**The influence of injection barriers on performance of organic solar cells studied by drift-diffusion model with transport layers**

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Organic solar cells (OSCs) are prospective technology because they are inexpensive, lightweight, flexible, and ideal for roll-to-roll large-scale processing. An impressive improvement in their power conversion efficiency (PCE) has been achieved in the past few years with the PCE reaching a certified value of 19.2% [1]. However, an adequate and comprehensive theoretical model which would explain the progress so far and indicate the direction of future performance improvement is still missing.

Along the path of further PCE improvement, the main goal is to achieve the best possible absorption, photogeneration, and transport of charge carriers in the active layer (AL), as well as to reduce recombination losses in it. However, contact phenomena which include effects of transport layers (TLs) have turned out to be very important and influential in OSCs [2]. The amount of the photogenerated electrons and holes that are brought to the corresponding electrodes as well as the efficiency of their extraction is strongly dependent on TLs. In contrast, the drift-diffusion models (DDMs) used for modeling the OSCs do not consider the existence of TLs [3].

Here, the DDM that includes the Poisson equation and continuity equations for electrons and holes was used. The domain was divided into three subdomains corresponding to the hole transport layer (HTL), AL, and electron transport layer (ETL) and each layer is described with its electrical and optical material parameters. The absorption profile was described by the Beer-Lambert law and photogeneration was assumed to take place only in the AL. The mobilities of electrons and holes were taken to be constant in each layer, and a reduced Langevin recombination was assumed. The Dirichlet boundary conditions (BCs) at TL/electrode interfaces were used. The BCs include the effect of injection barriers (IBs) through thermionic electron and hole concentrations [4].The system of equations was solved with use of the finite difference discretization improved by Scharfetter and Gummel approach and the Newton algorithm.

The TLs have the role to reduce IBs between the AL and electrodes, thus, it is important to apply exact values for the hole and electron IBs in the DDM. It is expected that lowering the IBs leads to a higher PCE, which was verified using our model. We also simulated the current density-voltage (J-V) characteristics for the ITO/P3HT:PCBM/Al solar cell (structure without TLs) and the ITO/PEDOT:PSS/P3HT/LiF/Al solar cell in which PEDOT:PSS is the HTL and LiF is the ETL.The simulated J-V curves for the ITO/P3HT:PCBM/Al device without taking into account IBs (zero IBs) and including IBs were compared to the experimental J-V curve taken from [5]. A better agreement with the experiment was obtained when the IBs were included. The same was done for the ITO/PEDOT:PSS/P3HT/LiF/Al solar cell. In this case, the model which doesn’t include IBs reproduced the experimental J-V curve, taken from [6], better. This was taken as evidence of the electrodes Fermi level pinning in the considered device.

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