On the maximum power conversion efficiency of organic photovoltaics

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Research and development on organic photovoltaics (OPV) technology is rapidly growing, especially in recent years. The promise of a low-cost mass product for sustainable electricity production, combined with the potential of an even 'triple green' technology, is the main driving force. On the other hand, OPV has been invariably associated with low power conversion efficiency and stability relative to inorganic technologies. The stability issue has been tackled mainly by industry during the last 5 years. This has led to tremendous progress, especially for bulk-heterojunction OPV ('plastic PV') devices, with reports of lifetimes of several thousands of hours under elevated temperatures and even without encapsulation.

The power conversion efficiency of OPV constitutes an appealing and challenging issue for researchers. General design rules for high efficiency OPV have been given by several groups. Such design rules are mainly based on a combination of materials and device properties that are on the one hand considered realistic and on the other are based on fairly specific mechanisms of how the devices should operate. Interestingly, the two most influential analyses thus far both focus strongly on optimization of the properties of the donor material and neglect charge carrier generation as the result of light absorption by the acceptor.[1,2] The main optimization parameters were the width of the donor bandgap and LUMO-LUMO offset between donor and acceptor. More fundamental theoretical analyses of OPV efficiency were reported by Sun et al., Rau, and Vandewal et al.[3,4,5], with the latter focusing on the origin of the open circuit voltage. At the other hand, there is the central dogma of the theoretical Shockley-Queisser efficiency limit for a single p-n junction PV device.[6]

Here, we report on our analysis of a single junction (molecular) donor/acceptor OPV device under standard AM1.5 illumination. We take an approach in which there is no fundamental difference between donor and acceptor materials other than the fact that they have the relationship that the frontier orbital energies of the donor are at higher energy than the corresponding ones of the acceptor. We argue that such a symmetrical version of OPV is desirable. First, we investigate in a semi-empirical way the influence of bandgap(s) and band offsets on the power conversion efficiency. Second, we also include the influence of the reorganization energy of the charge generation process. Using a slightly different approach, we then consider the influence of the exciton binding energy on the maximum power conversion efficiency. Finally, we introduce the dielectric constant as a parameter in the analysis.

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Our analysis suggests that there is no fundamental thermodynamic reason for OPV to have a theoretical efficiency limit lower than the Shockley-Queisser one. It simply shows that there is much work to do on improving molecular materials to overcome present limitations. The trivial conclusion is that in the limit of assuming a donor/acceptor combination of ideal organic materials the same result is obtained as when taking an ideal inorganic p-n junction.