Supplementary Information

High Open-Circuit Voltage Small-Molecule p-DTS(FBTTh$_2$)$_2$:ICBA Bulk Heterojunction Solar Cells - Morphology, Excited-State Dynamics, and Photovoltaic Performance

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***J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA solar cells**

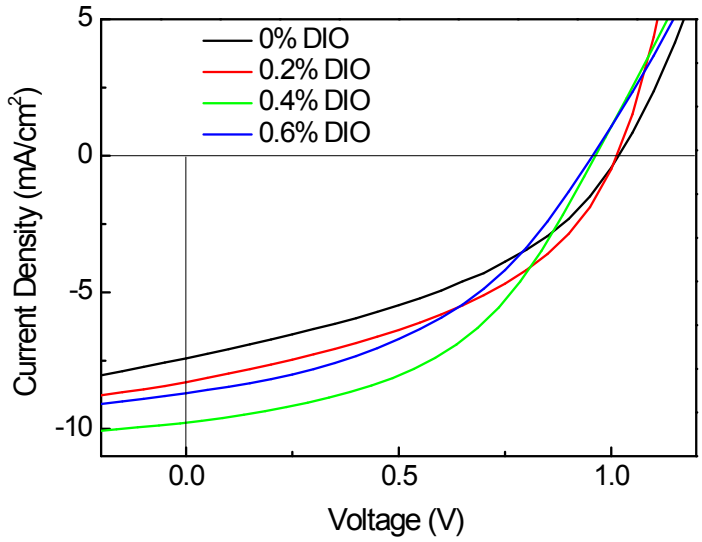

Fig. S1 *J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA solar cells processed with various contents of DIO (0%, 0.2%, 0.4% and 0.6%) under AM 1.5G irradiation at 100 mW/cm^2. The blend ratio of p-DTS(FBTTh$_2$)$_2$:ICBA is 1.5:1.

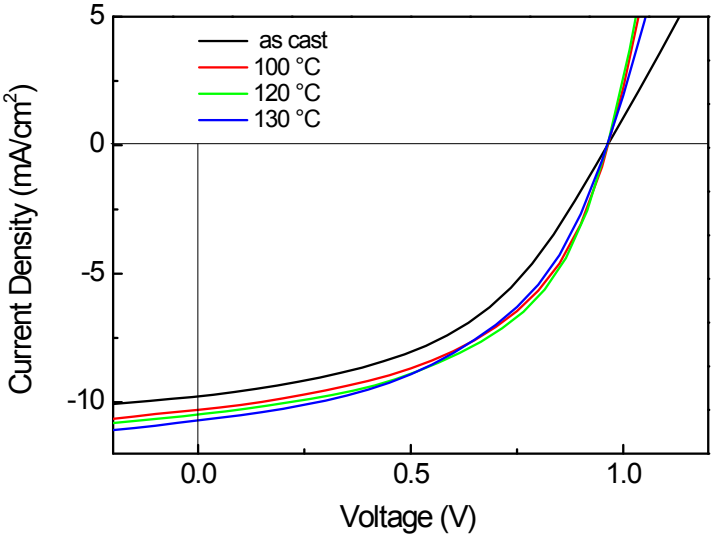

Fig. S2 *J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA solar cell after annealing at different temperatures. The solar cells were fabricated from 1.5:1 blend ratio of p-DTS(FBTTh$_2$)$_2$:ICBA with 0.4% DIO.

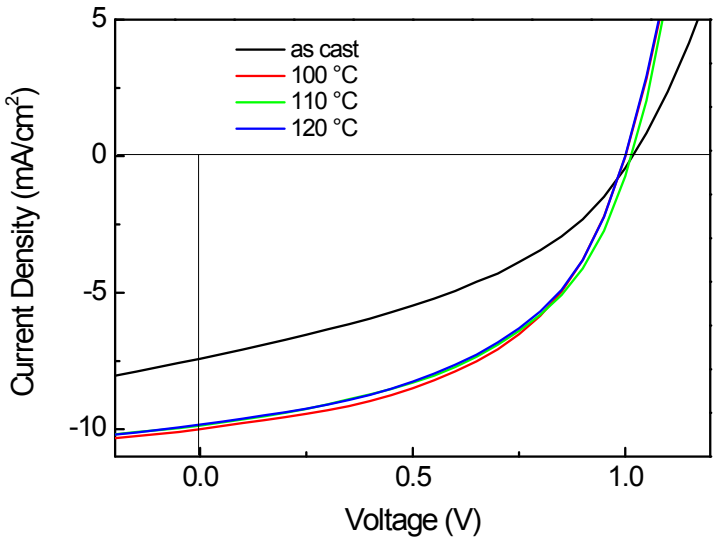

Fig. S3 *J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA solar cell after annealing at different temperatures. The solar cells were fabricated from 1.5:1 blend ratio of p-DTS(FBTTh$_2$)$_2$:ICBA without DIO.

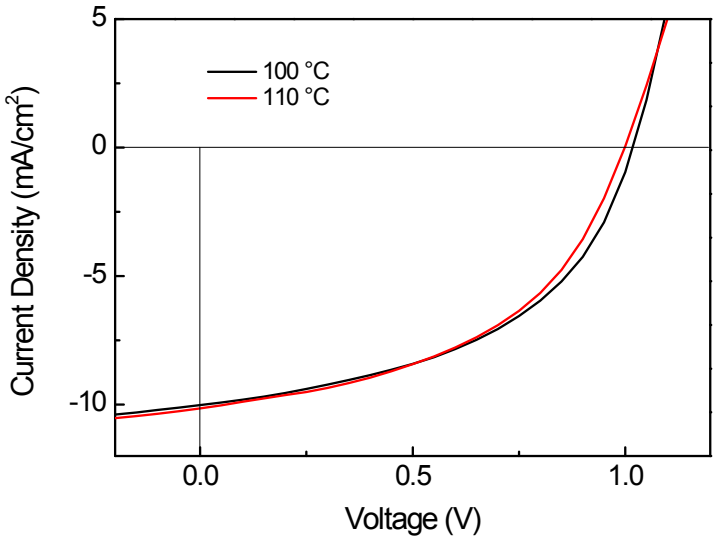

Fig. S4 *J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA solar cell fabricated from 2.3:1 blend ratio of p-DTS(FBTTh$_2$)$_2$:ICBA (without DIO) and annealed at different temperatures.

Comparison between p-DTS(FBTTh$_2$)$_2$:ICBA and p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM (Absorption and EQE spectrum)

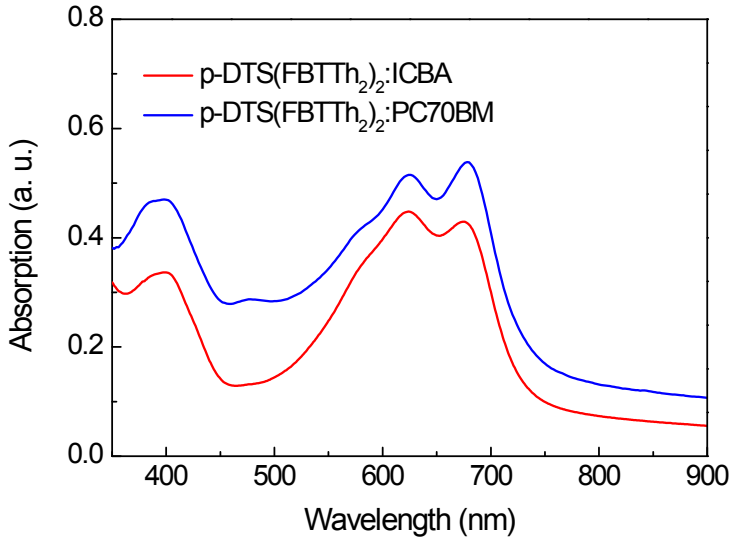

Fig. S5 UV-Vis absorption spectrum of p-DTS(FBTTh$_2$)$_2$:ICBA and p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM blend under optimized condition.

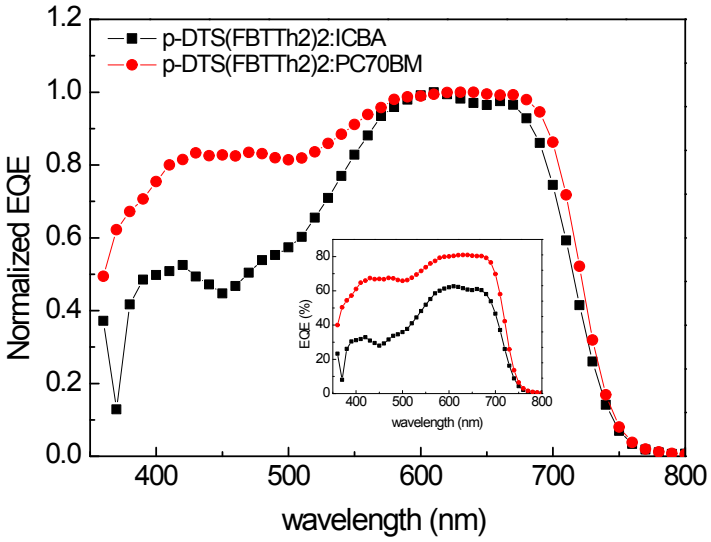

Fig. S6 Normalized EQE spectrum of p-DTS(FBTTh$_2$)$_2$:ICBA and p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM solar cells. Inset shows the absolute EQE spectrum of two cells.

U-Vis absorption spectra show that absorption of p-DTS(FBTTh$_2$)$_2$:ICBA is lower than that of p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM, especially in the region below 580 nm, owing to the lack of absorption tail of ICBA in visible region. The normalized EQE spectra (normalized by peak value of individual device) also reveal that EQE sharply drops below the wavelength of 580 nm. Since internal quantum efficiency (IQE) is pretty flat throughout the spectrum, EQE reflects the absorption of BHJ film. The sharp drop in absorption below the wavelength of 580 nm is the main reason for low Jsc in p-DTS(FBTTh$_2$)$_2$:ICBA solar cell.

Comparison between p-DTS(FBTTh$_2$)$_2$:ICBA and p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM solar cells (Dark J-V characteristics)

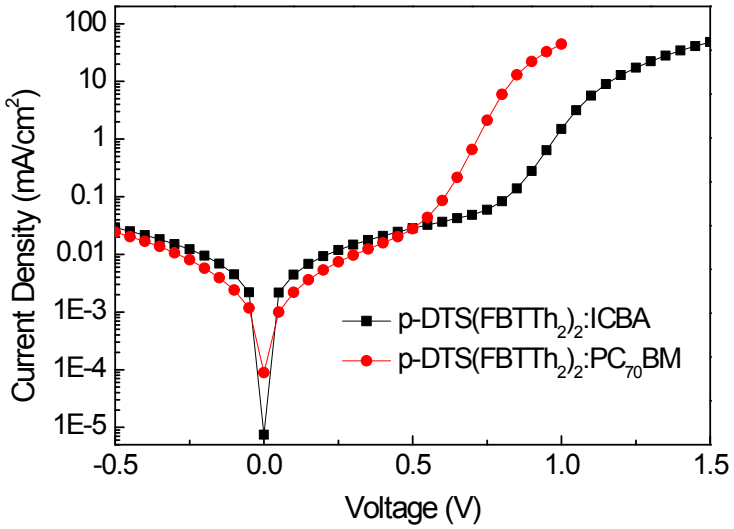

Fig. S7 *J-V* characteristics of p-DTS(FBTTh$_2$)$_2$:ICBA and p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM solar cells in the dark.

The dark *J-V* curve of p-DTS(FBTTh$_2$)$_2$:ICBA solace cell shows high rectification ratio and low leakage current which are comparable to that of p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM solar cell. The high rectification ratio and low leakage current ensure the good quality interface between the BHJ and electrodes.

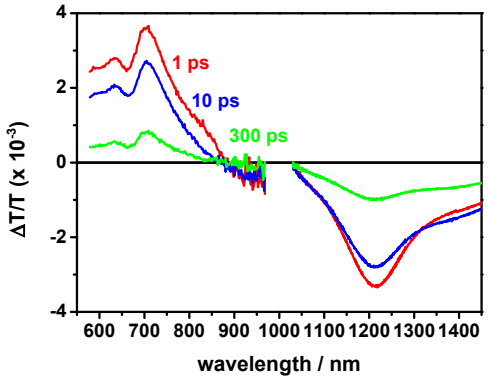

Fig. S8 Spectra of neat p-DTS(FBTTh$_2$)$_2$ film after excitation with 520 nm.

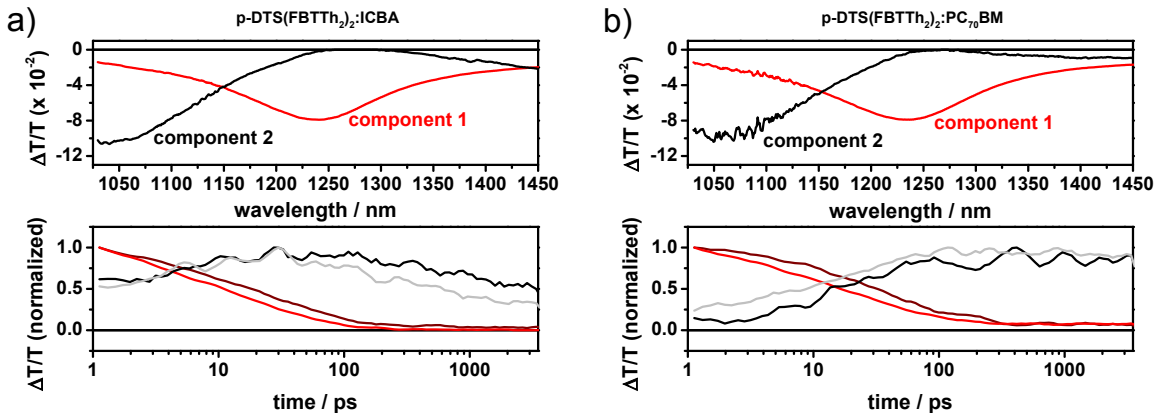

Fig. S9. Spectra (upper panel) and concentration profiles (lower panel) obtained from MCR-ALS analysis of a) p-DTS(FBTTh$_2$)$_2$:ICBA and b) p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM NIR data.

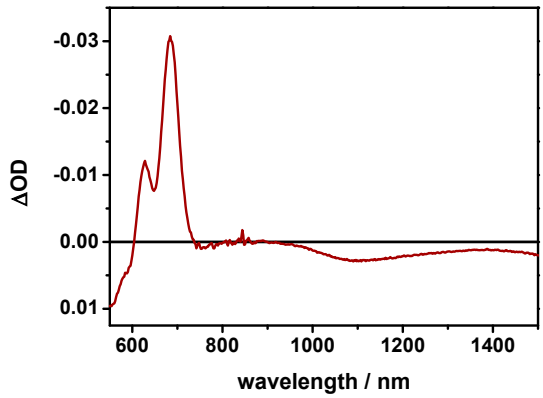

Fig. S10. Iodine vapour oxidized film of p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM

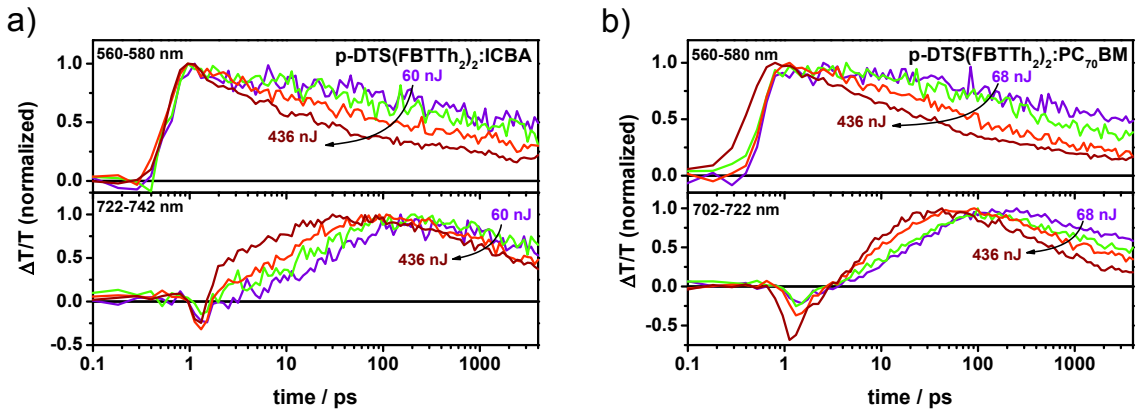

Fig. S11 Kinetics of p-DTS(FBTTh$_2$)$_2$:ICBA tracked at 560-580 nm (ground-state bleach, upper panel) and 722-742 (0-transition at 1 ps, lower panel) and b) p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM at 560-580 nm (ground-state bleach, upper panel) and 702-722 (0-0 transition at 1 ps, lower panel).

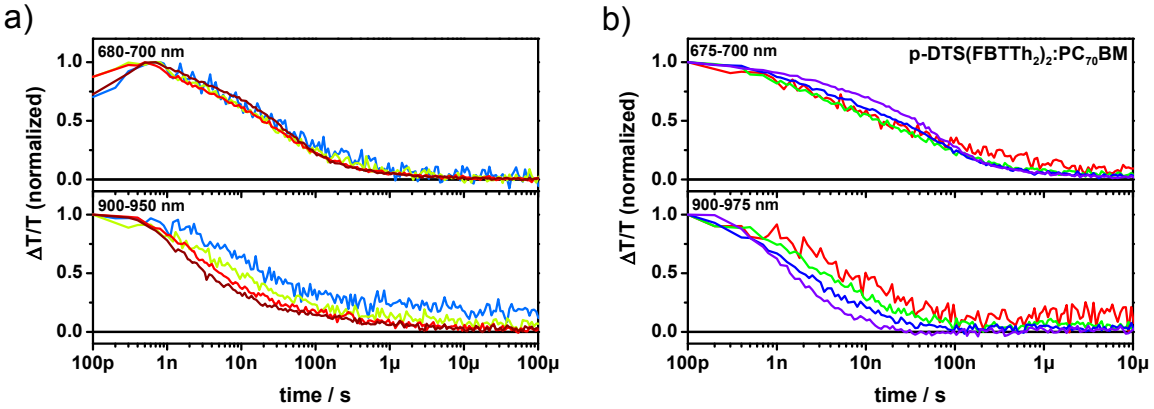

Fig. S12 a) Kinetics of p-DTS(FBTTh$_2$)$_2$:ICBA films tracked at 680-700 nm (upper panel, GSB) and at 900-950 nm (lower panel, PIA); b) Kinetics of p-DTS(FBTTh$_2$)$_2$:PC$_{70}$BM films tracked at 675-700 nm (upper panel, GSB) and at 900-975 nm (lower panel, PIA).