Supplementary information

Correlating triplet yield, singlet oxygen generation and photochemical stability in donor/acceptor blend films

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Experimental

Materials

The synthetic detail for the polymer DPP-TT-T has been previously published.[1] PTB7 was purchased from 1-Material and purified before use. Purification was carried out with soxhlet extraction by Shahid Ashraf, whereby the polymer was extracted with acetone, n-hexane and diethylether (each 12-24 hours). Then the polymer was extracted with chloroform (chloroform solution was concentrated and precipitated in methanol), filtered and redissolved in chloroform and precipitated again in methanol. Finally, the polymer was filtered and dried for two days under high vacuum. $PC_{71}BM$ was obtained from Solenne and used as received.

Films fabrication

Solutions for DPP-TT-T films were prepared with chloroform at ~10mg/ml for neat films and ~18mg/ml for DPP-TT-T:$PC_{71}BM$ (1:2) blend films. For PTB7 films, solutions were prepared with a mixture of 97% chlorobenzene and 3% 1,8-diodoctane at ~15mg/ml for neat films and ~25mg/ml for PTB7:$PC_{71}BM$ (1:1.25) blend films. The blend films' compositions were chosen from the optimum device performance. All polymer films were fabricated by spin coating onto glass substrate, which had been cleaned by sonication in acetone and isopropanol for 15 min respectively.

Measurements

Transient absorption data were collected on films with a microsecond transient absorption system under nitrogen atmosphere as detailed previously.[2]

The films were degraded by exposing to white light irradiation from Luxeon Star white LED (~80 $mWcm^{-2}$) under pure oxygen environment. Ground state absorption spectra were then obtained as a function of illumination time using a UV-1601 Shimadzu uv-vis spectrophotometer. Control data in the absence of illumination showed no measureable degradation.

The fluorescence probe used for singlet oxygen detection is the Singlet Oxygen Sensor Green (SOSG) reagent which was purchased from Molecular Probes. Stock solutions of concentration ~5 mM were prepared by dissolving one 100µg vial in 33µL of methanol. The stock solutions were then diluted with deionised water to 0.5µM as reported by Manceau et al.[3] The films were immersed into the SOSG solution and irradiated at ~80 $mWcm^{-2}$ (wavelength below 510 nm were filtered out to minimise self-excitation of the SOSG solution). Fluorescence spectra of the SOSG solution were then obtained using a Horiba Jobin Yvon spectrofluorimeter with an excitation wavelength of 504 nm.

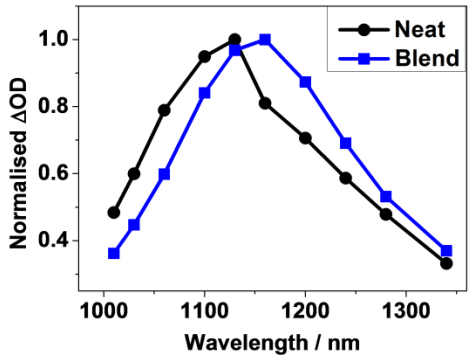

Figure S1: Normalised transient absorption spectra of PTB7 neat and PTB7: $PC_{71}BM$ blend films at 1µs after laser excitation at 630nm under nitrogen atmosphere, assigned to PTB7 triplet and polaron states respectively. These assignments are made on the basis of their decay dynamics (see Figures 1 and S2), and in particular upon the dependence of these decay dynamics on the presence of oxygen. The acceleration of the PTB7 neat film decay observed in the presence of oxygen is typical of that we have observed previously for polymer triplets states.[4] On the other hand, the blend film absorption decay kinetics are unaffected by the presence of oxygen, as we have typically observed for polaron signals.

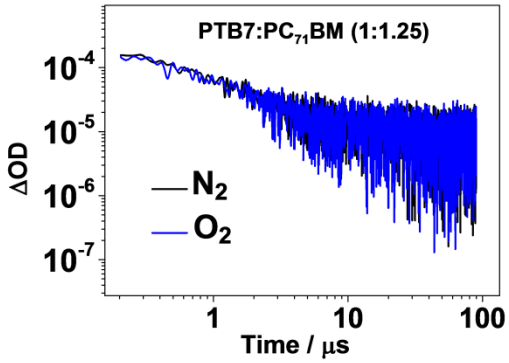

Figure S2: The transient absorption decay kinetics of PTB7: $PC_{71}BM$ blend film measured using 1.4 µJcm^{-2} excitation at 630 nm and probed at 1200 nm under nitrogen and oxygen environments. The decay kinetics followed a power law decay and are not quenched under the presence of oxygen, and are therefore assigned to non-geminate recombination of dissociated polarons.

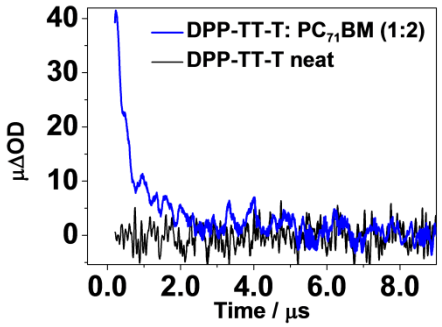

Figure S3: The transient absorption decay kinetics of DPP-TT-T neat and DPP-TT-T: $PC_{71}BM$ blend films measured using 3.3 µJcm^{-2} excitation at 640 nm and probed at 980 nm. The blend film follows power law decay kinetics (straight line on log/log plot, not shown) whereas no transient signal can be observed in the neat film.

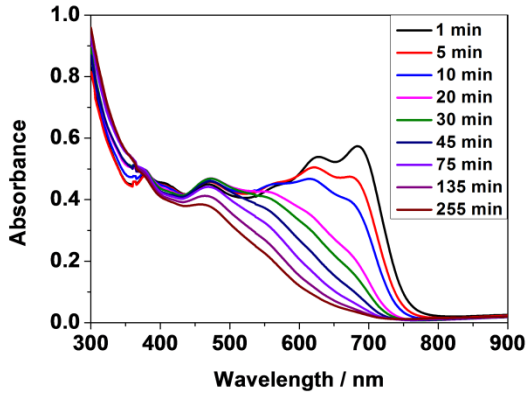

Figure S4: Change in uv-vis absorption spectrum of PTB7:$PC_{71}BM$ blend film under pure oxygen environment with white light ($\lambda > 410$ nm) irradiation time.

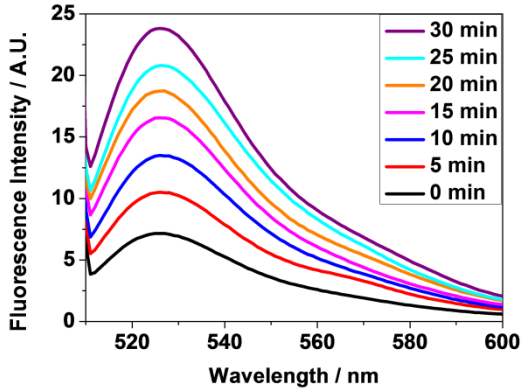

Figure S5: Change in fluorescence spectrum of the singlet oxygen sensor green (SOSG) solution with white light irradiation ($\lambda > 550$ nm) time on PTB7:$PC_{71}BM$ blend film.

1. H. Bronstein, Z. Chen, R. S. Ashraf, W. Zhang, J. Du, J. R. Durrant, P. Shakya Tuladhar, K. Song, S. E. Watkins, Y. Geerts, M. M. Wienk, R. A. J. Janssen, T. Anthopoulos, H. Sirringhaus, M. Heeney and I. McCulloch, *J. Am. Chem. Soc.,* 2011, ***133***, 3272-3275.
2. H. Xin, S. Subramaniyan, T.-W. Kwon, S. Shoaee, J. R. Durrant and S. A. Jenekhe, *Chem. Mater.,* 2012, ***24***, 1995-2001.
3. M. Manceau, A. Rivaton and J.-L. Gardette, *Macromol. Rapid Commun.,* 2008, ***29***, 1823-1827.
4. H. Ohkita, S. Cook, Y. Astuti, W. Duffy, M. Heeney, S. Tierney, I. McCulloch, D. D. Bradley and J. R. Durrant, *Chem. Commun.,* 2006, ***(37)***, 3939-3941.