Krūvininkų lokalizacija, judris ir atsiskyrimo greičiai polimeriniuose saulės elementuose

Charge carrier localisation, mobility and separation rates in polymer solar cells

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Organic photovoltaic cells can be assembled into lightweight and flexible solar panels which can be easily integrated into semitransparent windows, car roofs, etc. They are researched actively and small devices with power conversion efficiencies over 13% have been demonstrated. Photon absorption in organic semiconductor generates tightly bound excitons and charge generation occurs by electron or hole transfer at an interface between electron donor and acceptor materials. Most popular organic solar cells are made using conjugated polymers as electron donors and fullerene derivatives as acceptors which are blended together to fabricate bulk heterojunctions with large interface area. Because electron and hole transfer are short-range processes and the dielectric constants of organic semiconductors are low (typically between 3 and 4), the generated charge pairs are expected to be bound by Coulomb attraction. Yet the majority of pairs split into free carriers in the weak built-in electric field induced by a difference in the electrode work functions. The mechanisms of charge separation are still not understood and widely disputed [1].

We have combined broadband transient absorption spectroscopy with ultrafast carrier drift measurements to study the dynamics of charge separation in high performance solar cells based on the blends of the conjugated polymer PTB7 and the fullerene derivative $PC_{71}BM$ as the active layers [2]. We found that the photogenerated electron-hole pairs separate into free carriers on a picosecond time scale with the field-independent rate which is determined by electron mobility in fullerene clusters (Fig. 1). The photogenerated holes delocalise on PTB7 chains which decreases the Coulomb binding energy of charge pairs. We will also discuss how the entropy increase upon charge transport from a mixed donor-acceptor phase to the pure donor and acceptor domains provides the gain of the free Gibbs energy which drives charge separation. Pure domains are less than 10 nm in size in optimised morphologies and provide efficient carrier generation as well as separation [3].

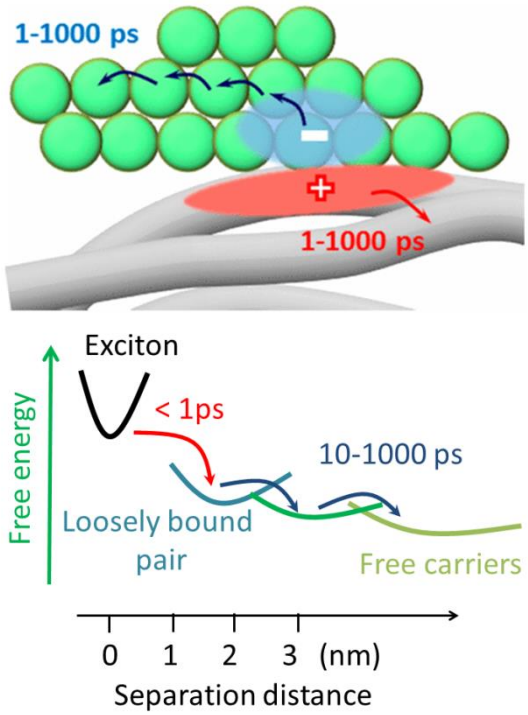

Fig. 1. Schematic illustration of the charge separation mechanism in efficient polymer-fullerene solar cells by electron hopping between fullerene molecules and hole hopping to a next polymer chain. The bottom panel shows hypothetic free energy surfaces of the electronic states along the charge separation coordinate and experimentally observed separation times.

Keywords: Organic semiconductors, bulk heterojunction, charge photogeneration, binding energy, transient absorption spectroscopy, ultrafast carrier drift.

References

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[3] G.J. Hedley, A.J. Ward, A. Alekseev, C.T. Howells, E.R. Martins, L.A. Serrano, G. Cooke, A. Ruseckas, I.D.W. Samuel, Nature Commun., **4**, 2867 (2013).