Correlating photovoltaic properties of PTB7-Th:PC71BM blend to photophysics and microstructure as a function of thermal annealing

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Supporting Information

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Figure S1. Atomic force microscopy height images of PTB7-Th:PC_{71}BM blends as a function of thermal annealing. Thermal annealing temperatures are given in inset.
Figure S2: Histogram of domain size distribution of PTB7-Th:CP22BM blend films estimated from AFM height images corresponding to two processing temperatures of (a) RT and (b) 150 °C.
Figure S3. (a) PL intensity comparison of the RT and 150 °C thermally annealed PTB7-Th:PC71BM blend films (b) Time-resolved PL decays of neat PTB7-Th (Blue dots) and PC71BM measured using excitation wavelength of 515 nm.
Figure S4: Absorption spectra of PTB7-Th:PC71BM blends measured at different emission wavelengths. The dotted lines shows the absorption spectra of the neat donor and acceptor films.
Figure S5. Fitted PL decay curves for the PTB7:PC71BM blends as a function of thermal annealing temperature (a) from 815 nm onwards and (b) 850 nm onwards.
Table S1: PL quenching efficiency of the PTB7-Th:PC71BM blend films annealed at different temperatures.

| Thermal annealing temperature (°C) | Φ_0 (720nm) (%) | Φ_0 (820nm) (%) |
|------------------------------------|-----------------|-----------------|
| RT                                 | 71.7±0.7        | 62.2±0.8        |
| 70                                 | 69.9±0.5        | 54.0±0.5        |
| 100                                | 68.4±0.6        | 52.6±0.6        |
| 120                                | 65.7±0.8        | 49.0±1.0        |
| 150                                | 61.4±1.1        | 41.6±1.3        |

Table S2: Domain size of PC71BM and the exciton decay life times of PTB7-Th:PC71BM blend films at different emission wavelengths as a function of thermal annealing.

| T (°C) | 1/e t (ps) | 1/e t (ps) | 1/e t (ps) | Domain size of PC71BM (nm) |
|--------|------------|------------|------------|----------------------------|
|        | \( \lambda_m \) (870-720 nm) | \( \lambda_m \) (815-900 nm) | \( \lambda_m \) (850-900 nm) |                           |
| RT     | 15.9±1.0   | 21.3±2.8   | 28.6±1.9   | 9.1±0.4                   |
| 70     | 19.9±1.6   | 30.1±1.5   | 29.1±2.1   | 10.2±0.7                  |
| 100    | 22±2       | 31.6±1.5   | 33.6±2.2   | 10.8±0.8                  |
| 120    | 23±1.5     | 37.3±1.9   | 43.0±2.0   | 12.3±1.1                  |
| 150    | 38±2       | 57.4±2.4   | 64.3±2.8   | 13.4±0.6                  |

Figure S6: PL ratio of PC71BM in blend to pristine PC71BM. Black lines are best fit achieved using model described in the main paper with diffusion coefficient of 1.6×10⁻⁴ cm²/s.
Figure S7. Normalised 1D diffraction data of PTB7-Th:PC71BM blends as a function of different thermal annealing temperatures for (a) in plane (b) out of plane directions.
Figure S8: Device architectures used for (a) hole mobility and (b) electron mobility measurements.