Light-To-Charge Conversion In Organic Photovoltaics: Mechanisms And Timescales

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Abstract. Recent years have seen an intense debate on the physical mechanisms and time scales of free-charge generation following photoexcitation of donor/acceptor organic solar cells, which initially produces strongly bound excitons in the donor material. The interpretation of ultrafast spectroscopic signatures suggests that free carriers are predominantly generated on a subpicosecond time scale following the excitation, the key role in this process being played by high-energy ("hot") delocalized interfacial charge transfer (CT) states [1]. However, other experimental studies indicate that the main precursor towards free charges is the strongly bound and localized ("cold") CT state, so that free-charge generation occurs on time scales ranging from tens to hundreds of picoseconds [2, 3].

We investigate charge separation in a one-dimensional model of an interface between two organic semiconductors, both on ultrashort and on much longer time scales. We conclude that free carriers present on a subpicosecond time scale following a pulsed photoexcitation are mainly directly optically generated from the ground state thanks to the resonant mixing between states of donor excitons and free charges [4]. However, on the same time scale, we find that the majority of photogenerated charges still remain bound in form of donor or CT excitons [5]. We obtain that their further separation on longer time scales is weakly electric field- and temperature-dependent and is enabled by the synergy between carrier delocalization and moderate disorder [6].

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