Dynamics of Charge Separation in Donor-Acceptor Heterojunction Photovoltaic Systems

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Electron transfer and subsequent charge separation through donor-acceptor heterojunctions remain the most important areas of study in the field of third-generation photovoltaics. In this context, it is particularly interesting to unravel the dynamics of individual ultrafast processes (such as photoinduced electron transfer, carrier trapping and association, energy transfer and relaxation), which prevail in materials and at their interfaces.

The formation of bound interfacial electron-hole pairs, the so-called charge-transfer states (CTS), following electron transfer from donor to acceptor and the subsequent charge recombination are among the dominant loss mechanisms hindering performance in molecular photovoltaic devices. Whether interfacial CTS dissociate to yield free separated carriers due to vibrational excess energy or to the electric field is still under debate.

Applying a combination of ultrafast time-resolved electroabsorption and THz spectroscopy techniques, we scrutinized the detailed mechanism of photoinduced charge separation in dye-sensitized solar cells, OPV systems (small molecule- and conjugated polymer-based), and in high-efficiency hybrid lead halide perovskite solar energy converters. CTS dynamics could be monitored in each case, suggesting a unified picture for free carrier generation and separation in all types of donor-acceptor heterojunctions.