Ultrafast spectroscopy of donor-acceptor organic molecules for photovoltaic applications: Minimizing charge recombination

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In the last ten years, many alternatives relying on organic molecules have been explored that could replace the traditional solar cells made by inorganic semiconductors. Organic cells are thin, flexible, and cheap-to-produce, but suffer from inherent limitations of organic materials, in particular their low carrier mobility. Nevertheless, the record power conversion efficiency recently reported is as high as 12% [1].

Solar cells using liquid crystal (LC) films of donor-acceptor (DA) molecules are a new approach, in which the ratio of DA interface-to-volume is maximized, leading to fairly good performances [2]. The motivation is to make the distance to the D-A interface shorter than the exciton diffusion length (typically 10 nm). We have studied LC films of bisthiophene-derivatives forming D and perylenediimide as A, by femtosecond transient absorption (TA) spectroscopy. Due to the strong electronic coupling between D's the initial laser excitation, selectively tuned in the absorption of D, excites a coherent superposition of many D molecules (exciton) that decays within 60 fs into a charge transfer (CT) state, that localizes on a slower 0.4 ps time scale. However, while the CT formation is ultrafast and efficient, the time-resolved spectroscopy shows that the CT states recombine within less than 50 ps, i.e. on a time scale too short to allow significant carrier transport [3].

We will present results obtained for a new type of donor family incorporated in the DA's that incorporate moieties with different electron-donating and -deficient character, thereby offering a handle to control the localization of HOMO and LUMO orbitals. A smectic liquid crystal state is formed at room temperature. CT lifetimes larger than 2 ns are now observed and the results are rationalized within the Marcus theory for charge transfer.