

PhD position

Synthesis, shaping and investigation of the barocaloric refrigeration ability of spin crossover compounds

Funding: ANR Bref

Laboratory: ICMCB, “Switchable Molecules and Materials” group, Bordeaux

Duration: 3 years from October 2024.

Spin crossover (SCO) materials are molecular switches between two electronic states upon the application of an external stimulus such as temperature, light, electric field or pressure. Already investigated applications included sensing and memory devices. Very recently, the huge entropy changes observed whenever abrupt crossovers occur, usually coupled with 1st order phase transitions, evidenced that this class of compounds is of utmost interest to be integrated in solid-state refrigeration technology, using either hydrostatic pressure (barocaloric refrigeration) or anisotropic strain (elastocaloric refrigeration) as the driving parameters. However, before their integration into devices, the full pressure/temperature phase diagrams of the selected systems must be known, and they must be shaped into large bulk materials with reasonable thermal conductivity, which can be challenging concerning molecular compounds. Potentially addressing those issues, our group has specifically developed an expertise on the fundamental applications of hydrostatic pressure on spin crossover materials and has recently devised a fundamental approach for sintering those soft materials into centimetric-sized ceramics.

Accordingly, the project aims first at preparing compounds adapted for barocaloric refrigeration, i.e., presenting an abrupt SCO with reduced to non-existent thermal hysteresis, ideally close to room temperature. The most promising systems will feed the preparation of ceramics firstly by Spark Plasma Sintering (SPS) at low temperature and then by other sintering techniques. A particular attention will be paid to the establishment of sintering maps to ensure reproducibility. All synthesized compounds and corresponding ceramics will be precisely characterized concerning their structural and physical properties under variable temperature and pressure conditions. The investigations will cover crystallographic and magnetic properties under variable temperature and pressure to explore the full P/T phase diagrams as well as calorimetric measurements under pressure to extract their refrigeration ability.

All those techniques are available in the lab. Especially, X-ray diffraction facilities host specific powder and single-crystal diffractometers that will be adapted for pressure measurements. Specific collaborations at the national (ANR projects) and European level (European Innovation Council Pathfinder Challenge project) are already in place to cover additional investigations and a new micro-calorimeter will be acquired in this context to perform mandatory calorimetry measurements under moderate pressure (1 – 1000 bar).

The selected candidate will be hired by CNRS and will be based at the Institute of Condensed Matter Chemistry of Bordeaux (ICMCB) where she/he will benefit from the entire technical platform. The “Switchable Molecules and Materials” group has a long-standing expertise in the synthesis and characterization of spin crossover compounds, with a renowned experience in magnetism, crystallography and pressure measurements. The PhD thesis is already funded in the context of the ANR Bref.

Contact: Guillaume Chastanet (Guillaume.chastanet@icmcb.cnrs.fr) and Mathieu Marchivie (Mathieu.marchivie@icmcb.cnrs.fr)

ICMCB: 87 avenue du Dr. A. Schweitzer, 33600 PESSAC, France

Switchable Molecules and Materials group (X: @SwitchMM2)