Identification of different pathways of electron injection in dye-sensitised solar cells of electrodeposited ZnO with an indoline sensitiser

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Supplementary Material

Data analysis

The transient absorption data displayed in Figure 1 have been recorded in several measurements with probe pulses in different wavelength ranges. The displayed transient spectra below 1300 nm were taken with white light continua, and the data at longer wavelength with nearly transform limited pulses from a non-collinear optical parametric amplifier NOPA. We note, that the entire range between 1200 and 2300 nm has been scanned with individual NOPA probed measurements. For clarity, we only plot two examples, selected at wavelengths where the identified states are not spectrally overlapping: the neutral CT state around 1600 nm, and the ZnO conduction band around 2100 nm.



Figure: A transient absorption spectrum simulation generated by means of a reverse global analysis using the measured transient spectral signatures and their corresponding temporal evolutions as depicted in Table 1. The series of NOPA probed measurements above 1300 nm were spectrally narrow; therefore an informed assumption was made with respect to the broadness of the NCT and ICT states' absorption. When compared to the measured transient absorption spectra, of which only four example spectra are displayed in Figure 1, an excellent agreement is found.

We first determine the temporal evolution and time constants of known spectral signatures such as the dye's ground state (GSB), its excited and its oxidized states (ESA and OX), and the ZnO conduction band. We then identify all other spectral components in the entire set of data with their respective temporal evolution and assign them to transiently populated states, or depleted or fluorescing states, depending on the sign of the absorption changes. We link equal time constants to the same process, and build a consistent model, which can be understood in terms of reasonable electronic states and charge dynamics between them, as shown in Figure 3. The analysis is very much guided by this last step - the assignment of transient spectral signatures to physical states, and therefore is able to reveal previously spectroscopically unknown states. As a final control, we perform a reverse global analysis, by plotting the determined spectral components and their temporal evolution in a two-dimensional representation as the measurement, see Figure below. If both agree, we conclude that we have properly deconvolved

the transient data.