

Interface loss mechanisms in organic bulk heterojunction solar cells

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Organic bulk heterojunction (BHJ) devices are a promising solar cell technology but their cell efficiency needs to be increased. The BHJ cell is a complex structure and in order to improve the efficiency it is essential to understand in detail the various loss mechanisms, so that these might be overcome by better materials or better device geometry. This work focuses on the efficiency loss associated with the electron-hole pair separation at the heterojunction interface and the subsequent recombination, both of which have been the subject of much debate. We show that the energy loss when the exciton is split, and the evident absence of Langevin recombination at the interface, are both related to the magnitude of the electron-phonon interaction and the wave-function extent of the electron and hole. In contrast to some recent publications, we conclude that structurally well-ordered, high mobility organic materials provide the best chance for higher efficiency cells.[1]

The solar cell open circuit voltage, V_{OC} , should be as close as possible to the optical band gap energy. However, when the exciton splits at the interface, the energy loss reduces V_{OC} . We show that in addition to the band offsets at the heterojunction, the Stokes shift arising from the electron-phonon coupling is a significant contribution to the reduction in V_{OC} . Each mechanism contributes about 0.5 eV in present BHJ solar cells and together are a major cause for the low cell efficiency. It is therefore important to minimize the energy loss at the hetero-junction by choosing materials with appropriate energy levels with respect to the exciton energy, and to find an organic semiconductor with as small as possible electron-phonon coupling of the exciton, so that the optical gap is as close as possible to the exciton zero-phonon energy. Increased conjugation length in well-ordered polymers is known to give delocalized excitons with smaller Stokes shift. The effect of structural order to reduce the phonon coupling is also known for polarons in the organic semiconductors.

According to the Langevin recombination mechanism, which is typically associated with low mobility materials, efficient geminate electron-hole recombination across the heterojunction should be expected even after the exciton has split. The efficiency of the BHJ solar cells shows that the interface recombination is strongly suppressed. We analyze the Langevin mechanism and describe the conditions when it is suppressed, which depends on the relative rates of recombination or thermal ionization of the exciton, rather than on the magnitude of the carrier mobility. A simple recombination model indicates that the recombination rate is mostly determined by the exciton binding energy and consequently on the magnitude of the electron-phonon coupling. Analysis of the model gives insight into the material properties that are needed for low recombination at the interface. We also discuss the various other recombination mechanisms that contribute to the cell fill factor.

[1] R. A. Street Appl. Phys. Lett., 93, 133308 (2008)