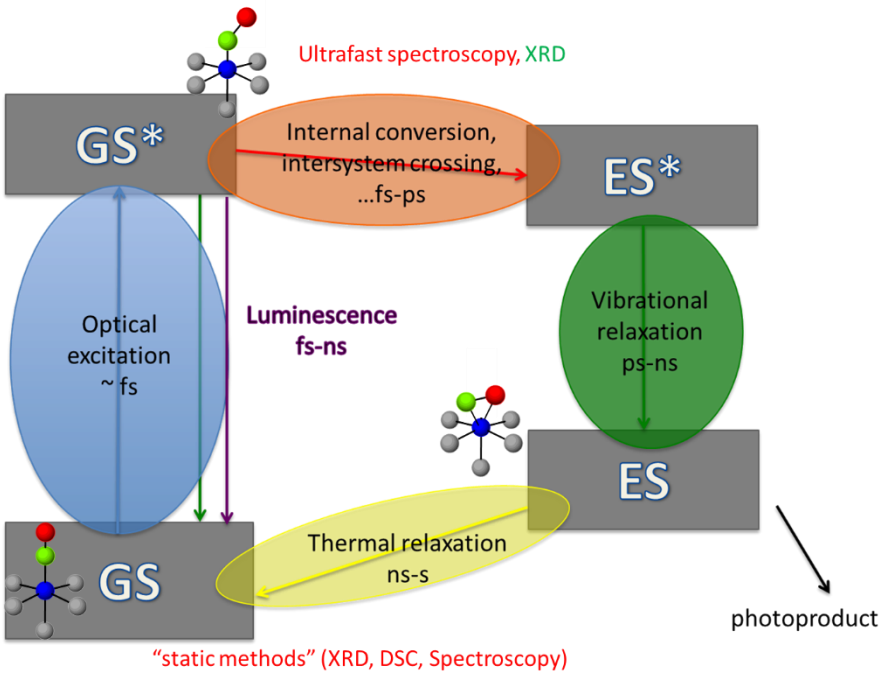
# PhD Thesis position

**Structural dynamics of photoswitchable complexes: from seconds to femtoseconds**


Summary

The main goal of this project is to follow the structural evolution during photoisomerisation of the NO ligand in photoswitchable molecules (see scheme below) by X-ray diffraction (XRD). This will allow to verify the models elaborated from ultrafast spectroscopy [1,2] for the complete photocycle of the photoisomerisation process in the family of $ML_5NO$ (M=metal, L=ligand) complexes, starting from the electronic excitation of the order of a few femtoseconds to the thermal relaxation of the order of milliseconds to seconds. The photoisomerisation process will be monitored in real-time by XRD measurements, from which the structure of the intermediate states will be determined. This requires XRD measurements on all time scales, from femtoseconds to seconds. For this purpose, different experimental facilities will be used : (i) on the millisecond to second time scale, XRD measurements will be performed in the CRM2 laboratory, where we dispose of a XRD setup allowing for this kind of measurement [3] ; (ii) on the submicrosecond time scale, the XRD measurements will be performed at synchrotron sources, e.g. on the CRISTAL beamline at the synchrotron SOLEIL (France), where measurements down to a few picoseconds are possible ; (iii) for the fastest XRD measurements, experiments at an X-ray free electron LASER are envisioned.

A second important aspect of the thesis project will be the improvement of our in-house XRD facility, in order to access time scales of a few tens of microseconds.

Candidate profile

We are looking for highly motivated candidates with a degree in Physics. The candidate should have a keen interest in experimental techniques and characterisation methods, especially X-ray diffraction and optical spectroscopy. Furthermore, she/he should be at ease with programming (languages like C or python, and tools like LABVIEW will be used). The project will include travel to large scale facilities, probably in different countries, the candidate should therefore be willing to participate in such endeavors.

References

[1] D. Schaniel, M. Nicoul, T. Woike, *Ultrafast reversible linkage isomerization in $Na_2[Fe(CN)_5NO[2H_2O$*, Phys. Chem. Chem. Phys. 12, 9029-9033 (2010).

[2] G. Galle, M. Nicoul, T. Woike, D. Schaniel, E. Freysz, *Unraveling the mechanism of NO photoisomerism by time-resolved infrared spectroscopy*, Chem. Phys. Lett. 552, 64-68 (2012).

[3] N. Casaretto, D. Schaniel, P. Alle, E. Wenger, P. Parois, B. Fournier, E.-E.Bendeif, C.Palin, S. Pillet, *In-house time-resolved photocrystallography on the millisecond timescale using a gated X-ray hybrid pixel area detector*, Acta Cryst. B73, 696-707 (2017).

Keywords

Time-resolved diffraction, photocrystallography, photoswitchable materials

Supervisor

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Application procedure

Please send a CV with a motivation letter as well as the grades of your master's degree (1st and 2nd year) along with a recommendation letter from your master's thesis supervisor (or equivalent).

Deadline for the application: 20th of July 2019

Starting date of PhD contract: 1st of October 2019