Charge transfer phenomena at organic and inorganic heterojunctions

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Abstract

Blends between conjugated polymers and fullerene derivatives constitute a promising material combination for organic photovoltaics. Currently efficiencies up to 8% have been reached, with the potential for better performances. To further advancing this technology and make it competitive, a thorough understanding of loss mechanisms in carrier photogeneration is mandatory. Recombination via charge transfer excitons (CTEs) appears to be a fundamental loss impacting both the open circuit voltage and the short circuit current of solar cells.
In this communication we unravel the origin of CTEs forming in such blends and we discuss their importance in recombination processes considering the role of binding energy [1], polymer conformation [2], and energetic position [3]. CTE photoluminescence (PL) can be observed in several material combinations such as poly3-hexylthiophene and poly(phenylene-vinylene) when blended with the fullerene acceptor PCBM. By combining electron microscopy images and PL spectroscopy, we show that CTE recombination is only slightly influenced by the mesoscopic morphology. Surprisingly, large differences in CTE recombination have origin in the polymer chain conformation [2]. Additionally, we correlate the CTE PL of different polymer/fullerene blends with the short circuit current and open circuit voltage of the corresponding devices. By shifting the lowest unoccupied molecular orbital of different fullerene acceptors, we tune the CTE emission energy and the open circuit voltage. CTE emission at high energies results in cells with high open circuit voltages but poor short circuit currents. The latter cell parameter correlates with the CTE PL intensity which can be enhanced by energetic resonance effects or poor phase separation in the blend. The results highlight a fundamental limit in the efficiency of organic solar cells with CTE recombination.

In the second part of this presentation we will consider the recombination via CTE in inorganic heterostructures made of II-VI semiconductors such as CdSe/CdTe tetrapods. First we will review our recent work on the fundamental excitations in these nanocrystals of complex geometry [4,5], then the binding energy of these excitations and their importance in nanocrystal based photovoltaics. In addition, we will discuss the potential nanocrystals made out of earth abundant elements, such as copper sulfide for renewable energy applications [6].

References

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