- «Photo-NMR » characterization of photoactive systems

This research axis focusses on the study of photoactive systems. The molecular structural changes induced by light irradiation can provide exceptional properties such as color changes (photochromism), conversion of light energy into chemical energy, or triggering of complex chemical processes.

The understanding of the interactions between the photo-commutators and their environment (solvent or porous matrices) therefore represents a key step towards the development of advanced functional materials. We thus developed a setup allowing the *ex-situ* generation of photoinduced states in solids and the subsequent low temperature transfer inside the NMR spectrometer. By complementing our NMR studies with photo-crystallographic studies of the CRISP team, we can study the effect of molecular structure on the generation and thermal relaxation of photo-induced states (e.g. in nitrosyl complexes).

Additional DFT calculations are also performed to give access to the charge density distribution on the different atoms. On top of providing the assignment of the NMR signals, these calculation can also provide the assignment of IR spectra in order to identify the photo-induced states of *in-situ* photo-IR experiments.

In order to study photochromism and solvatochromism of photo-commutators in solution, we also developed a setup for *in-situ* irradiation that we apply to study our photoswitches (e.g. cyclocurcumine, spyropiranes, …). In these studies, the NMR allows the observation of photo-isomerization reversibility upon subsequent irradiation cycles and the identification of degradation by-products. The *in-situ* follow up also allows the study of photoisomerization kinetics and the determination quantum yields.