Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information to

Initiator free crosslinking of oxetane functionalized low bandgap polymers: An approach towards stabilized bulk heterojunction solar cells

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A. Cationic ring-opening polymerization of oxetane

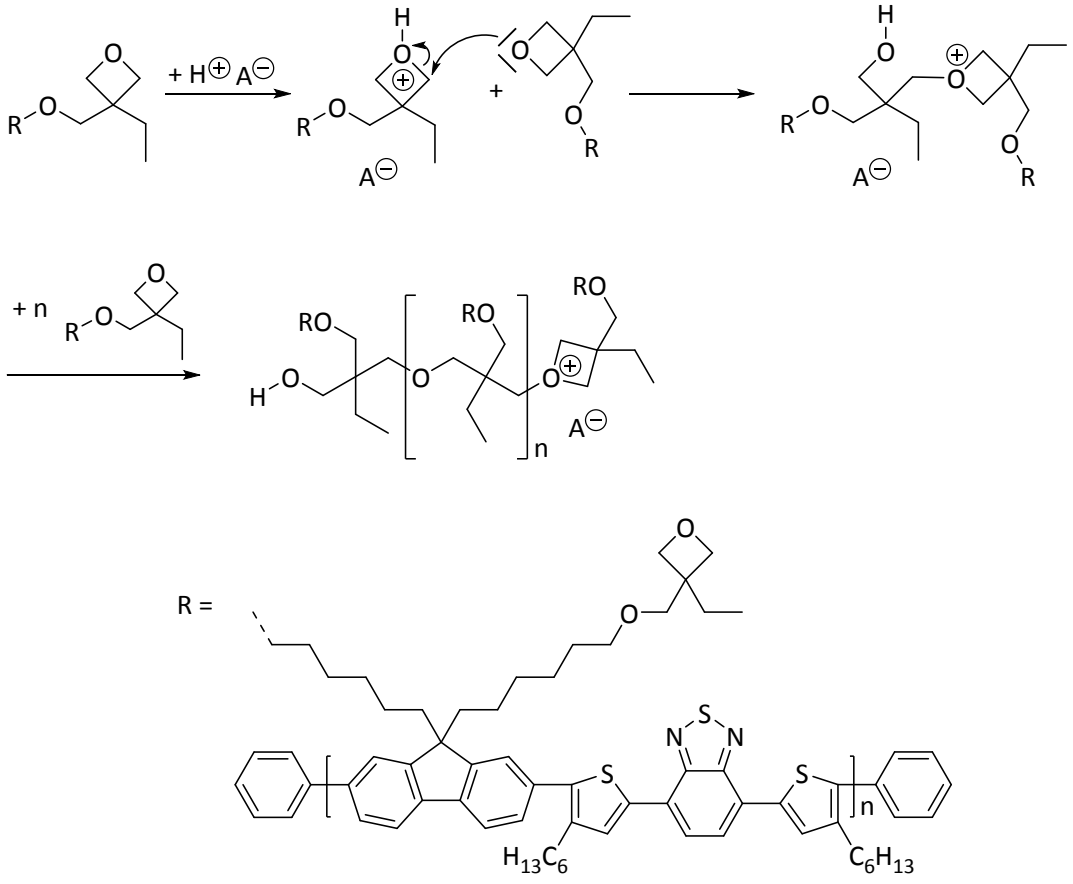

Figure S 1. Mechanism of the cationic ring-opening polymerization of oxetane after reference [1].

B. Crosslinking in the presence of PCBM

The crosslinkable polymer PFDTBTOx and the fullerene derivative PCBM (1:2 w/w, 30 mg ml^{-1}) were mixed in a solution of chlorobenzene. After spin coating and drying, absorption spectra were recorded. In an inert argon atmosphere films were exposed to TFA at 100 °C followed by storage in vacuum at 60 °C for 30 minutes. To estimate the crosslinking efficiency, the optical densities before and after rinsing with solvent were compared.

The absorption spectra are shown in Figure S 2. In the range of 280 to 400 nm most of the optical density is lost after rinsing. However, the remaining absorption spectrum matches the spectrum of neat PFDTBTOx. The low bandgap polymer is crosslinked successfully, remaining as insoluble layer. All the loss of optical density during rinsing is assigned to PCBM. The low-molar mass acceptor is not incorporated into the polymer network by chemical bonds. PCBM is easily washed out of the thin samples, leaving behind the polymer scaffold.

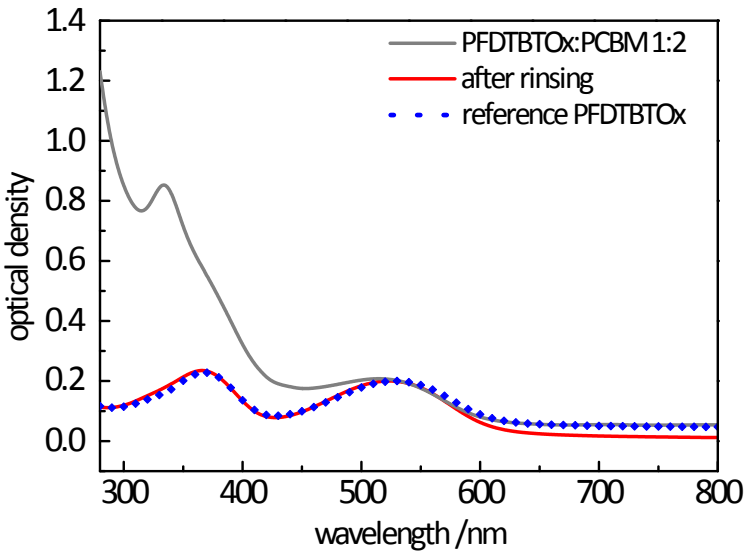

Figure S 2. Crosslinking of PFDTBTOx in a blend with PCBM. The sample was exposed to TFA vapor at 100 °C for five minutes. The reference spectrum of PFDTBTOx was normalized to the maximum at 530 nm.

C. Accelerated aging

Blends of PFDTBTOx:PCBM and PFDTBT:PCBM were cast on glass slides. The films were annealed at 100 °C under inert atmosphere for up to 100 hours. By polarization microscopy the samples were checked for PCBM aggregates.

PFDTBTOx:PCBM 1:2 crosslinked in TFA vapor

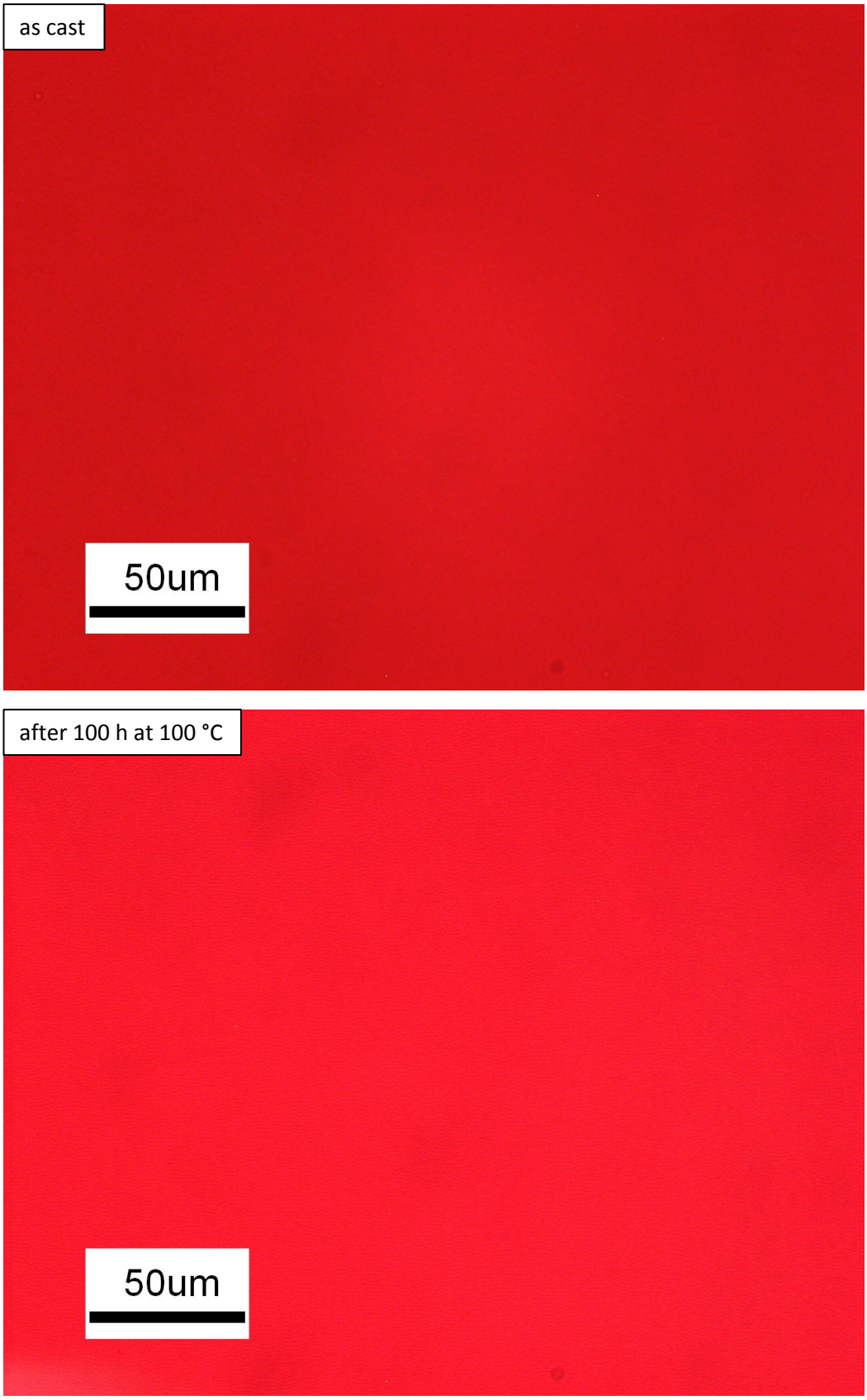

Figure S 3. Optical micrographs of a PFDTBTOx:PCBM 1:2 blend. The films were crosslinked in TFA vapor prior to annealing at 100 °C for 100 hours.

PFDTBTOx:PCBM 1:2

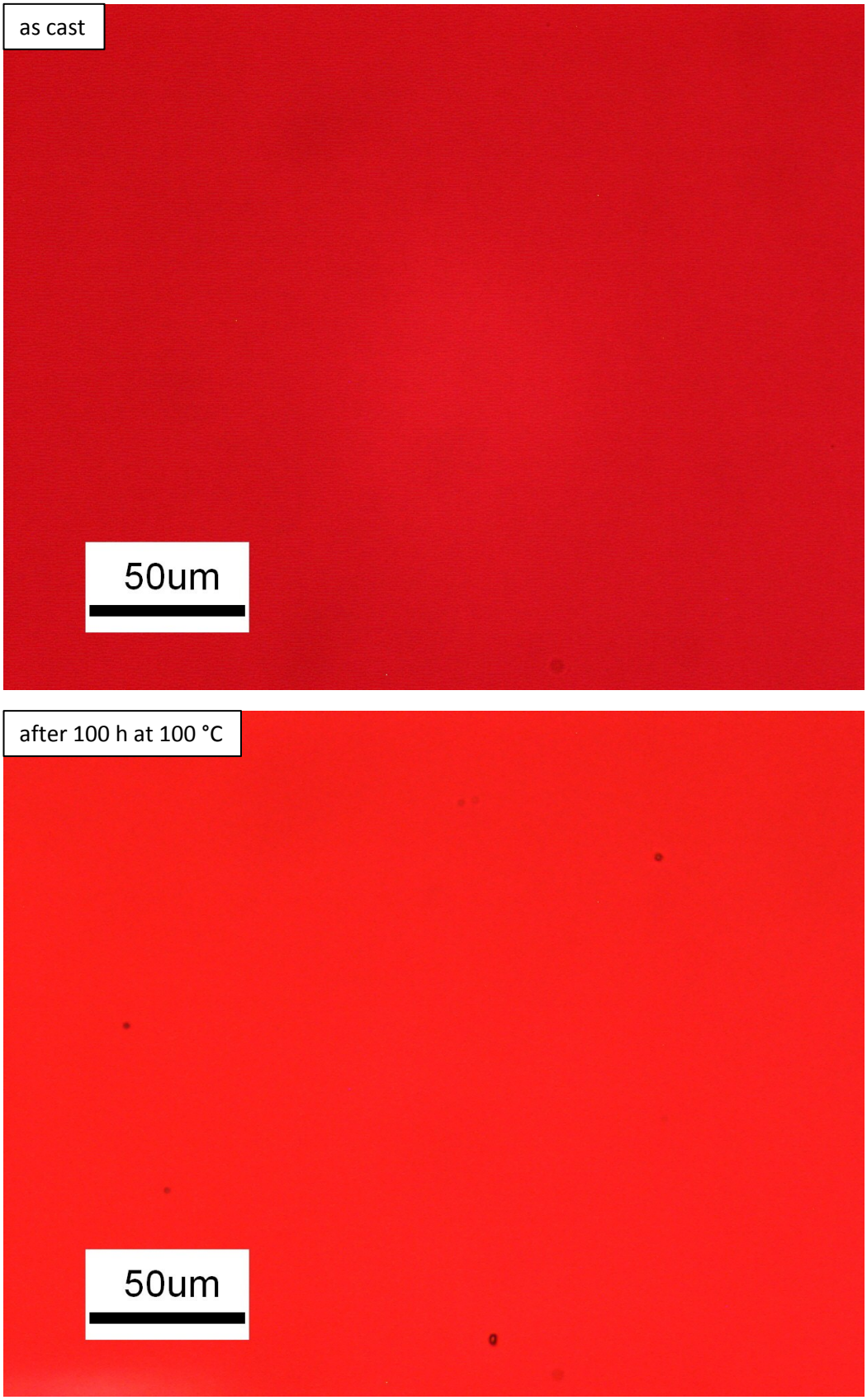

Figure S 4. Optical micrographs of a PFDTBTOx:PCBM 1:2 blend.

PFDTBT:PCBM 1:2

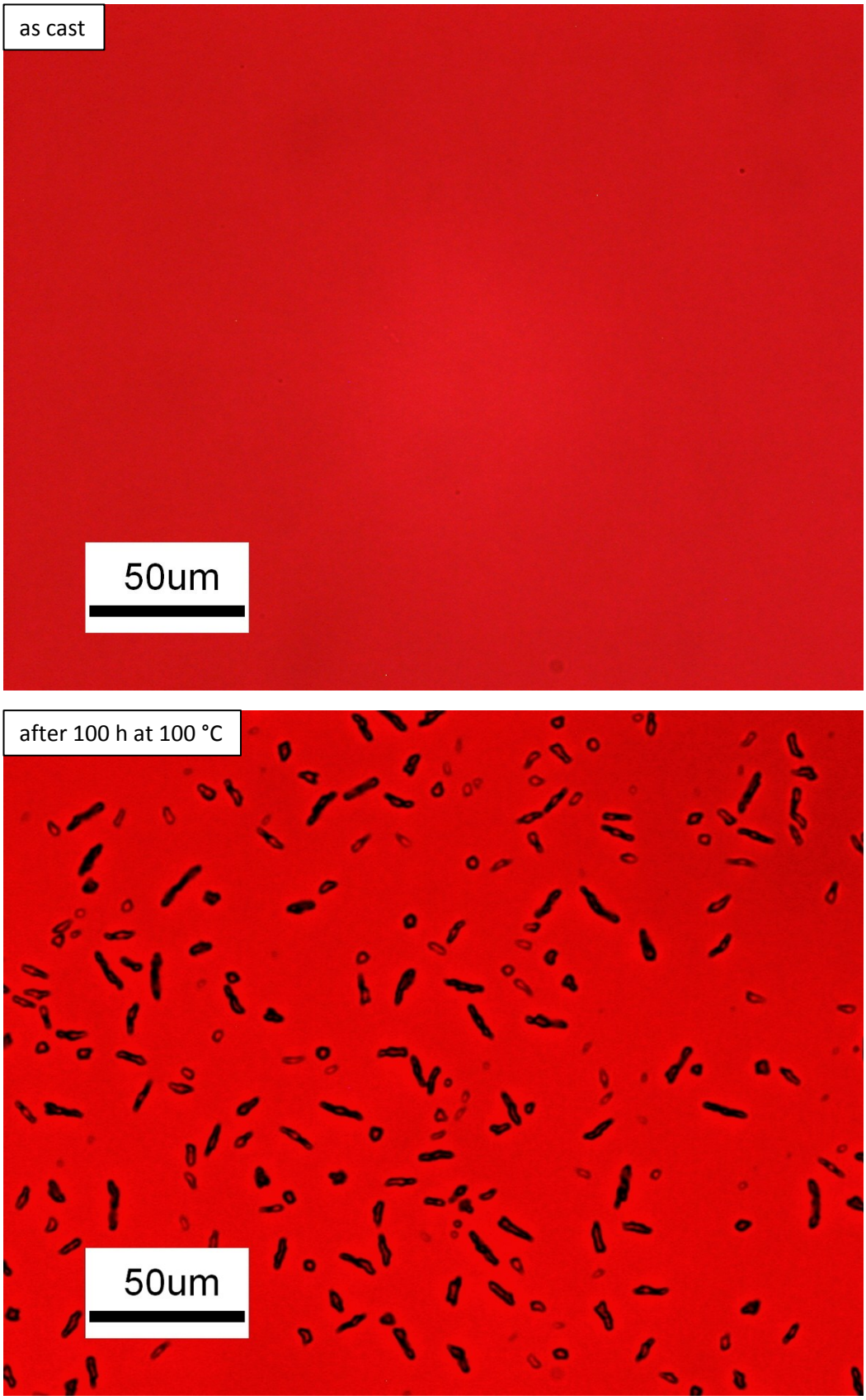

Figure S 5. Optical micrographs of a PFDTBT:PCBM 1:2 blend.

D. Accelerated aging of BHJ solar cells

The current-voltage (*J-V*) characteristics of the solar cells were measured for every single interval of annealing. Figure S 6 shows the *J-V* curves.

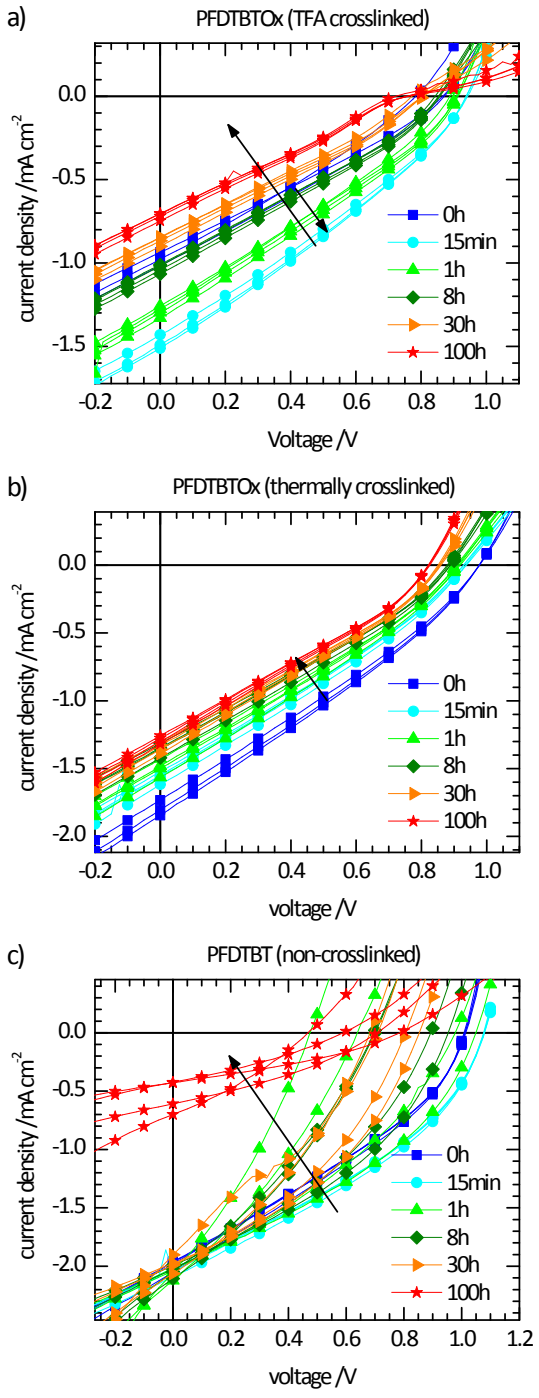

Figure S 6. *J-V* characteristics from accelerated aging tests of the TFA crosslinked PFDTBTOx (**a**), thermally crosslinked PFDTBTOx (**b**), and non-crosslinkable PFDTBT (**c**) in a polymer:PCBM blend with a 1:2 ratio. For each material combination four solar cells were measured.

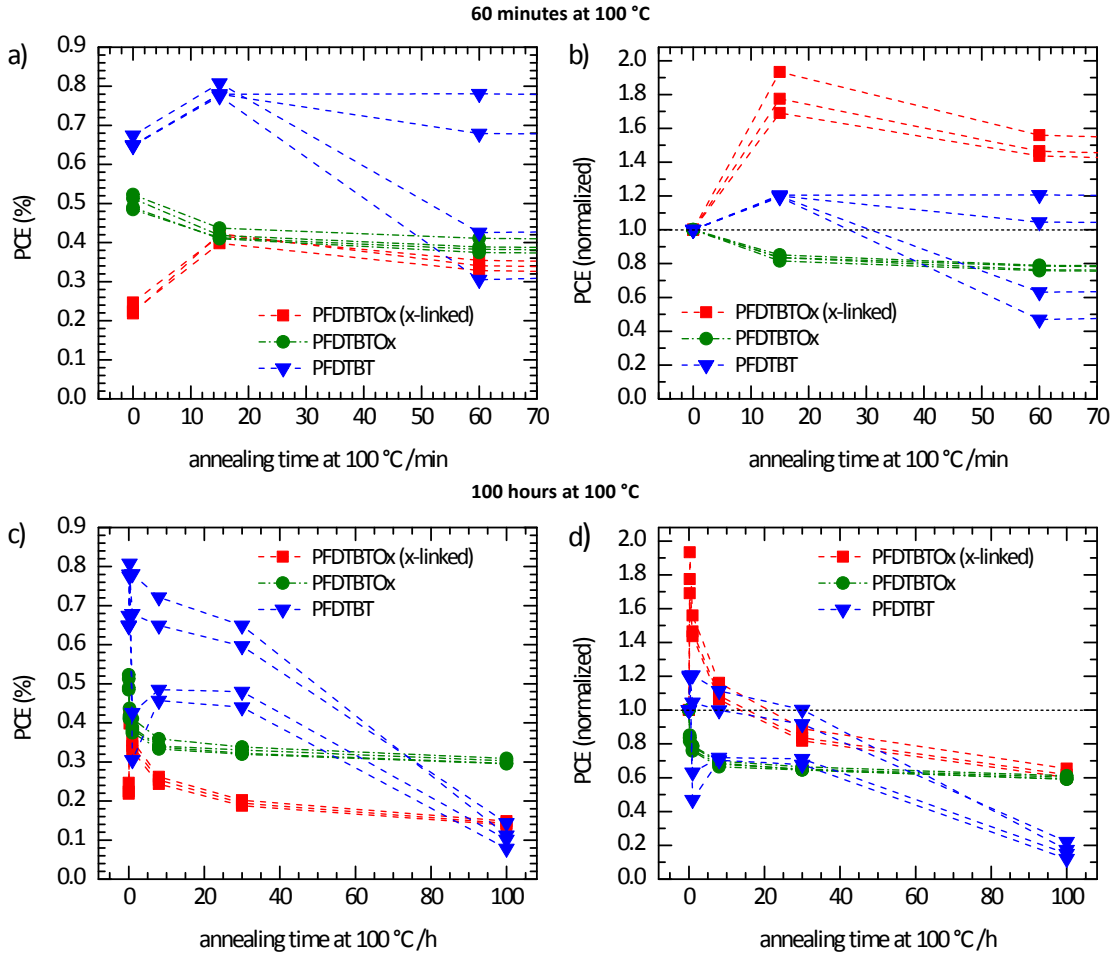

Figure S 7. Development of the PCE for the TFA crosslinked PFDTBTOx, thermally crosslinked PFDTBTOx and non-crosslinkable PFDTBT in a 1:2 blend ratio with PCBM. At the top the PCE during the first 60 minutes of annealing at 100 °C is displayed. At the bottom the development for up to 100 hours at 100 °C is shown. Absolute PCE values are shown on the left (a, c). On the right the relative PCE normalized to the starting value is displayed (b, d). For each system four different cells were measured.

References

1 M. C. Gather et al., *Adv. Funct. Mater.*, 2007, **17**, 191–200.