

# Interligand Electron Transfer Dynamics in Ruthenium Polypyridyl Dyes for Sensitized Solar Cells Determined with Femtosecond IR Transient Absorption Anisotropy

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The intriguing simplicity, yet powerful technique behind dye sensitized solar cells (DSSCs) has resulted in years of attempts to improve its energy efficiency in making sunlight into electricity or fuels. It has become clear that to further improve the energy conversion of DSSCs the influence of various recombination paths has to be diminished.<sup>[1,2]</sup> Most paths cannot be fully eliminated, however they may be out-competed. It demands that the desired processes are favorable and occur at such a rate that the recombination is circumvented.

The first essential step in a DSSCs after the initial excitation of the dye is the injection of the charge (electron for n-type) into the semiconductor. If this injection is slow the excited state of the dye might decay or reduce the surrounding electrolyte. For many years, the most impressive DSSCs were sensitized with polypyridyl ruthenium dyes for which injection has shown to vary from sub-ps to ns duration.<sup>[3-5]</sup> With a ns injection recombination becomes more apparent and therefore it is crucial to fundamentally study the underlying reasons behind this slow charge transfer. One feature which may impair the injection is the localization of the charge far from the semiconductor surface.

In this study interligand electron transfer (ILET, see Figure 1) dynamics of N712 (cis-diisothiocyanato-bis(2,2'-bipyridyl-4,4'-dicarboxylate) ruthenium(II)) is studied using fs Transient Absorption Anisotropy Spectroscopy in the IR region. The anisotropy decay allows for the determination of whether the excitation remains localized on the photoselected ligand or is randomized over the available bipyridyl ligands. To make a prediction of the obtain anisotropy for the localized as well as the randomized state, ongoing DFT calculations are being performed. Noteworthy is that previous studies within the N3 family, using the same technique in the visible region, show contradicting results.<sup>[6-8]</sup> This study therefore aims to elucidate the true time scale of ILET in these well-known dyes.

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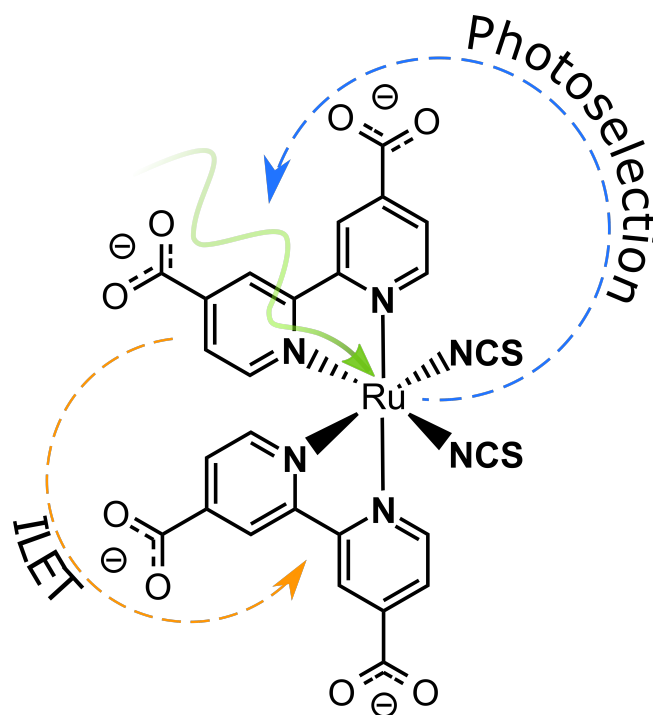


Figure 1: Interligand electron transfer in N712 between the two bipyridyl ligands after initial photoselection.

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