Supporting Information

Charge carrier mobility of the organic photovoltaic materials PTB7 and $PC_{71}BM$ and its influence on device performance

Bernd Ebenhoch, Stuart A. J. Thomson, Kristijonas Genevičius, Gytis Juška, Ifor D. W. Samuel^{*}

Figure S1 shows the hole mobility of PTB7:PC₇₁BM as a function of temperature. The hole mobility (μ) depends almost exponentially on the temperature (*T*) as shown by the red fitting line. A simple equation of $\mu = a \ge e^{(T/b)}$ revealed a fit parameter of $a = 2.75 \ge 10^{-9} \text{ cm}^2/\text{Vs}$ and b = 29.2 K. This relation was used to convert the temperature to the hole mobility



Figure S1: Hole mobility of PTB7:PC71BM vs. temperature on a semi-log scale.

Figure S2 shows the open circuit voltage, extracted charge and the integral of the short circuit current for the turn-on behavior of $PTB7:PC_{71}BM$ solar cells. (This measurement was done on a separate device batch with similar performance.) The extracted charge was measured using a microsecond switch and the method described in the literature [1]. At 77 K the extracted charge reaches saturation at a much longer time scale compared to at room temperature. The steady state value at 77 K is 2.5 times higher than at 295 K.



Figure S2: Extracted charge and open circuit voltage vs. illumination time. Increasing light intensity from 0.12 (black) sun to 0.93 sun (magenta)

Figure S3 presents the series resistance of the devices obtained by the slope at high voltage (1.5 V), at the open circuit voltage and from a method based on two JV-curves with different intensity. The method using two JV-curves, which is recommended by the standard for testing solar cells (IEC 60891) [2], agrees well with the slope at V_{OC} . All curves show an increase of the series resistance with reducing hole mobility. The series resistance obtained from the two-curve method is approximately proportional to $\mu^{-1/4}$ (grey line).



Figure S3: Series resistance of PTB7:PC71BM solar cells as a function of temperature and hole mobility.

The fill factor is strongly influenced by the intensity of illumination as shown in **Figure S4**. At 77 K the fill factor increases from 33 % to 66 % when the light intensity is reduced from 1 sun to 0.01 sun, these values are comparable to the literature [3]^{\cdot} Increased light intensity

leads to a higher density of charge carriers and higher bimolecular and trap-assisted recombination rates, giving rise to a decay of the fill factor.



Figure S4: Fill factor as a function of light intensity for varying temperature.

Figure S5 shows the collapsed JV-curves of PTB7:PC₇₁BM solar cells of varying light intensity from 0.01 sun to 1.01 sun. The curves were normalized at -0.5 V. The spread at short circuit was attributed to trap-assisted recombination and the spread at open circuit to bimolecular recombination [4,5]. Cooling from 325 K to 77 K shows an increase of trapassisted recombination.



Figure S5: Collapsed JV-curves normalized at -0.5 V for different temperatures.

Figure S6 shows the fit parameters of the exponent of J_{SC} vs. intensity and the slope of V_{OC} vs. intensity. In the region between 200 K and 325 K the mobility has not much influence on the trap-assisted and bimolecular recombination. From 200 K to 77 K bimolecular recombination increases slightly, whereas trap-assisted recombination increases strongly.



Figure S6: Fit values of the exponent of JSC vs. intensity and the slope of VOC vs. intensity as a function of temperature and mobility

References:

- 1 C.G. Shuttle, A. Maurano, R. Hamilton, B. O'Regan, J.C. de Mello, J.R. Durrant, Charge extraction analysis of charge carrier densities in a polythiophene/fullerene solar cell: Analysis of the origin of the device dark current, Applied Physics Letters. 93 (2008) 183501. doi:10.1063/1.3006316.
- 2 A. Wagner, Peak-power and internal series resistance measurement under natural ambient conditions, in: Proceedings EuroSun, 2000. http://2012.interempresas.net/FeriaVirtual/Catalogos_y_documentos/80319/Medidade-Rs-y-Potencia-pico.pdf.
- R. Mauer, I.A. Howard, F. Laquai, Effect of Nongeminate Recombination on Fill Factor in Polythiophene/Methanofullerene Organic Solar Cells, The Journal of Physical Chemistry Letters. 1 (2010) 3500–3505. doi:10.1021/jz101458y.
- 4 S.R. Cowan, A. Roy, A.J. Heeger, Recombination in polymer-fullerene bulk heterojunction solar cells, Physical Review B. 82 (2010). doi:10.1103/PhysRevB.82.245207.
- 5 A.K.K. Kyaw, D.H. Wang, V. Gupta, W.L. Leong, L. Ke, G.C. Bazan, et al., Intensity Dependence of Current–Voltage Characteristics and Recombination in High-Efficiency Solution-Processed Small-Molecule Solar Cells, ACS Nano. 7 (2013) 4569–4577. doi:10.1021/nn401267s.