PhD position

New solid state-based refrigeration processes: (*p*,*T*) phase diagrams of spin crossover materials

Funding: European Innovation Council Pathfinder Challenge *FROSTBIT*

Laboratory: ICMCB, "Switchable Molecules and Materials"

Duration: 3 years from October 2024.

Spin crossover (SCO) materials can switch between two electronic states upon the application of an external stimulus, most interestingly temperature and pressure. It has been only recently evidenced that with the huge entropy changes observed whenever sharp abrupt crossovers occur, usually coupled with structural 1st order phase transitions, this class of compound is of utmost interest for innovative solid-state refrigeration technologies only recently developed, using either hydrostatic pressure (barocaloric refrigeration) or anisotropic strain (elastocaloric refrigeration) as the driving parameters. We have specifically developed expertise in the fundamental applications of hydrostatic pressure on spin crossover materials and recently devised a fundamental approach for sintering soft molecular materials in centimetric sized ceramics.

In the context of a very ambitious European-driven innovation project aiming to develop innovative refrigeration technologies to address the GreenHouse Gas emission of current vapour compression technology, we aim to use those materials to design and develop a heat exchanger. Our sintering approach is key to raise a technological hurdle towards the incorporation of spin crossover materials. Nevertheless, it necessitates a thorough understanding of the (*p*,*T*) phase diagram of materials of interest: Before the sintering process to solve varied issues e.g. polymorphic transformations, or differences in behaviour between the low *T* high *p* Low-Spin phase vs. the high *T* low *p* High-Spin one; During the sintering process to understand its mechanisms; After sintering to correlate the refrigeration capability of the final ceramics with the initial powder properties. This project will first select and synthesize materials adapted for barocaloric refrigeration, that is that present an abrupt SCO with reduced to non-existant thermal hysteresis close to room temperature (molecular materials). The investigations will cover crystallographic, calorimetric and magnetic properties under variable temperature and pressure to extract the (*p*,*T*) phase diagram and refrigeration ability. All those techniques are available at ICMCB, and through collaborations at the national (ANR projects) and European level.

The selected candidate will be hired by CNRS and will be based at the Institute of Condensed Matter Chemistry of Bordeaux (ICMCB). 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.

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