Effect of pressure and irradiation on the properties of photoisomerisable spin transition compounds

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Scientific background

Determining and analysing the structural organisation of a material is a prerequisite for any understanding of its physical or chemical properties. The study of structure-property relationships is therefore an important step in materials science in order to improve properties or bring out new ones. X-ray diffraction (XRD) is the key technique in this process. In addition to structural analysis of materials in their fundamental state, it is now possible to study structural changes in materials subjected to light irradiation using photocrystallography (X-ray diffraction under in situ light irradiation). In particular, this approach allows to determine changes in intra/inter-molecular bonds, such as ligand isomerisation or photo-induced phase transitions. Applying pressure to a crystal is another external stimulus that can change the properties of a material by modifying its structure in a 'clean' way, i.e. by altering the inter-atomic distances and bond angles without changing the chemical nature of the atoms of the structure. This application of pressure can induce phase, magnetic and/or electrical transitions. In situ XRD can be used to trace the structural origins of such pressure-induced transitions. At CRM2, we have experimental setups to measure DRX under pressure and DRX under light irradiation.

Aim of the thesis

The aim of this thesis is to combine the two constraints (pressure/irradiation) in order to study materials that respond to both stimuli and thus establish structure-property relationships as a function of pressure and irradiation.

To achieve this goal, we are planning two phases:

- the first will be methodological and instrumental, with the aim of setting up devices enabling in situ XRD and infrared (IR) spectroscopy measurements to be carried out simultaneously under the application of pressure and light irradiation.
- The second part aims to apply this methodology to materials that show a dual response, under pressure and irradiation.

We are focusing on iron nitroprusside materials with organic pillars, the choice of which offers great flexibility and structural diversity.

This family of compounds exhibits interesting properties, in particular an atypical kinetic behaviour during the temperature-induced spin crossover (SCO): we observe a broadening of the hysteresis when the cooling/heating rate is reduced [1]. Pressure XRD combined with pressure IR spectroscopy measurements with and without light irradiation will enable a detailed study of the structural evolution of these compounds. By exploring the pressure-irradiation-temperature diagram, we can establish the structure-property relationships by identifying the different mechanisms at work.

Work of the person recruited:

- Instrumental development
- Synthesis of crystals and selection of those with the best responses.
- Study by X-ray diffraction and infrared spectroscopy under pressure/light irradiation of the selected compounds.
- Data processing and presentation of results in oral and written form.

Bibliography:

[1] Y. Plasencia et al., J. Phys. Chem. Sol. 150, 109843 (2021). Y. Avila et al., Eur. J. Inorg. Chem. 24, e202200252 (2022).

Thesis grant (3 years)

Funded by Université de Lorraine (>€2100 gross/month)

Application open: from February 21th - April 14th

Pre-selection and interviews: April - May 2024

Start of thesis: October 2024

Candidate profile:

- Master in physics, chemistry or materials science

- Skills in crystallography, X-ray diffraction and spectroscopy

- Scientific curiosity, autonomy, a taste for experimentation and instrumental development, good communication skills and a taste for teamwork.

Application: Send us

- CV and covering letter,

- Transcripts of Master and Bachelor grades

- Two reference letters (Master's supervisor, internship supervisors, etc.) or the contact details of two referees.

Selection process :

Stage 1: pre-selection on the basis of applications

Stage 2: interview by a panel (these supervisors + external experts)