

Molecular and microstructural factors influencing the open-circuit voltage of organic photovoltaics

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Electronic processes at organic hetero-interfaces between electron donating and electron accepting molecules determine the photocurrent, photovoltage and ultimately, the power conversion efficiency of organic solar cells. Solar cells with incident-photon-to-extracted-charge conversion yields of over 85%, and absorbed photon-to-extracted-charge conversion yields of 90-100% have been achieved, using organic materials. However, the difference between the optical gap of main absorber and open-circuit voltage (V_{oc}) is much larger than for inorganic and perovskite based solar cells. The main improvements of the V_{oc} of organic solar cells have so far been made by tailoring donor-acceptor interfacial energetics, taking advantage of well-known principles of molecular design. Nevertheless, for most material systems we consistently find a large, almost constant difference (~ 0.6 eV) between eV_{oc} and the energy of the intermolecular charge transfer (CT) state, E_{CT} . Added to this, electron transfer losses are very often larger than 0.1 eV, resulting in overall voltage losses larger than 0.7 eV. We present experimental evidence that the $E_{CT}-eV_{oc}$ difference can be reduced by reducing the physical interfacial area available for free charge carrier recombination. We further discuss the influence of measurable molecular properties, such as the electronic coupling, molecular reorganization as well as non-radiative recombination pathways on free carrier recombination and the V_{oc} of organic solar cells.