Ultrafast dynamics of charge generation in efficient organic photovoltaics

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In an organic solar cell (OPV), the key photophysical process is free charge carrier generation. Ultrafast long-range charge separation have been proposed¹, there is however no universal consensus about the role of the charge-neutral electron-hole pairs (excitons) and charge transfer (CT) state in this process^{2, 3}.

Previous work on CTS formed at early times through the ionization of excitons at heterojunctions suggested that their dissociation was mediated by charge wave function delocalization⁴. Through using different molecular weights, and optimizing the donor phase loading ratios in a $D_1:D_2$: A blend with respect to the binary blend, allowing us to get different blend with varied delocalization.



Figure 1. a) Transient absorption spectra of films excited at 700nm, b) Time-resolved photoluminescence of binary and ternary blends.

Here, we aim at getting more insight on the timescale and process leading to the formation of the charge carriers from thermalized excited states, by using ultrafast transient absorption spectroscopy with sub 50fs time resolution and other steady state optical measurements based on one efficient ternary D_1 - D_2 -A OPV system. The transient absorption signal created by the pump are clearly visible from the TA data (fig.1, a). Compared to binary blend, the ternary blend generate more charges at initial time (before 10ps). For T-H blend, charge generated instantly with pump, this phenomena could not explained simply by charge transfer state (CT) involved only. Time-resolved photoluminescence data (fig.1, b) showing that exciton in the ternary blend dissociate almost totally in the initial 10ps, while the binary blend still emitted photons after 1ns. In combination with other time –resolved and steady state optical measurements, we can identify that compared to binary blend, the ternary blend show less charge transfer state and more charge carriers come from exciton directly. This shows that thermalized excited states is not hindering charge generation as the vibronic coupling accelerates ultrafast charge separation dynamics.

References:

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