Optical optimization for high performance polymer solar cells

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When using low-bandgap polymers with extended solar spectrum harvesting properties, efficiencies above 7% have been reached when a fine tuning of the electrical material properties or an optimized architectural device construction has been implemented. In direct architecture bulk heterojunction devices, the work function of ITO and the metal electrodes can be finely tuned by an electron blocking layer and a hole blocking layer (HBL), respectively.



Figure 1: Calculated J_{SC} as a function of the PBDTTT-C:PC71BM blend thickness (solid lines) and experimentally determined J_{SC} for devices with top electrode composed of: 3.5 nm of BCP and 90 nm of Ag (red squares), 10 nm of BCP and 90 nm of Ag (blue squares) and 10 nm of Ca and 90 nm of Ag (black dots).

In the current work we show that the optical material constants of the HBL play a key role in determining the final power conversion efficiency (PCE) of the device. We demonstrate that by a proper selection of the imaginary and real parts of the refractive index. light harvesting can be largely optimized. For the study. we chose benzodithiophene derivatives (PBDTTT-C, PTB7) as the low-bandgap donor materials. Its low laying HOMO energy level is ideal to achieve a large difference with the LUMO of the acceptor. Indeed, PCEs of 6.4% for PBDTTT-C [1] and up to a 7.4% for PTB7 [2] has been reported when using the direct ITO/PEDOT:PSS/POLYMER:PC71BM/Ca/Al architecture. We performed a numerical optical optimization of the light harvesting which demonstrated that a reduced extinction coefficient (k) for the HBL is essential to achieve an optimal light absorption by the active layer. In accordance, in the device architecture indicated above, we replaced the typical back metal electrode composed of a thin 10-20 nm Ca layer and a thicker Al layer by a few nanometer thick bathocuproine (BCP) layer and a thick Ag layer.

BCP, which is a widely used exciton blocking layer in organic devices such OLEDs and small molecule solar cells, possess a k value that is close to zero for a broad range of wavelengths. This enhanced the reflectivity of the back Ag electrode which resulted in an increase of the short circuit current. Light harvesting could be further improved by adjusting simultaneously the thickness of both the BCP and the active layer to achieve an optimal optical interference. Such combined tuning of k and the real part of the refractive index (n) implied an 8% increase in short circuit current. In addition, we observed that when using the BCP/Ag electrode, the photovoltaic parameters of the cell not directly related to photon harvesting such as the open circuit voltage and fill factor also improved. Taking advantage of the optical optimization and the slight improvement in the electrical properties, we were able to fabricate cells with PCEs of 7.5% for the PBDTTT-C and up to 8.1% for the PTB7. In conclusion, we demonstrated that an optimization of the optical properties of the layers in the polymer solar cell is essential to achieve high performance thin film OPV devices.

References

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