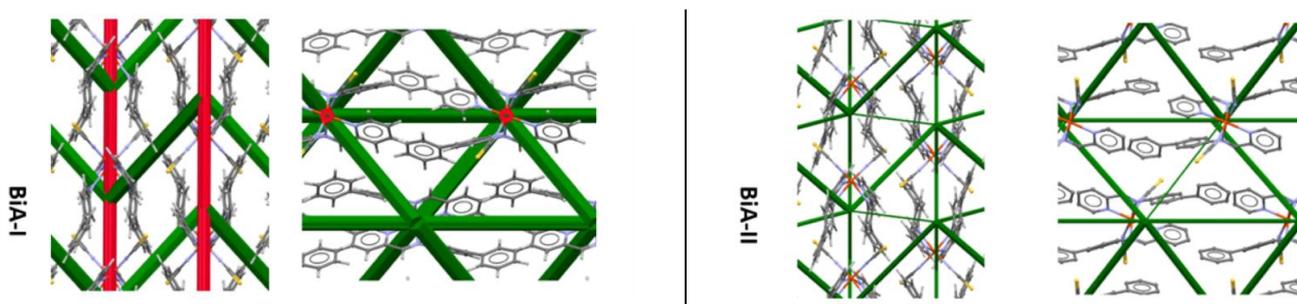


PhD position available

Beyond the usual structure-property relationships: Classifying and quantifying interatomic interactions in molecular switches.

Spin CrossOver (SCO) complexes have interested the scientific community for decades. Their reversible switching between two electronic states has applications in information storage, temperature, pressure, and chemical sensors, as well as in displays and actuators and they are even being considered as an alternative to barocaloric refrigeration.

It is now well established that certain structural characteristics govern the switching characteristics¹. The distortion of the coordination sphere of transition metals has been deeply investigated, demonstrating its crucial role in thermal and light-induced switching features for example. However, these correlations were based on a limited number of complexes within specific families until we recently developed a tool to explore a set of thousands of compounds². In addition to exploring the coordination sphere influence, the concept of cooperativity linked to the strength of the intermolecular interactions and responsible for the abruptness of the transition or the presence of a hysteresis loop, is still debated and lacks experimental quantification. Moreover, the presence of competing interactions that give rise to symmetry breaking, multi-step transitions, and metastable states has not been analysed in terms of any experimental energy data. The study of the non-covalent intermolecular interactions responsible for these phenomena is yet to be fully explored, as the methods of evaluating the nature and energy of these interactions are still in their infancy. Lately, however, we demonstrated that it's possible to map these intermolecular interactions (Figure below)³ and such new tools are now being implemented on dedicated software (CrystalExplorer, NCIPLOT, CrystalOptimiser, etc.), enabling the analysis of a larger number of compounds to improve structure-property correlations.



Energy difference frameworks for polymorphs of $[\text{Fe}(\text{PM-BiA})_2(\text{NCS})_2]$.

The thesis project plans to use these tools to evaluate the intermolecular interactions of several selected SCO families which exhibit a wide range of behaviours (gradual, cooperative, multistep...). The main data source of the crystal structures of these derivatives will be the Cambridge Structural Database (CSD). Any missing or additional structural data will be obtained through X-ray diffraction, on which the recruited doctoral student will be trained. Moreover, we will extract additional properties of crystal lattices, such as thermal expansion tensors. This will enable us to generate new structural descriptors to form the basis of a more extensive structure-property relationships' analysis, well beyond the coordination sphere on the initial few families of SCO complexes studied. The results will, at least, provide a 3D map of the energy landscape of intermolecular interactions in several families of SCO complexes. This will unlock a unique detailed understanding of the cooperativity and thermodynamic aspects of SCO, which are key factors in its use in devices. This methodology can then be extended to other types of compounds (molecular conductors or organic-inorganic hybrid crystals, etc.) and/or used to feed machine learning algorithms to identify more universal trends.

Profile and skills required: We are looking for a highly motivated student with a master's degree in physical chemistry, physics, or materials science with basic knowledge on crystallography and X-ray diffraction.

Location: Institute of Condensed Matter Chemistry of Bordeaux (ICMcb), in the "Switchable Molecules and Materials" group, CNRS- University of Bordeaux.

Type of contract: The PhD is funded by the University of Bordeaux for 3 years

Tentative start date of the PhD: September or October 2026

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