Active layer materials properties for a new efficiency regime of molecular solar cells

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We present three different theoretical approaches to identify pathways to organic solar cells with power conversion efficiencies in excess of 20%. We take off after reasoning why the Shockley-Queisser limit is applicable to OPV. The arguments are based on previously reported analyses by others. A radiation limit for organic solar cells is introduced that elucidates the role of charge-transfer (CT) state absorption. Provided this CT action is either sufficiently weak or present in its maximized form throughout the active layer material, organic solar cells can be as efficient as their inorganic counterparts.

Next, we analyze what the ideal combination of band gaps is for a donor/acceptor pair of materials in OPV. We make this more quantitative in a model based on Marcus theory of electronic transfer that considers exciton generation by both the electron donor and electron acceptor. We use this model to show how reduction of the reorganization energies in the processes of electron and hole transfer can lead to substantial power conversion efficiency gains. This analysis, together with optimizing the energy level offsets between the donor and acceptor materials accordingly, clearly indicates that optimization along these lines can easily yield devices with >20% AM1.5 power conversion efficiency.

Third, and by far most important, we introduce the dielectric constant as a central parameter for efficient organic solar cells. We have reported on the very first steps of this analysis in 2011. Recently, we have made a much more thorough investigation. Now, we analyze how the dielectric constant influences every fundamental step in OPV. We analyze and model the case of the 2009 world record PTB7:[70]PCBM cell of 7.4%, using a drift-diffusion model. Based on the model and based on the fact that the exciton binding energy diminishes with increasing dielectric constant of the medium, we find that efficiencies of more than 20% are within reach upon increasing the dielectric constant ε_r of the material to 10 (Figure 1). The next step is to make the translation from the desired materials properties to actual molecular design. The transition towards high-k molecular semiconductors can also pave the road towards a 'triple green' technology, in which the materials are made by green (bio)chemical processes, produce green energy in their device application, and can be fully recycled after use.

If time allows, we will present some first results on the design of high OPV performance molecular materials.

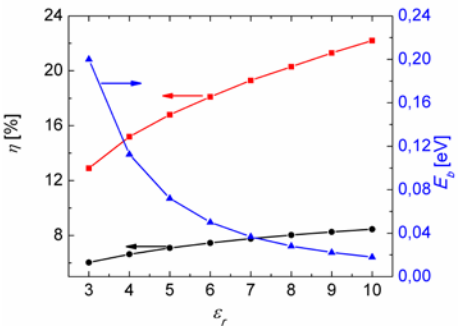

Fig1: (black line) $\eta_{(PTB7:[70]PCBM)}$ as function of ε; (blue line) exciton binding energy E_b as function of ;(red line) η of OPV with E_b optimized for each value of ε.

(1) L. J. A. Koster, S. E. Shaheen, J. C. Hummelen, *Adv. Energy Mater.* **2**, 1246-1253 (2012)
(2) R.C. Chiechi, J.C. Hummelen, *ACS Macro Lett.* **1**, 1180−1183 (2012)