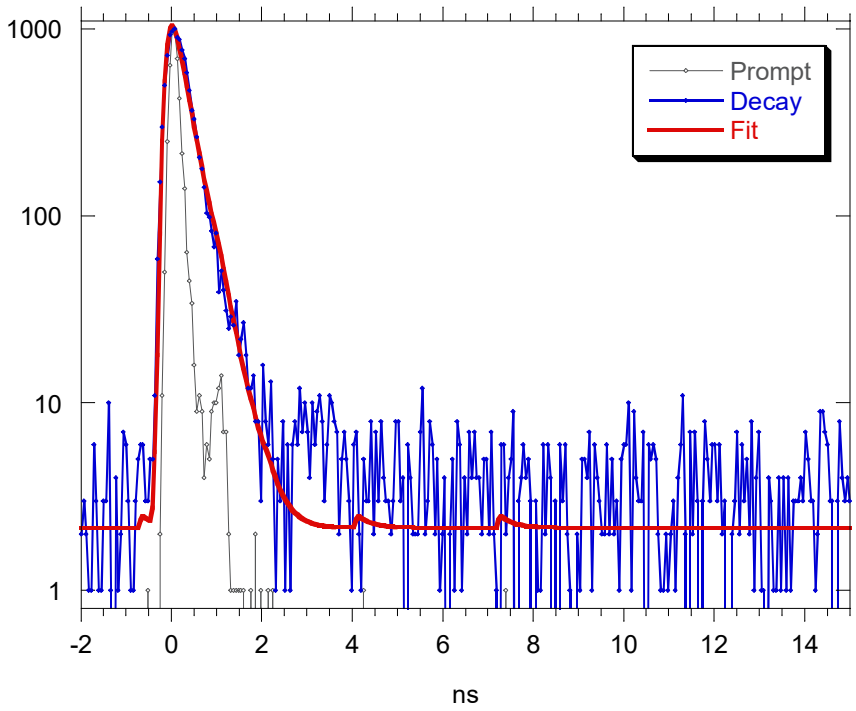

Fig. S7. PL decay of a cast film of DTDPAB at 840nm, excited at 407nm. The red line is a monoexponential fit (lifetime 304 ps, CHISQ = 1.778482). Fitting parameters T1 = 3.04299E-10 sec, S. Dev = 5.709041E-12 sec, A = 1.996751, S. Dev = 5.288644E-02, B1 = 0.4585481, [100.00 Rel. Ampl], S. Dev = 4.40858E-03, CHISQ = 1.778482, [829 degrees of freedom].

Table S2. Oxidation and reduction potentials derived from ciclovoltammetry, HOMO and LUMO energy levels, absorption maxima and energy band gaps derived from optical and electrochemical measurements of F8BT, F8BT-TTBT and DTDPAB. HOMO and LUMO energy levels were estimated according to $E_{HOMO/LUMO} = -\ 4.39 + (0.34 + E_{ox/red})$, where $E_{ox/red}$ are the onset oxidation and reduction potential, respectively, vs Ag/Ag^{+} electrode (0.34 V vs SCE).[1] The precision of the measurement was ± 0.01 V.

Sample	**E_{ox} (V)**	**E_{red} (V)**	**HOMO (eV)**	**LUMO (eV)**	**λ_{max} (nm)**	**E_{gopt} (eV)**	**E_{gel} (eV)**
F8BT	0.99	-1.84	-5.72	-2.89	324; 455	2.73	2.83
F8BT-TTBT	0.97	-1.8	-5.70	-2.93	319; 450; 530	2.34	2.77
DTDPAB	0.57	-0.65	-5.30	-4.08	321; 453	1.72	1.22

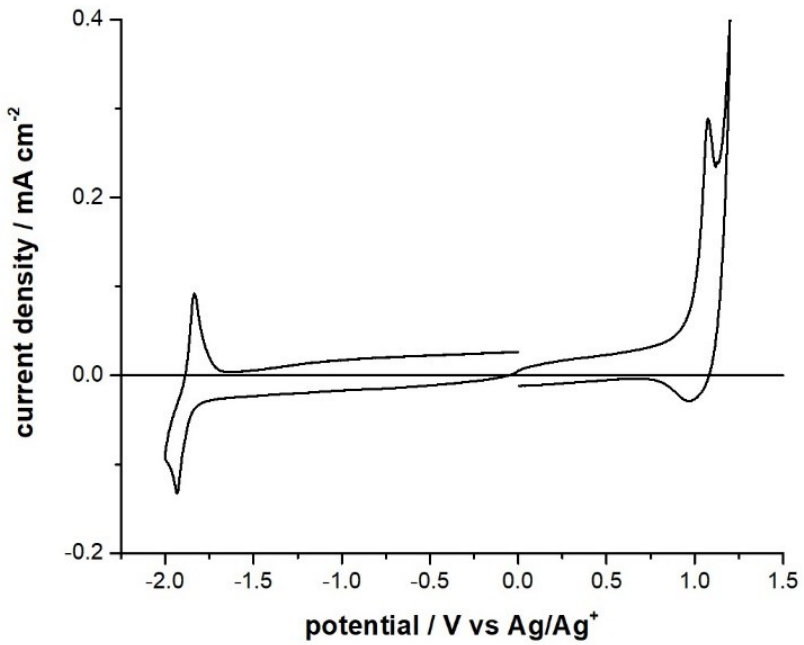

Fig S8. Cyclic Voltammogram of F8BT polymer in acetonitrile + 0.1 M Bu_4NClO_4. Scan rate: 0.1 V s^{-1}.

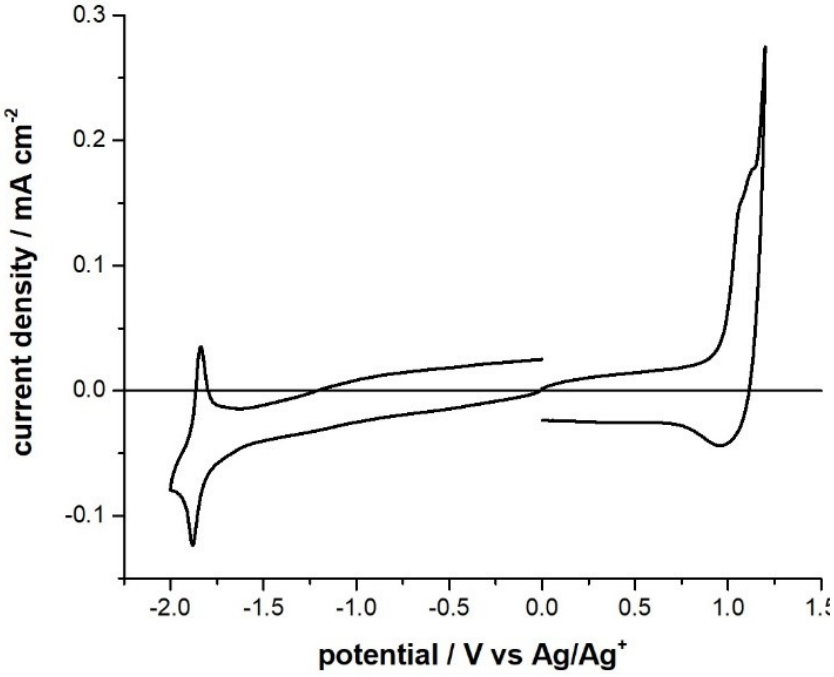

Fig. S9. Cyclic Voltammogram of F8BT-TTBT polymer in acetonitrile + 0.1 M Bu_4NClO_4. Scan rate: 0.1 V s^{-1}.

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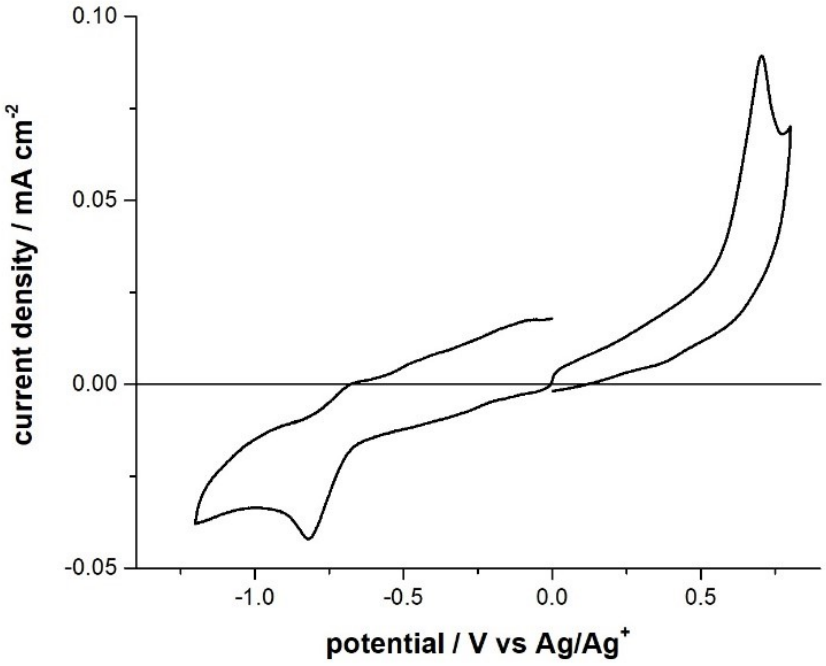

Fig S10. Cyclic Voltammograms of DTDPAB molecule, in acetonitrile + 0.1 M Bu_4NClO_4. Scan rate: 0.1 V s^{-1}.

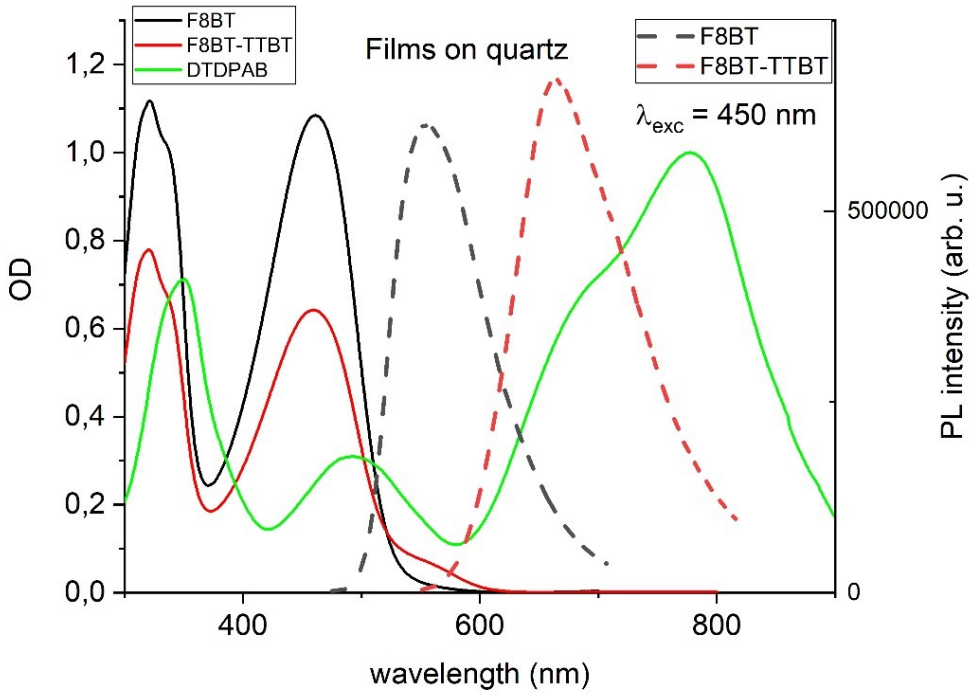

Fig. S11. Absorption of F8BT, F8BT-TTBT and DTDPAB films (solid lines) and PL of F8BT and F8BT-TTBT films (dashed lines). The overlap of DTDPAB absorption and the polymers PL is better for F8BT-TTBT.

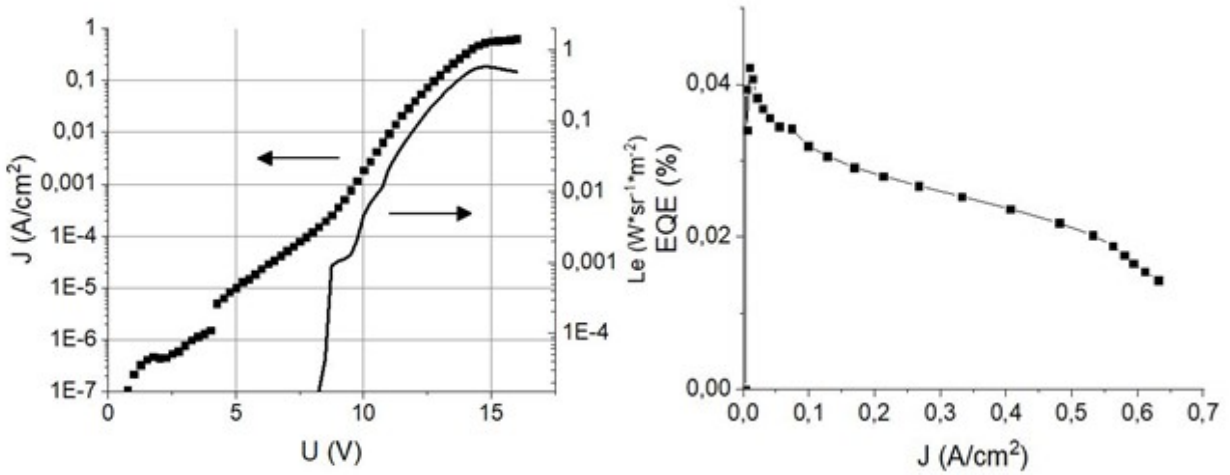

Fig. S12. J-V-L_e curves and EQE of ITO / PEDOT:PSS / PVK / 95% F8BT : 5% DTDPAB / Ba / Al device.

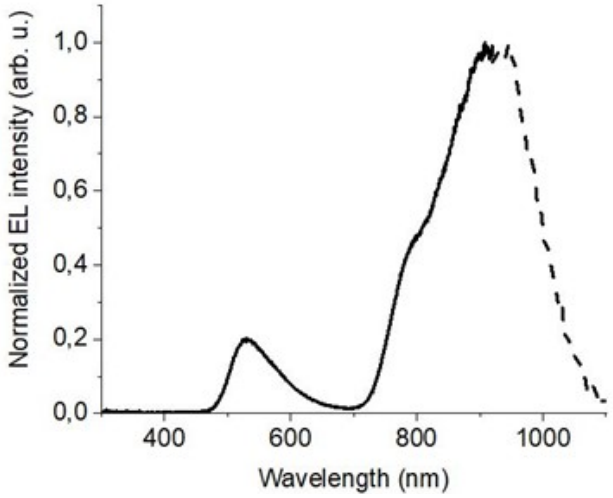

Figure S13. EL at 100 mA/cm^2 of ITO / PEDOT:PSS / PVK / 20% F8BT : 80% DTDPAB / Ba / Al device. Dashed line shows simulated extrapolation of the spectrum.

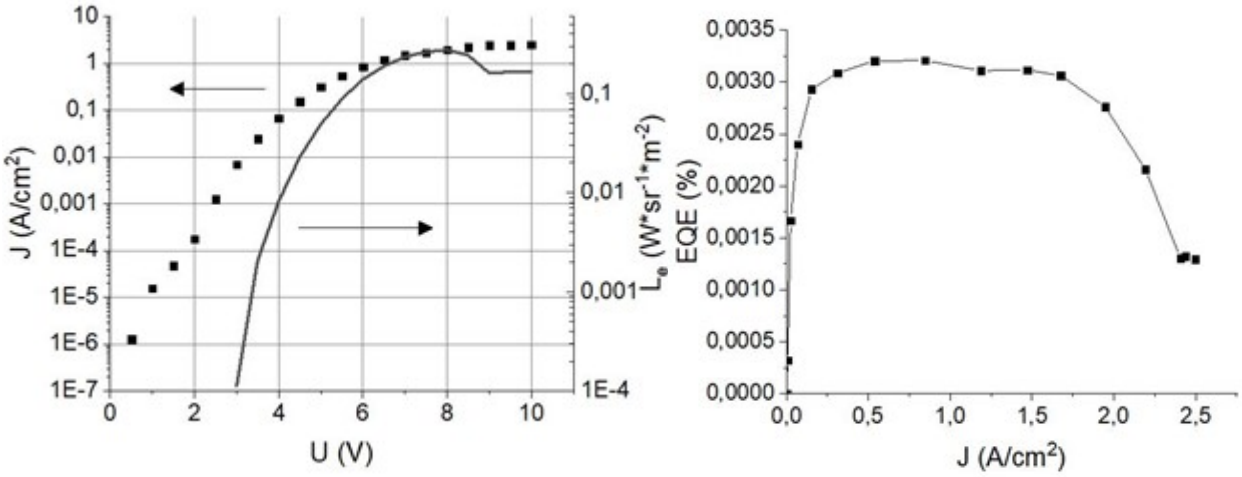

Figure S14. J-V-L_e curves and EQE of ITO / PEDOT:PSS / PVK / 20% F8BT : 80% DTDPAB / Ba / Al device.

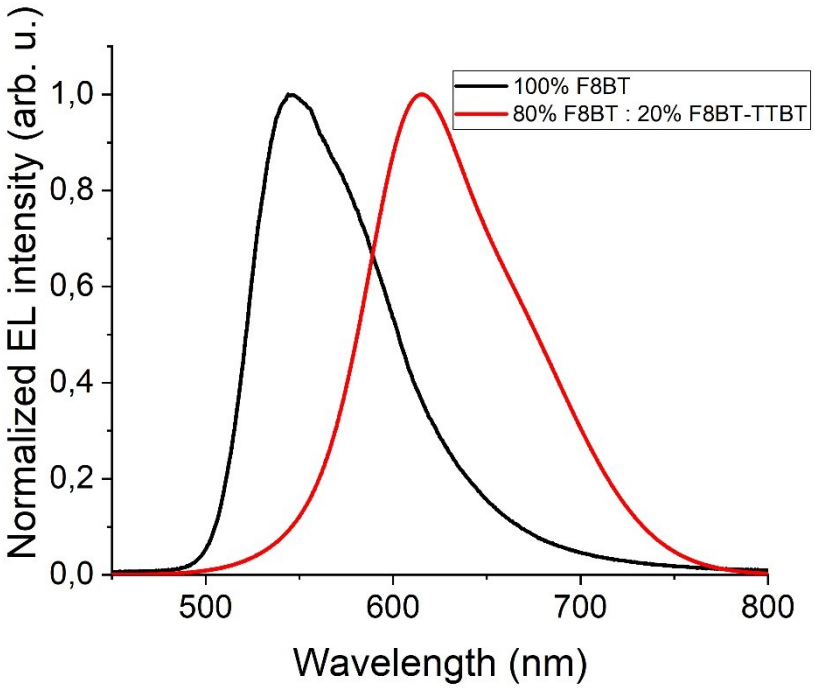

Fig. S15. Normalized electroluminescence spectra of devices with the emitting layers consisting of 100% F8BT and 80% F8BT : 20% F8BT-TTBT.

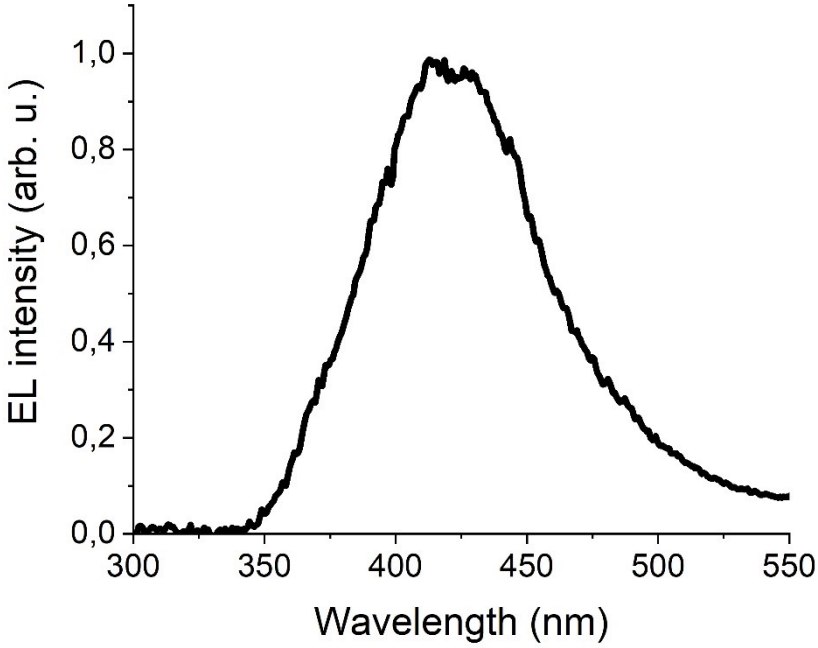

Figure S16. EL spectrum of a device with neat PVK as the emitter.

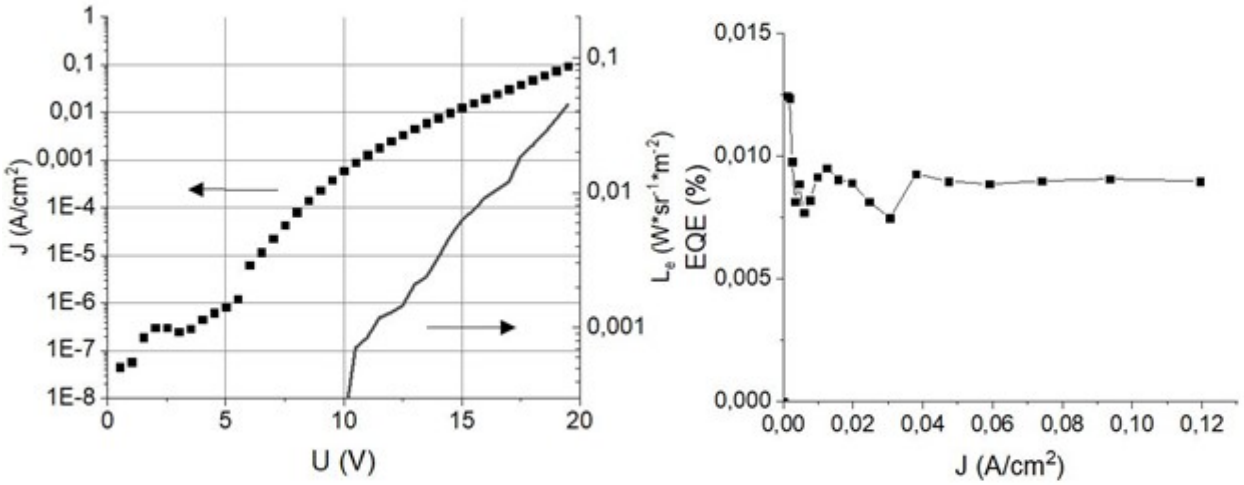

Figure S17. J-V-L_e curves and EQE of ITO / PEDOT:PSS / PVK / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / TPBi / Ba / Al device.

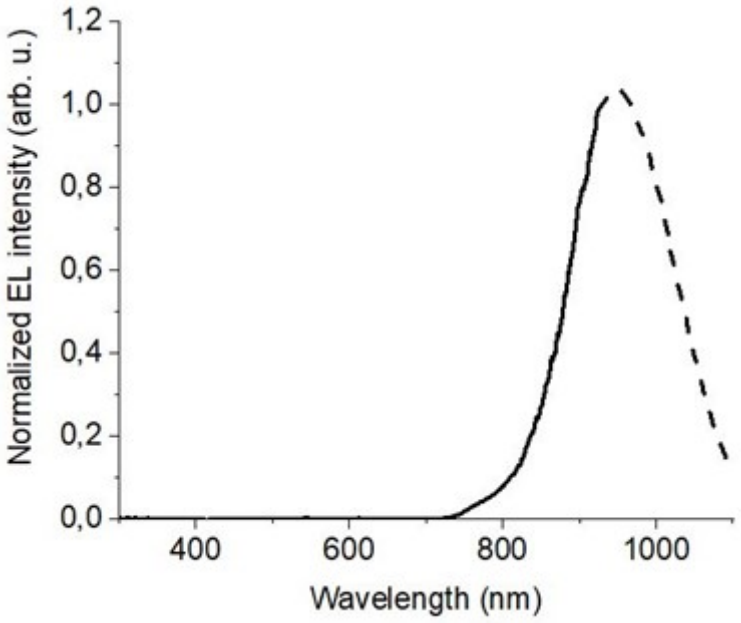

Figure S18. EL at 100 mA/cm^2 of ITO / ZnO / PEIE / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / CBP / MoO_3 / Al device. Dashed line shows simulated extrapolation of the spectrum.

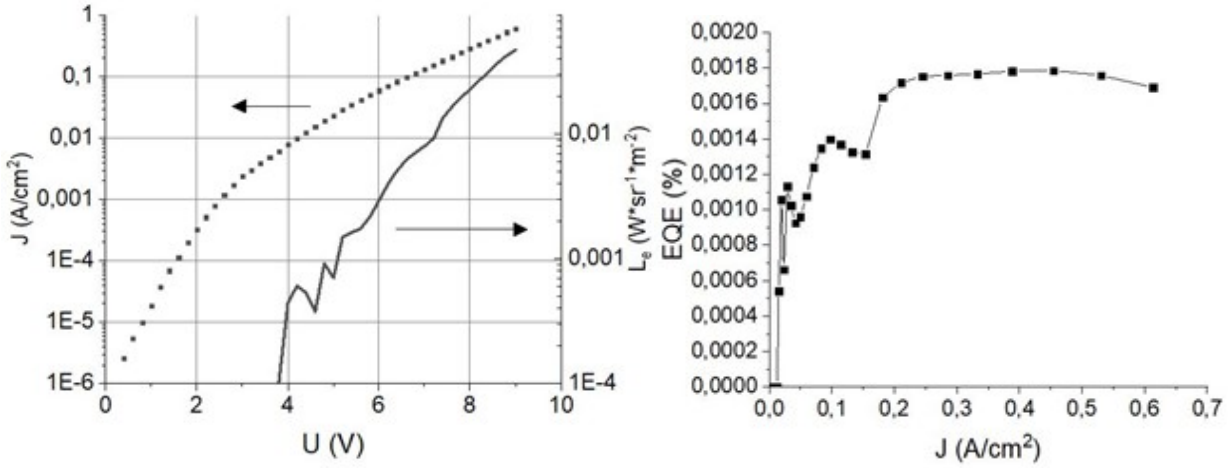

Figure S19. J-V-L_e curves and EQE of ITO / ZnO / PEIE / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / CBP / MoO_3 / Al device.

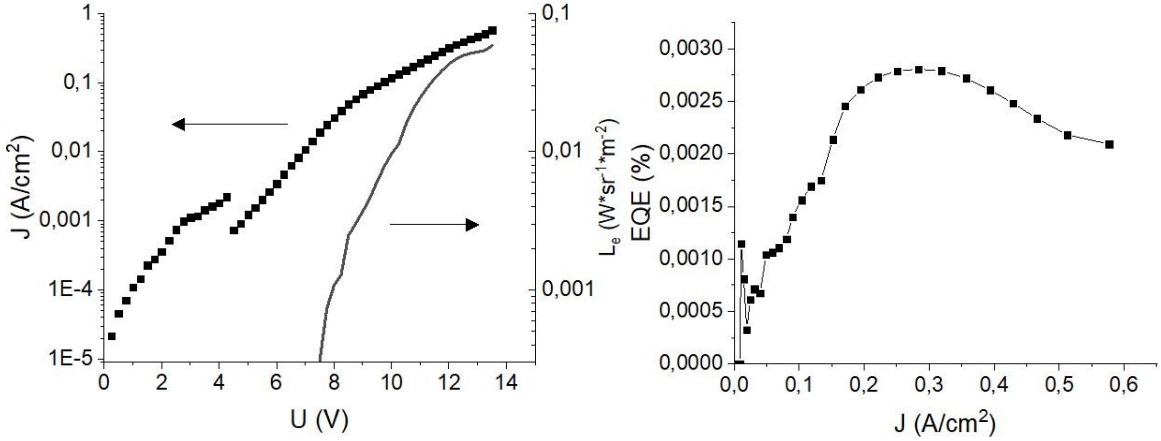

Figure S20. J-V-L_e curves and EQE of ITO / ZnO / PEIE / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / CBP / Au device.

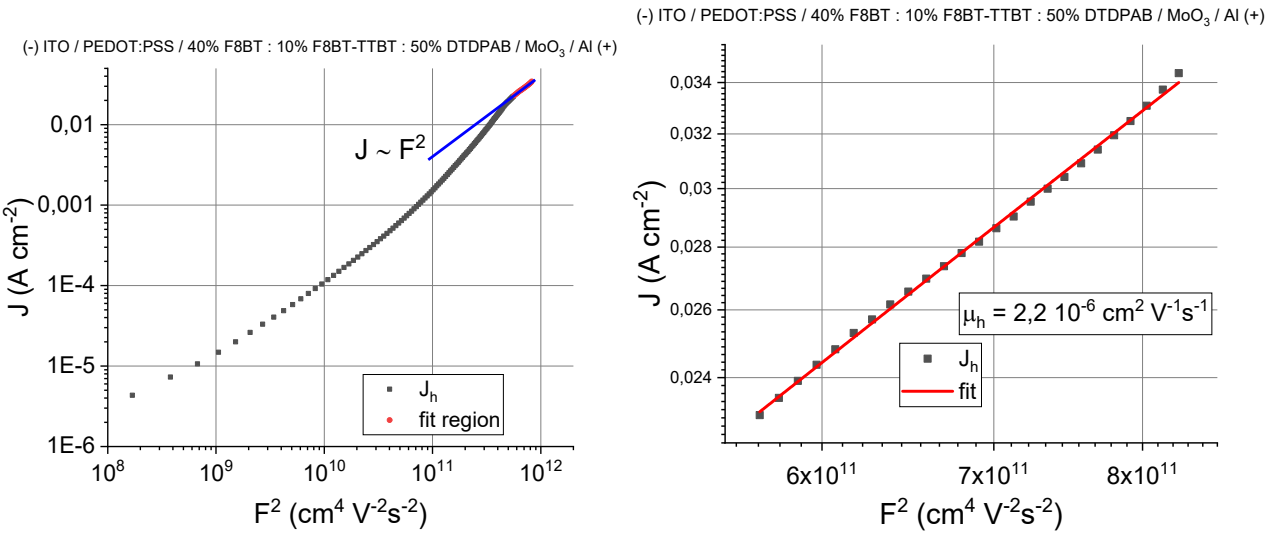

Figure S21. J-F^2 curve of the hole-only device ITO / PEDOT:PSS / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / MoO_3 / Al and the best linear fit with the Mott-Gurney law to the hole current density in the electric field range where space charge limited current was recorded ($J \sim F^2$).

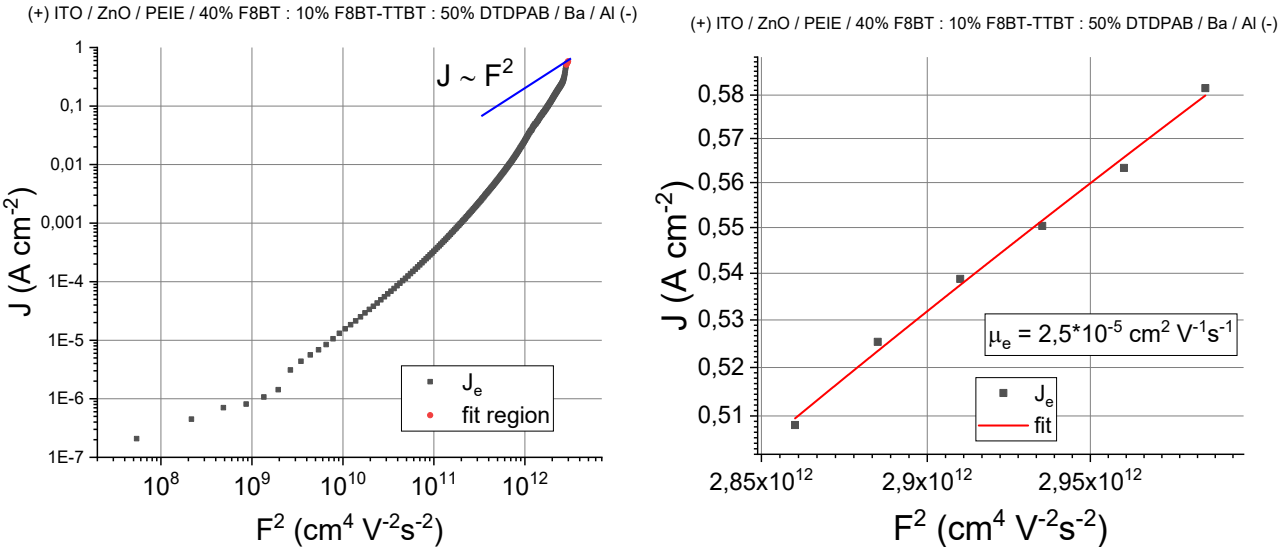

Figure S22. J-F^2 curve of the electron-only device ITO / ZnO / PEIE / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / Ba / Al and the best linear fit with the Mott-Gurney law to the electron current density in the electric field range where space charge limited current was recorded ($J \sim F^2$).

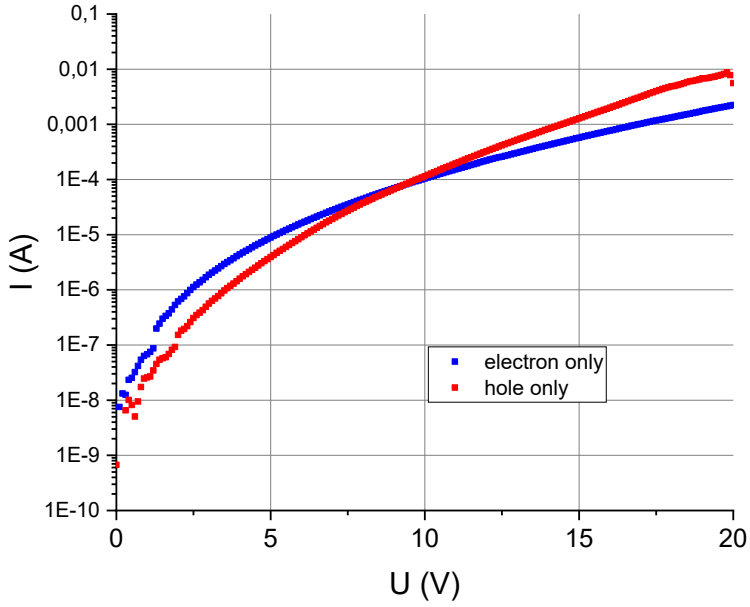

Figure S23. Electron and hole currents in the electron-only device ITO / ZnO / PEIE / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / CBP / Ba / Al and hole-only device ITO / PEDOT:PSS / 40% F8BT : 10% F8BT-TTBT : 50% DTDPAB / CBP / MoO_3 / Al.

References

1 M. D. Iosip, S. Destri, M. Pasini, W. Porzio, K. P. Pernstich and B. Batlogg, *Synthetic Metals*, 2004, **146**, 251–257.