
# Photo-NMR methods for the Dynamic & Structural analysis of Photoswitches@MOF.

A 18 month postdoctoral fellowship on the development and application of solid-state nuclear magnetic resonance (NMR) under *in situ* photoirradiation is available at the University of Lorraine in Nancy.

**Starting date: end of 2025/ Starting 2026.**

**Background and motivation**:

Light and optical technologies are increasingly central to our society in the 21st century. Optoelectronics has the potential to highly contribute to sustainability and to the energy transition thanks to renewable energy production, energy-efficient lighting, high-efficiency data communication and data storage, environmental sensing, efficient manufacturing process and efficient transportation. We aim to contribute to these challenges by investigating materials enabling better energy efficiency and device sensitivity.

The combination of photoswitches (PS) and Metal-Organic Frameworks (MOFs) results in materials with extraordinary properties. Understanding interactions occurring inside such host-guest systems represents a key step to pave the way towards advanced functional materials. Since the properties of the guest molecules are determined by their structure and host/guest interactions, adapted characterization techniques are mandatory to draw a full picture of material properties as a function of structural parameters.

One of the expertise of CRM2 laboratory is the characterization of photosensitive molecules and nanoparticles. To perform the NMR study of molecular photo-switches, we therefore developed strategies allowing the *ex situ* generation of photoinduced states and the subsequent low temperature transfer inside the NMR spectrometer[1] in solids. In parallel We also developed *in situ* irradiation devices for the study of photochemical reactions in solution[2–4]. By complementing our NMR studies with photo-crystallographic studies developed at CRM2, we can therefore study the effect of molecular structure on the generation and thermal relaxation of photo-induced states and thereby unravel the molecular processes at the origin of the optical properties.

**Approach:** Great challenges lie in the analysis of crystalline, semi-crystalline, or even dynamic host materials with possibly dynamic or disordered guest molecules. The aim of this postdoctoral fellowship is to establish a robust analytical workflow combining experimental and theoretical methods to fully characterize PS@MOF composites in order to derive the structure-property relationship. The hired candidate will further develop and apply Solid State NMR characterization to study the structure and the dynamics of MOF host matrices, along with the confined guest photoswitches. Solid State NMR methodology (such as dipolar recoupling techniques) will also be confronted to calculations based on theoretical models in order to characterize host-guest interaction. This project also implies the development of novel *in situ* irradiation strategies, in particular for MAS (magic angle spinning) solid state NMR experiments, as well as setting up combined NMR/UV-vis measurements to directly link the structural features to the optical properties of the new hybrid materials. The hybrid host-guest materials will be synthesized in our group as well as by our international partners at the Institute of General, Inorganic and Theoretical Chemistry (Innsbruck University, Austria).

**Hosts and research infrastructure**: This project is funded by the DYSPHOM ANR PRCI project. The postdoctoral researcher will work in the CRM2 laboratory and will be supervised by Axel Gansmüller of the CRM2 NMR team ( https://crm2.univ-lorraine.fr/recherche/equipes/rmn/), in the framework of a collaboration with the University of Innsbruck.
The researcher will have access to the platforms for structural (NMR, XRD, TEM, etc.) and optoelectronic (spectroscopies, microscopies, ellipsometry, calorimetry, etc.) characterization of our interdisciplinary initiative with LUE, fostering the research for sustainable solutions for the digital world. The development will be carried out on the NMR platform at CRM2, equipped with 6 spectrometers covering the range from 200-600 MHz for liquid and 300 & 600 MHz solid-state NMR with 1.3, 2.5, 3.2, 4 and 7mm MAS NMR probeheads along with solution and solid state “in-situ” irradiation setups with LEDs covering the 275-1300 nm range. In particular, this project will benefit from unique NMR instruments available in our group such as a brand-new 3.2 mm photo-MAS NMR probehead operating on a 600MHz NMR spectrometer.
**The candidate**: We seek application from national and international candidates, who have a PhD in chemistry, physics or materials science, and previous experience in Solid State NMR spectroscopy.
**Contact**: Applications (cover letter, CV and names for recommendation) and informal queries about the lab and research projects should be directed by email to axel.gansmuller@univ-lorraine.fr

**Selected publications**:


[1] A. Gansmüller, A. A. Mikhailov, G. A. Kostin, J. Raya, C. Palin, T. Woike, D. Schaniel, *Anal. Chem.* **2022**, *94*, 4474.
[2] J. Pecourneau, R. Losantos, A. Gansmuller, S. Parant, Y. Bernhard, M. Mourer, A. Monari, A. Pasc, *J. Photochem. Photobiol. Chem.* **2023**, 114583.
[3] E. Cortelazzo-Polisini, M. Boisbrun, A. H. Gansmüller, C. Comoy, *J. Org. Chem.* **2022**, *87*, 9699.
[4] G. Angelini, A. Gansmüller, J. Pécourneau, C. Gasbarri, *J. Mol. Liq.* **2021**, *333*, 116000.