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On the Origin of Charge Separation at Donor-Acceptor Interfaces in Organic Solar Cells: Energy Bending versus Energy Disorder

Gjergji Sini
Chemistry Departement, University of Cergy-Pontoise, Cergy-Pontoise, (France)

gjergji.sini@u-cergy.fr

Among the great diversity of solar cell technologies, organic solar cells (OPV) are outstanding with respect to their mechanical flexibility and unique optoelectronic tunability. Within the past three years the long-lasting dominance of fullerene-based acceptors has been overcome, which has been made possible by the development of new polymeric acceptors and by introducing different strategies to combine donor and acceptor polymers. However, a general mechanism that could explain this enormous boost in solar cell efficiency has not been identified so far.

Here, a brief overview of the main mechanisms proposed to explain the charge generation in the OPVs will be discussed, followed by recent developments using a combined experimental and theoretical (density functional theory,DFT, and Kinetic Monte-Carlo, KMC) approach. Clear structure-property relationships will be discussed, allowing to demonstrate (i) the presence of a substantial driving force (energy bending, EB) between the donor-acceptor interface and pure domains of the donor and acceptor polymer, and (ii) identify some factors being at the origin of this driving force. [1] (iii) Highlight the relative impact of EB and disorder on the charge generation efficiency.[2] Correlation between molecular structure and polymer deformations at the interface, will be highlighted, providing guidelines for designing the next generation of conjugated polymers and small molecules.

Références

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