

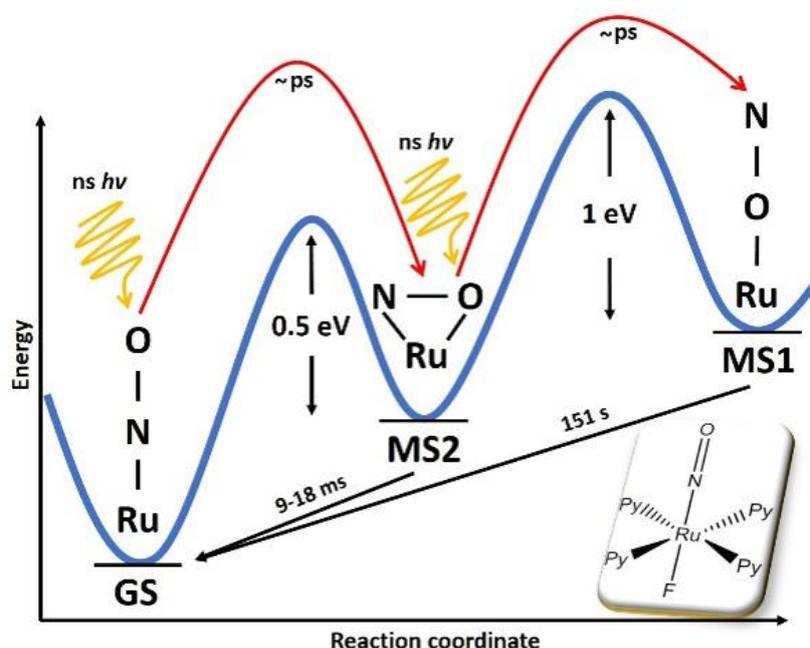
Postdoctoral position

Structural dynamics of photoswitchable solids

Summary

The objective of the project is a detailed study of the photoinduced isomerization of ruthenium nitrosyl complexes [1] in the solid state in order to understand the underlying mechanism, explore the potential energy surface and identify all metastable states and their properties, and establish the principles allowing for selectively driving the system towards one or the other structural configuration.

The photoisomerisation process will be monitored in single crystals by real-time by Xray diffraction (XRD) and spectroscopic measurements, from which the structural and electronic properties of the intermediate and metastable states will be determined. This requires XRD and spectroscopic measurements on various time scales and temperatures. For this purpose, different experimental facilities will be used: XRD measurements on the millisecond to second time scale will be performed in the CRM2 laboratory, where we dispose of a XRD setup allowing for this kind of measurement [2], while submicrosecond XRD measurements can be performed at synchrotron sources and XFELs (if necessary). Nanosecond and femtosecond optical spectroscopy can be performed on laboratory based setups.



Scheme illustrating the two-step mechanism $GS \rightarrow MS2 \rightarrow MS1$ in the photogeneration of nitrosyl linkage isomers in $[RuF(py)_4NO]^{2+}$ according to Ref. [3]



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Candidate profile

We are looking for highly motivated candidates with a PhD degree in Physics or Chemistry. The candidate should be familiar with experimental techniques and characterisation methods, especially X-ray diffraction and optical spectroscopy. Experience with photocrystallography and/or optical spectroscopy of photoinduced states under cryogenic conditions would be welcome. 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, T. Woike, *Necessary conditions for the photogeneration of nitrosyl linkage isomers*, Phys. Chem. Chem. Phys. 11, 4391-4395 (2009).
- [2] 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).
- [3] A. Mikhailov, W. Wenger, G. Kostin, D. Schaniel, *Room-temperature photogeneration of nitrosyl linkage isomers in ruthenium nitrosyl complexes*, Chem. Eur. J. 25, 7569-7574 (2019).

Keywords

Time-resolved diffraction and spectroscopy, photocrystallography, photoswitchable materials

Post-Doc duration: initially 12 months, extendable to 24 months. Salary of the order of 2100-2500 Euros per month, depending on the researcher's experience (funding by ANR-21-CE30-0045-01).

Project leader: Dominik Schaniel, CRM2, Université de Lorraine & CNRS, Nancy, France, Dominik.schaniel@univ-lorraine.fr; Web: www.crm2.univ-lorraine.fr

Application procedure

Please send a CV with a motivation letter to Dominik Schaniel.

Deadline for the application: Applications will be considered until the position is filled. Interviews will start on mid-April 2022.

Starting date of the contract: as soon as a suitable candidate is found.