High performance polymeric charge recombination layer for organic tandem solar cells

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Supporting information:

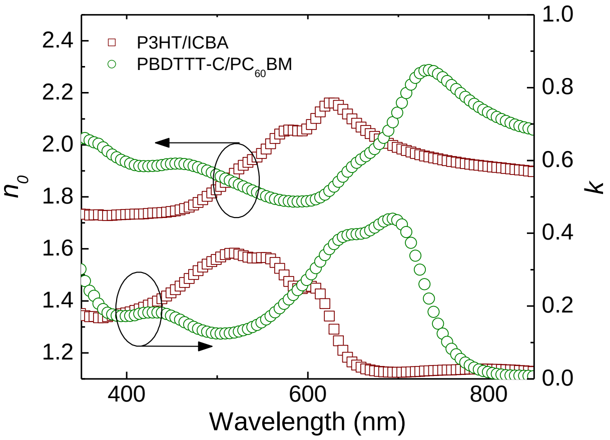

Fig. S1 Complex refractive index spectra derived from spectroscopic ellipsometric measurements on P3HT:ICBA and PBDTTT-C:$PC_{60}BM$ films deposited on glass and annealed as described in the experimental section.

The transfer matrix method was used to conduct simulations of the absorptance spectrum of the two active layers used in the tandem solar cell by assuming smooth single layers on glass and using refractive index values derived from spectroscopic ellipsometry, as shown in Fig. S1. The spectra were normalized (Fig. 2a) with respect to the maximum absorptance value found on the spectral range from 400 to 800 nm.

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Simulations of the short-circuit current density (J_{SC}) in tandem solar cell devices were carried out as follows: the absorptance of reference cells was measured and simulated by adjusting the thicknesses of individual layers using the transfer matrix method; a breakdown of the contribution to the total absorptance of each layer in the solar cell structure was carried out for reference single-junction solar cell devices (A and B) using the transfer matrix method. The absorptance of the active layer, $A_{AL}(\lambda)$, was multiplied by the spectral photon solar irrandiance (AM 1.5), $S_{AM1.5}(\lambda)\left[photons \cdot cm^{-2} \cdot s^{-1} \cdot nm^{-1}\right]$, and its product integrated spectrally. The internal quantum efficiency *IQE* was then approximated as a constant given by:

$$IQE \approx \frac{J_{sc,measured}}{q\int A_{AL}(\lambda) S_{AM1.5}(\lambda) d\lambda}$$

Where $J_{sc,measured}\left[A \cdot cm^{-2}\right]$ represents the average measured short circuit current and q is the elementary charge. In this way, *IQE* values of 0.61 and 0.86 were estimated for Devices A: ITO/PEIE/P3HT:ICBA/PH1000/Ag and Devices B: ITO/PEIE/PBDTTT-C:$PC_{60}BM$/MoO_3/Ag, respectively.

For tandem cell devices, the following expresion was used to estimate the J_{SC} in each subcell:

$$J_{sc,ALx} = \int q \cdot IQE_{ALx} A_{ALx}(\lambda) S_{AM1.5}(\lambda) d\lambda$$

The J_{SC} of the tandem solar cell was taken as the minimum value between $J_{SC,AL1}$ and $J_{SC,AL2}$.

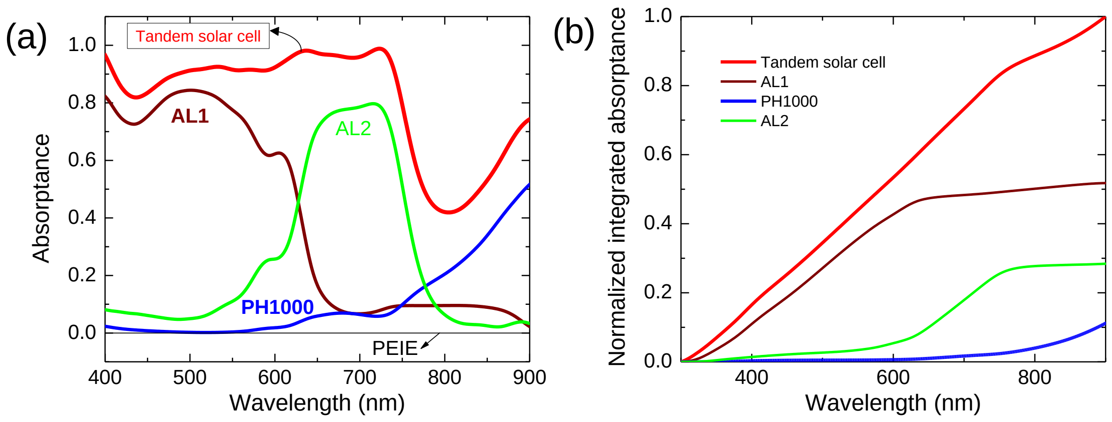

Fig. S2 (a) Simulation of the absoprtance in a tandem solar cell with optimized geometry and a breakdown of the individual contributions of the AL1: P3HT/ICBA (wine), PH1000 (blue), PEIE (black) and AL2: PBDTTT-C/$PC_{60}BM$ (green) layers. (b) Integrated absortance per layer.

Fig. S2a shows the simulated total absorptance in the tandem solar cell with optimum geometry: glass/ITO/PEIE(10 nm)/ P3HT:ICBA(220 nm)/PH1000(40 nm)/PEIE(10 nm)/PBDTTT-C:PCBM(80 nm)/MoO_3(10 nm)/Ag(150 nm), and a breakdown of the absorptance in each of the AL1, PH1000, PEIE and AL2 layers. Fig. S2b shows that the integrated absorptance in the PH1000 layer accounts for less than 4.5% of the total absorptance of the tandem cell for wavelengths below 800 nm.

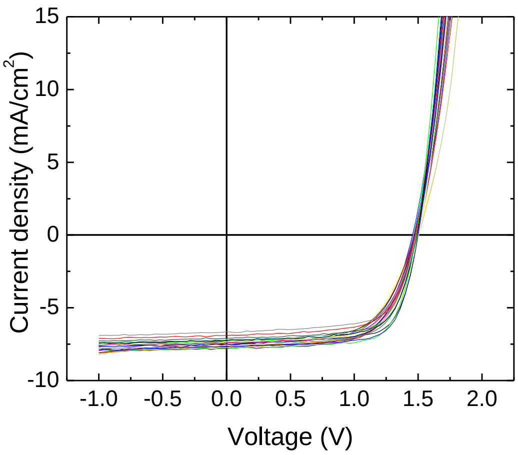

Fig. S3 *J-V* characteristics of 25 tandem solar cells measured under 100 mW/cm^2 AM1.5 illumination with an aperture area of 9.2 mm^2.

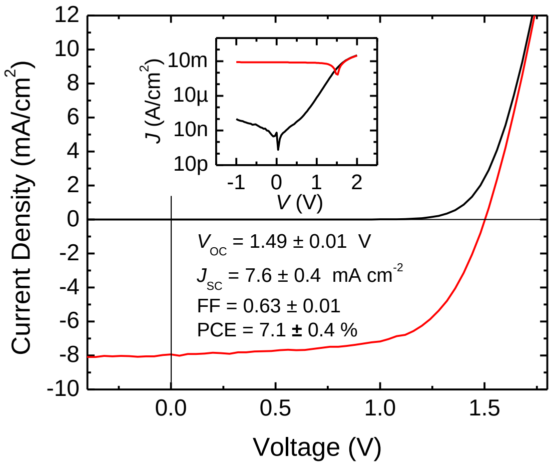

Fig. S4 *J-V* characteristics of champion tandem solar cells with a PH1000/polyethylenimine (PEI) recombination layer measured in the dark and under 100 mW/cm^2 AM1.5 illumination. Inset shows the same data on a semilogarithmic plot. Performance paramenters are given as averages over 4 devices.

Fill factor calculations

As mentioned, the *J-V* characteristics of solar cells can be fitted using Eq. 1 in the main text which is derived from an equivalent circuit model. Under ideal conditions where $R_S = 1/R_P = 0$, the fill factor of a solar cell is given by Eq. 2 in the main text (reproduced here for completeness):

$$\mathrm{FF}_0 = \frac{v_{OC} - \ln\left(v_{OC} + 0.72\right)}{v_{OC} + 1}$$

where $v_{OC} = qV_{OC}/nkT$. To incorporate the effects of R_S and R_P, a characteristic resistance for the device is defined as $R_{CH} = V_{OC}/(J_{SC}A)$ and normalized series resistance (r_S) and normalized shunt resistance (r_P) defined by $r_S = R_S/R_{CH}$ and $r_P = R_P/R_{CH}$, *respectively*. Using these quantities, the following semiempirical expresions have been shown to be good approximations to the experimental values of FF:

$$\mathrm{FF}_S = \mathrm{FF}_0(1 - 1.1 r_S) + 0.19 r_S^{\,2} \qquad \left(0 \le r_S \le 0.4, 1/r_P = 0\right),$$

$$\mathrm{FF}_{SP} = \mathrm{FF}_S\left\{1 - \frac{\left(v_{OC} + 0.7\right)}{v_{OC}} \frac{\mathrm{FF}_S}{r_P}\right\} \quad \left(0 \le r_S + 1/r_P \le 0.4\right)$$

Using these equations the parameters are calculated and shown in Table S1.

Table S1 Calculated values of r_S, r_P, FF_0, FF_S and FF_{SP}.

Device	r_S	r_P	FF_0	FF_S	FF_{SP}
Device A	0.037	30.64	0.67	0.64	0.63
Device B	0.041	11.34	0.62	0.60	0.56
Device C	0.017	18.95	0.74	0.72	0.69