Supplemental Material

for the paper

The $\alpha\mu\tau$-Product as a Figure of Merit for Solar Cell Absorber Materials

Pascal Kaienburg[1,2]*, Lisa Krückemeier[1], Dana Lübke[1], Jenny Nelson[3], Uwe Rau[1] and Thomas Kirchartz[1,4]*

[1] IEK5-Photovoltaics, Forschungszentrum Jülich, 52425 Jülich, Germany

[2] Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, OX1 3PU Oxford, UK

[3] Department of Physics and Centre for Plastic Electronics, Imperial College London, London SW7 2AZ, UK

[4] Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

Pascal Kaienburg* – pascal.kaienburg@physics.ox.ac.uk

Thomas Kirchartz* – t.kirchartz@fz-juelich.de

* Corresponding author

1. Extinction coefficient of organic materials

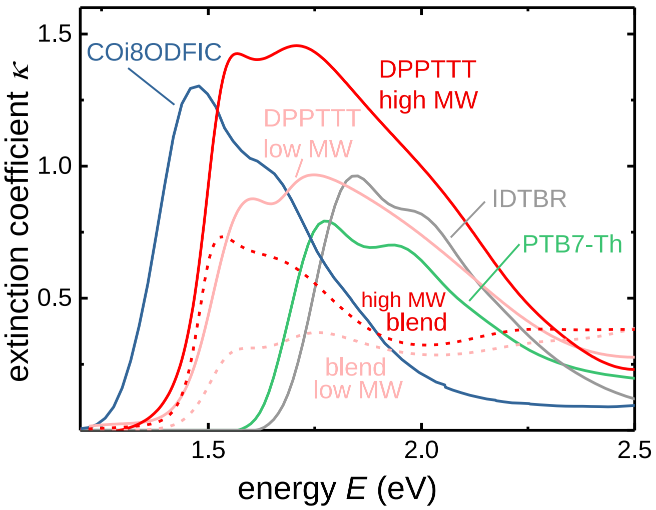

Figure S1: Extinction coefficient κ of several organic materials, which relates to the absorption coefficient via $\alpha = 4\pi\kappa/\lambda$ and allows comparing absorption strengths of different materials independent of the band gap. The maximum extinction coefficient varies for different organic semiconductors but mostly does not exceed one [1], except for certain polymers (e.g. high MW DPPTTT) and non-fullerene acceptors (e.g. COi8ODFIC). The dashed lines show the extinction coefficient of the DPPTTT polymers blended with PCBM (color matches that of the pure materials), which decreases the maximum extinction but broadens the spectra due to absorption in the PCBM. The data for IDTBR and PTB7-Th is taken from ref. [2].

2. Influence of band gap

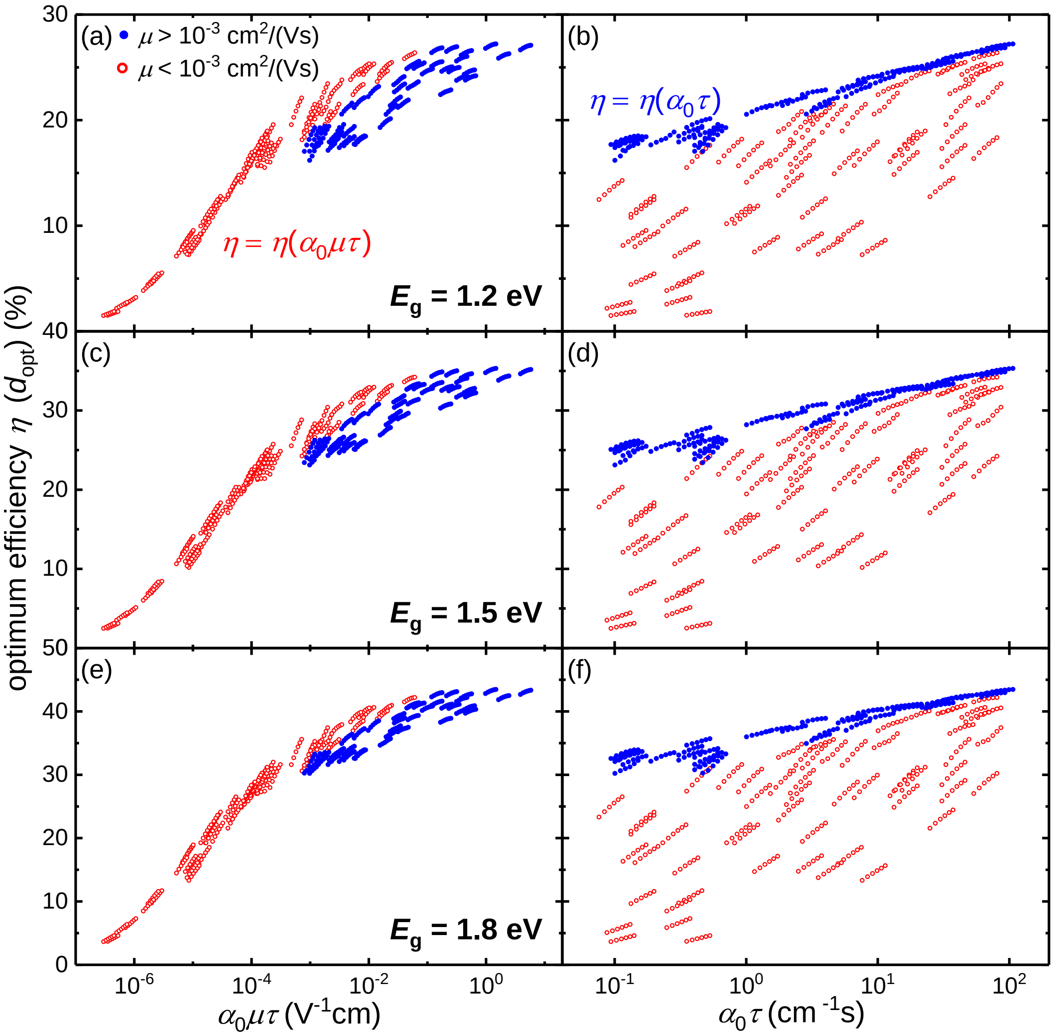

Figure S2: Variation of the electric band gap E_g in drift-diffusion simulations for trap-assisted recombination and inert surfaces ($S = 10^{-3}$ cm/s). The ($\alpha_0\mu\tau$)- and ($\alpha_0\tau$)-product remain good figures of merit for different values of E_g. Note that the optical band gap was not varied along with the electrical band gap in order to use the same absorption spectrum applied in all other simulations. Therefore, the simulated efficiencies reach unrealistic high values that exceed the Shockley-Queisser limit. The simulations nevertheless illustrate that our analysis and results are independent of the specific band gap value.

3. Modified *FOM*s

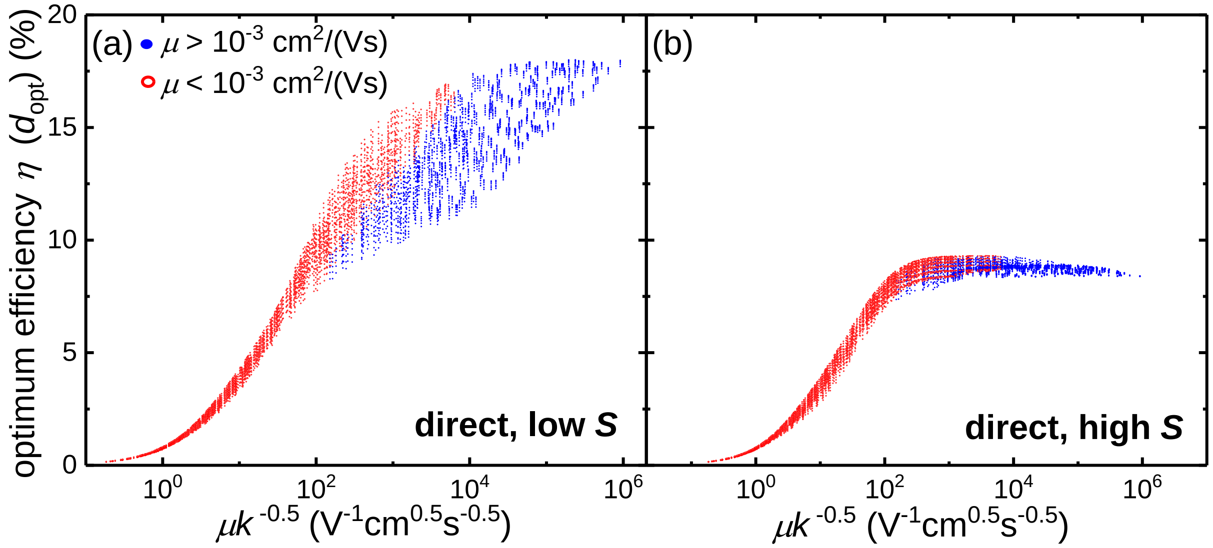

Figure S3: Although α_0 is only varied over a comparably small range - the largest factor is $c_\alpha = 1.5$ – the scatter increases significantly in the linear regime if α_0 is excluded from the respective FOMs on the x-axis. Exemplary data for bimolecular recombination (Compare with fig. 7) in the low mobility regime is shown for (a) low and (b) high surface recombination velocity.

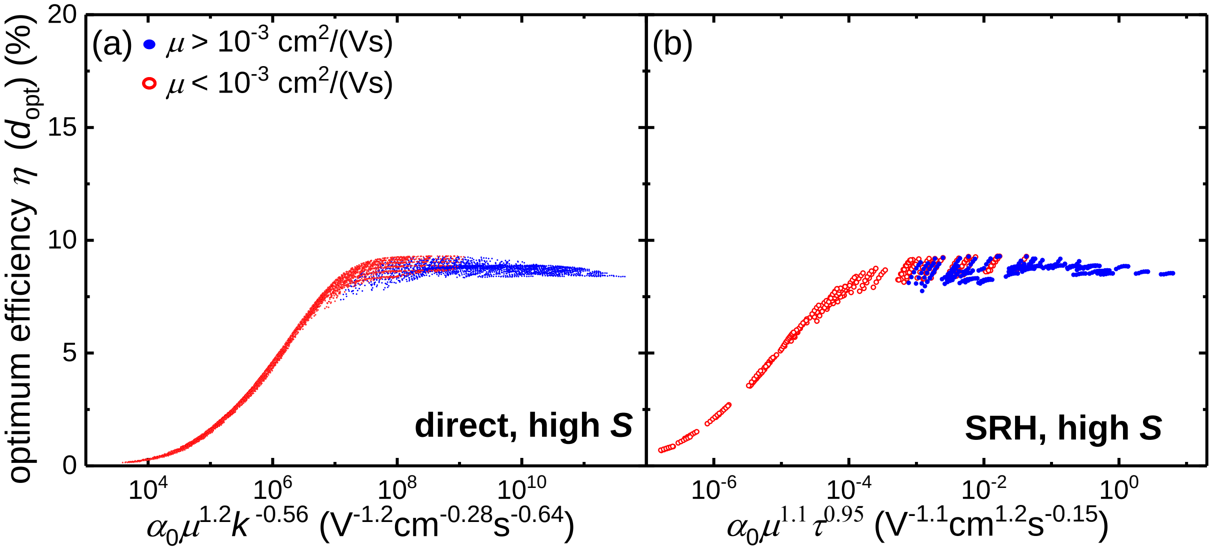

Figure S4: For the case of high surface recombination velocities and low mobilities, the correlation of the efficiency to a FOM depending on α_0, μ and k (or τ) is slightly improved in the linear regime by altering the weights and emphasizing the mobility. Compare (a) with fig. 7(c) and (b) with fig. 5(a).

4. Bimolecular (direct) recombination and the case of organic solar cells

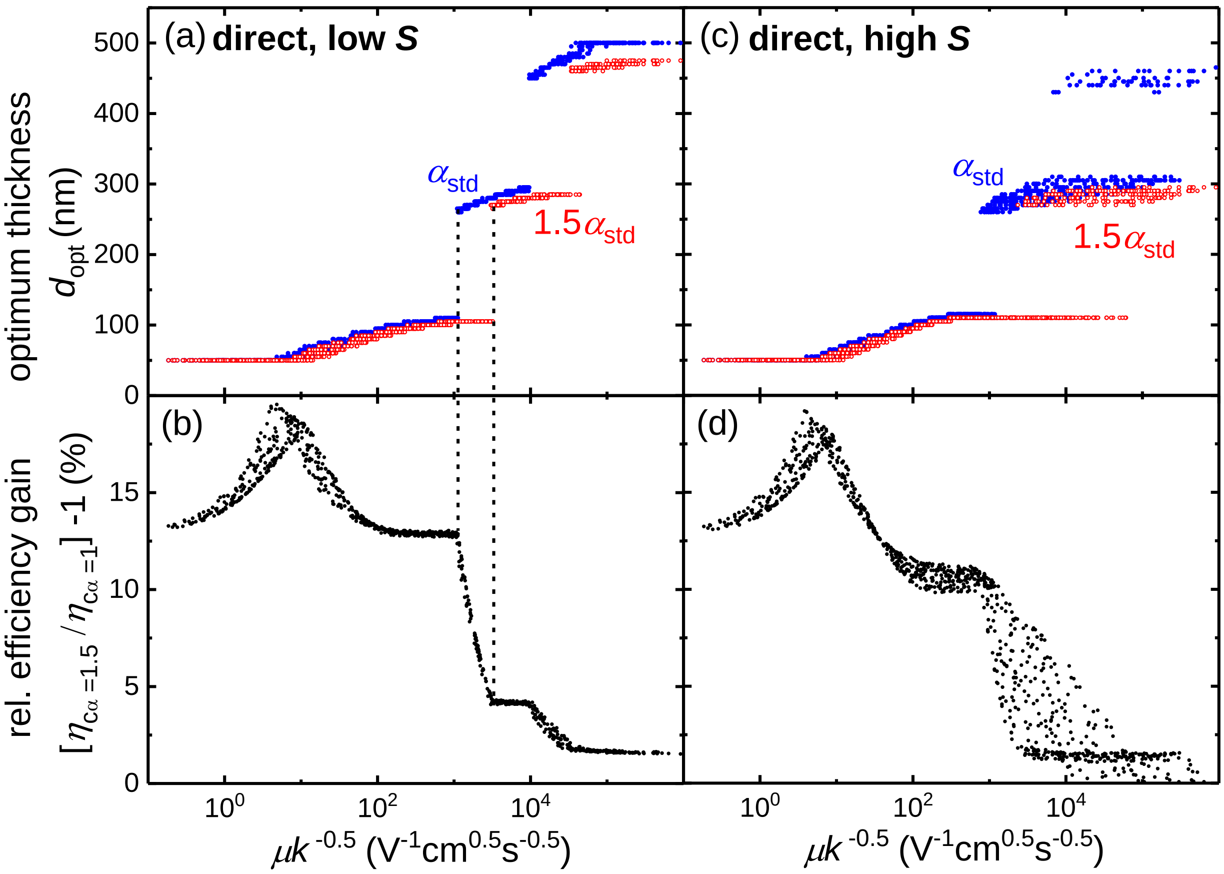

Figure S5: Connection between (a,c) optimum absorber thickness and (b,d) efficiency gain for simulated organic solar cells. (b) is identical to fig. 8(d). The case of strong surface recombination in (c,d) is similar to that of low surface recombination in (a,b) discussed in the following. The discretization of the optimum thickness stems from the presence of absorption maxima visible in fig. 8(a). The optimum thickness should in principle tend towards 0 nm for the lowest values of $\mu k^{-0.5}$ but saturates at 50 nm simply because thinner devices were not simulated. For increasing $\mu k^{-0.5}$, d_{opt} increases continuously until the first absorption maximum at 100 nm is reached. No further increase of d_{opt} with $\mu k^{-0.5}$ is observed until an abrupt jump to the second absorption maximum occurs. The features in (b) coincide with the jumps to higher absorption maxima in (a) as can be seen from the guiding dashed lines. The $\mu k^{-0.5}$ value at which a jump to higher maxima occurs, results from the tradeoff between a higher absorptance and lower collection efficiency when the absorber thickness increases. The non-monotonous behaviour for the lowest $\mu k^{-0.5}$ can be attributed to the fact that no devices with thickness below 50 nm were simulated in accordance with experimentally realized absorber thicknesses, although the optimum thickness for such low $\mu k^{-0.5}$ values is actually lower. The gain in absorptance with thickness is higher at a lower absolute value of the absorptance, but charge collection is mostly independent of the absorption strength. Consequently, for the weaker absorbing blend, the tradeoff becomes favorable at lower $\mu k^{-0.5}$ values. We observed a similar effect in a previous work, where we studied the interplay between absorber thickness, absorptance, charge carrier collection and efficiency for non-fullerene acceptor blends with different absorption bandwidth [2].

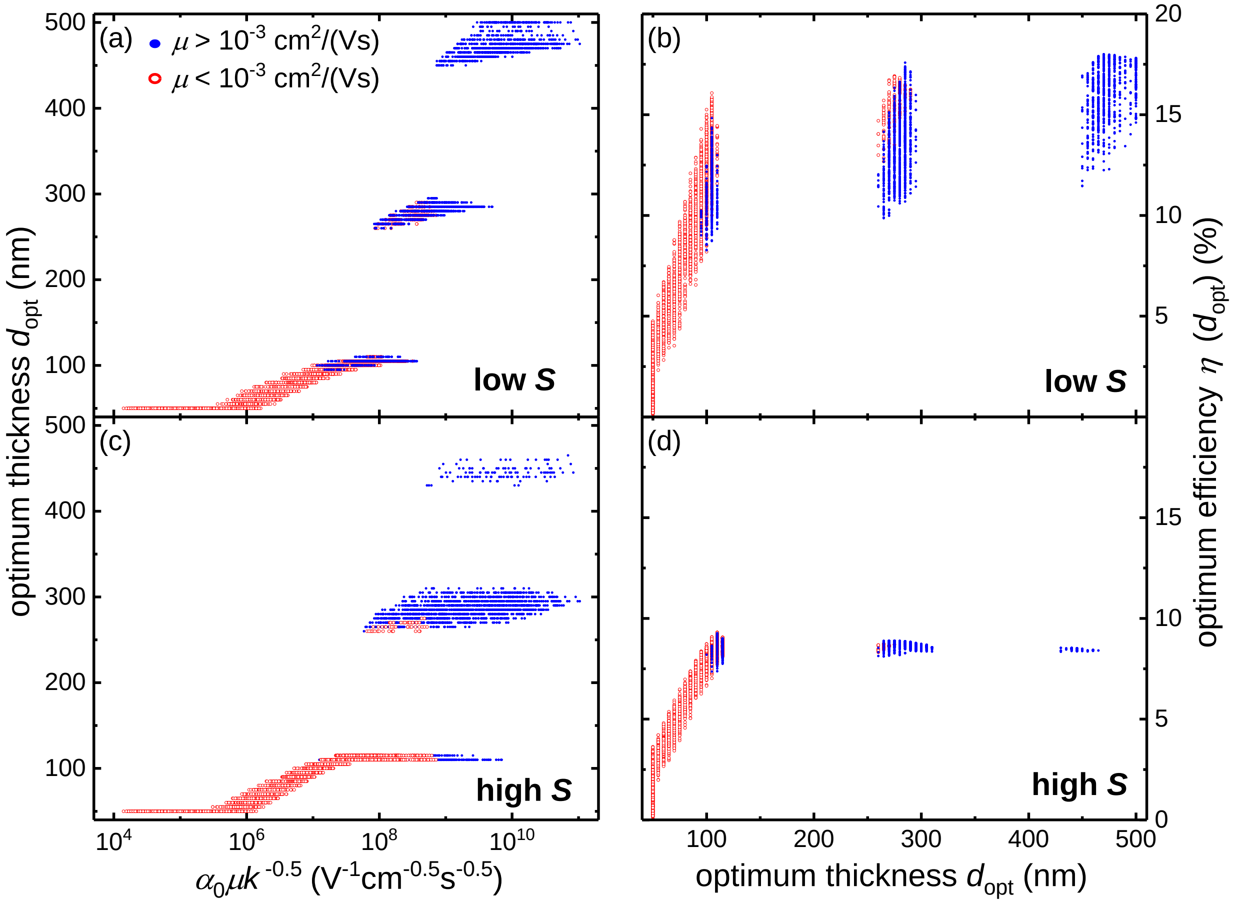

Figure S6: Optimum thickness in the case of bimolecular recombination. The optimum thickness is discretized due to optical interference in the thin-film layer stack as shown in fig. 8. Larger values of $\alpha\mu k^{-0.5}$ in (a,c) enable best performance for thicker absorber layers. Experimental studies of organic solar cell performance typically include the optimization of the active layer thickness as it is fairly easy to vary.

References

[1] M. S. Vezie, S. Few, I. Meager, G. Pieridou, B. Dörling, R. S. Ashraf, A. R. Goñi, H. Bronstein, I. McCulloch, S. C. Hayes, M. Campoy-Quiles, and J. Nelson, *Exploring the origin of high optical absorption in conjugated polymers*, Nat. Mater. **15**, 746 (2016).

[2] L. Krückemeier, P. Kaienburg, J. Flohre, K. Bittkau, I. Zonno, B. Krogmeier, and T. Kirchartz, *Developing Design Criteria for Organic Solar Cells Using Well-absorbing Non-fullerene Acceptors*, Commun. Phys. **1**, (2018).