

# FACTORS CONTROLLING LIGHT HARVESTING EFFICIENCY, ELECTRON INJECTION AND CHARGE-SEPARATION IN RUTHENIUM(II)-POLYPYRIDYL-TiO<sub>2</sub> SYSTEMS RELEVANT TO SOLAR ENERGY CONVERSION

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Coordination compounds that efficiently harvest solar energy are of great importance for molecular solar energy conversion applications such as dye-sensitized solar cells. Ru(II)-polypyridyl compounds have attracted much interest in this area due to their favorable excited state properties. They have a broad MLCT absorption in the visible region with molar extinction coefficients around 15 000 M<sup>-1</sup>cm<sup>-1</sup> which is low compared to many natural pigments that absorb solar photons ( $\epsilon > 100\,000\text{ M}^{-1}\text{cm}^{-1}$ ).

By using ligands based on the dafo-dithioline motif (figure 1 and 2), Ru(II)-compounds with considerably higher extinction coefficients (30 000 – 44 000 M<sup>-1</sup>cm<sup>-1</sup>) in the visible spectral region have been obtained. When attached to nanocrystalline TiO<sub>2</sub> thin films and excited with pulsed laser light, the formation of a long-lived charge-separated state was observed. These results are explained by an intra-ligand charge transfer band that can be utilized both for promoting hole transfer and enhancement of the extinction coefficients.

However, in contrast to the Ru(II)-trisbipyridine type of compounds, the compounds based on the dafo-motif are essentially non-emissive and excited state lifetimes are generally less than 10 ns in acetonitrile solution at room temperature. This behavior is most probably due to low-lying ligand field states that enhance non-radiative decay. This behavior make this family of compounds well suited for studying how differences in the excited state manifold of the dye influence important properties such as electron injection efficiency and charge recombination rates in systems relevant to dye-sensitized solar cell applications. Comparative studies with standard Ru(II)-sensitizers will be reported.

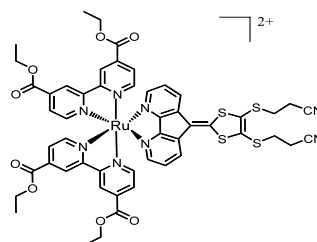
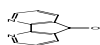


Figure 1. The dafo motif

Figure 2. Ru(deeb)<sub>2</sub>(dafo-dithioline)<sup>2+</sup>  
 $\epsilon=44\,000\text{ M}^{-1}\text{cm}^{-1}$  at 470 nm

## Selected references:

1. Kalayanasundaram, K. Photochemistry of Polypyridine and Porphyrin Complexes, 1992, Academic Press, London.
2. Staniszewski, A., Heuer, W. B. and Meyer G. J. *Inorg. Chem.* **2008**, *in press*.