

## PhD Thesis project & position

## Photo-energy conversion with Iron compounds: Watching the Ultrafast Molecular Events

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As the central part of metal-organic complexes, transition metals, Pt, Ir and Ru, are used in many electro-optical devices such as OLEDs and dye-sensitized solar cells (DSSCs). However, these metals are toxic and scarce thus expensive. Their replacement by earth-abundant elements like Fe or Cu is challenging since the photophysical properties of the latter are completely different and unfavorable for applications. Indeed, Fe-pyridine complexes undergo a very fast change of spin states that deactives the excited state within less than a picosecond. This is by far too rapid for the energy to be transferred onto a nearby molecular or nanomaterial acceptor. However, since very recently a new approach based on a new chemical design allows increasing the ligand field strength. The use of Nheterocyclic carbene (NHC) ligands was reported to lead to a prolonged excited state triplet lifetime, and solar cell or photo-catalysis applications come into reach.

Ultrafast femtosecond UV/VIS spectroscopy allows to « watch » and understand the charge transfer and other molecular processes in real time, and thus to improve the

molecular processes in real time, and thus to improve the molecular processes in real time, and thus to improve the molecular processes in real time, and thus to improve the molecular spectroscopy in the present (SRSMC, Nancy) we investigate these processes using laser spectroscopy in thin films mimicking DSSCs. Within the present PhD project, we will investigate new molecular constructs and the influence of their grafting on  $TiO_2$  on the charge transfer processes and solar cell performances.

The PhD project has two phases

- 1. in collaboration with another PhD student, she or he will learn femtosecond spectroscopy (transient absorption and fluorescence spectroscopy) and apply these techniques to isolated molecules in solution and to thin films.
- 2. Contribution to the development of a new method termed "two-dimensional" femtosecond spectroscopy. This technique allows obtaining new insights on why the charge generation processes depend on the excitation wavelength.

PhD position is open from October 2016, and has a 3-years duration. The net salary is approx. 1600€/month. This collaborative project is funded for four years, and involves partners in France and Germany. Applications must be sent to

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Top: Panels of DSSC's Bottom: Schematic of charge generation in a DSSC. The Fe-complexes work as the DYE. © Wikipedia