

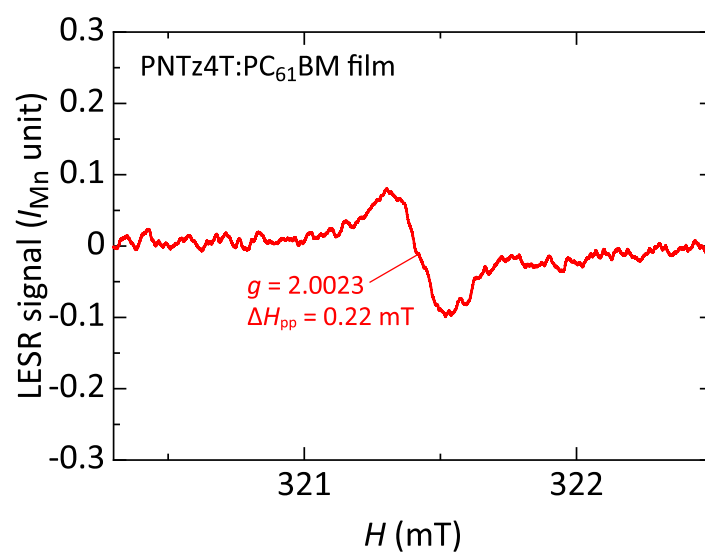
Supplementary Information for

**Microscopic investigation into higher efficiency and stability
of inverted organic solar cells compared to conventional cells**

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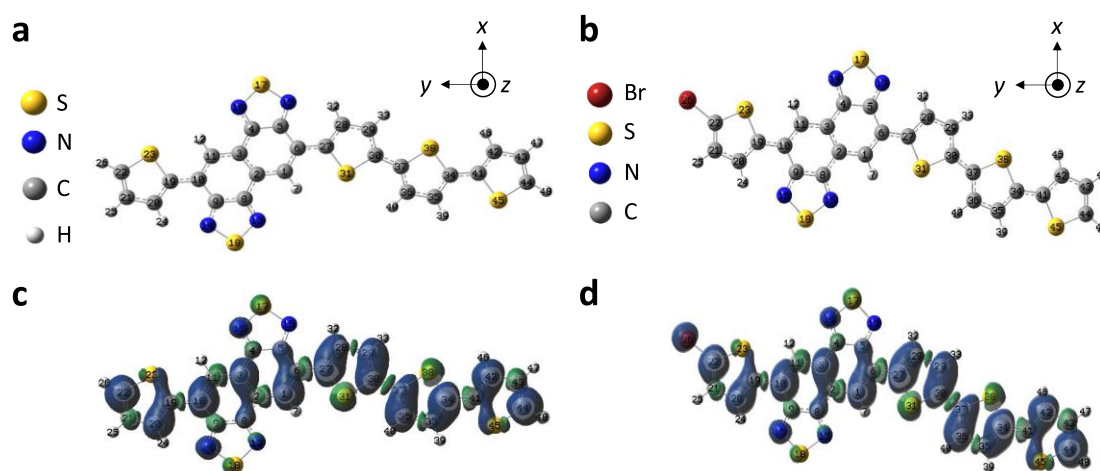
S1. Light-induced ESR spectrum of a PNTz4T:PC₆₁BM film.



Supplementary Figure 1 | Light-induced ESR spectrum of a PNTz4T:PC₆₁BM film.

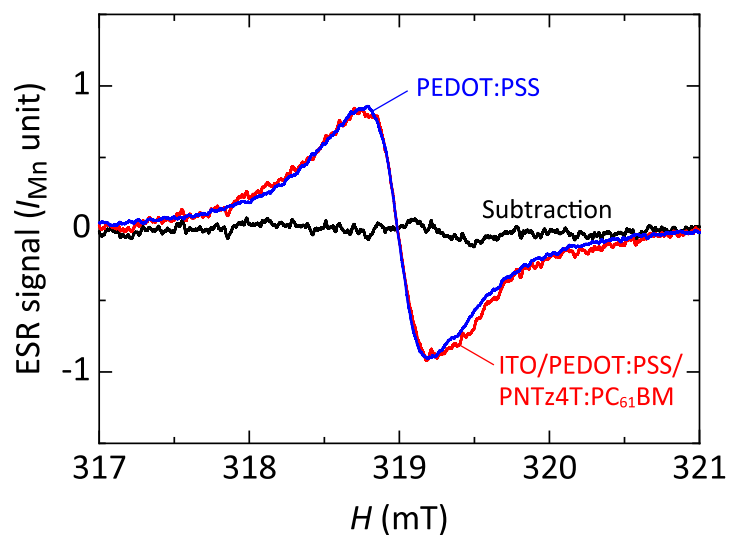
S2. Density functional theory (DFT) calculation.

All calculations were performed with Gaussian 09W with UB3LYP functional and 6-31G(d,p) basis set.



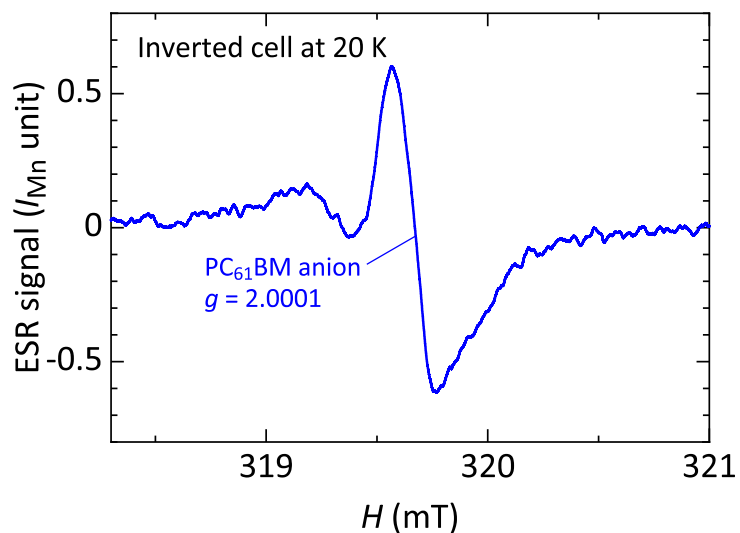
Supplementary Figure 2 | Model monomer molecules of PNTz4T for DFT calculation and spin density distribution in cationic states. a,b, Chemical structures of model monomers of PNTz4T with chain ends of H (**a**) and Br (**b**) used in the DFT calculation. **c,d,** Spin density distributions of the cationic monomers with the chain ends of H (**c**) and Br (**d**) obtained from the DFT calculation.

S3. Charge transfer at organic/organic interface under dark conditions.



Supplementary Figure 3 | ESR spectra of an ITO/PEDOT:PSS/PNTz4T:PC₆₁BM stacked film and a PEDOT:PSS film. No charge transfer at the interface between the layers of PNTz4T:PC₆₁BM and PEDOT:PSS under dark conditions is confirmed by a negligibly small ESR subtraction spectrum (black line), which is obtained by subtracting the ESR spectrum of a PEDOT:PSS film (blue line) from that of an ITO/PEDOT:PSS/PNTz4T:PC₆₁BM stacked film (red line). These spectra were observed under dark conditions at room temperature.

S4. Electron accumulation in an inverted cell by light irradiation at room temperature.



Supplementary Figure 4 | ESR spectrum of an inverted cell in the dark at low temperature after one-sun irradiation at room temperature. ESR spectrum of an inverted cell measured at 20 K shows the signal with a g -factor of 2.0001 originating from long-lived PC₆₁BM anions in addition to the signal due to long-lived PNTz4T cations. Low temperature ESR measurements at 20 K were conducted after one-sun irradiation at room temperature.