VISUALIZATION, CONTROL AND MODELLING OF SPATIOTEMPORAL ASPECTS OF THE DYNAMICS OF PHASE TRANSITIONS IN SPIN TRANSITION MOLECULAR CRYSTALS

Contact person : kamel.boukheddaden@uvsq.fr

This phd thesis will take place in the PMFM (Physics of Multifunctional Materials) group of GEMAC laboratory.

This is a multidisciplinary and fundamental thesis project, concerning the investigations on new multi-functional switchable molecular materials, based on transition metals (mainly Fe) combining in the synergistic way the spin-crossover (SCO) including photoinduced and hysteretic effects with fluorescence. Starting from a certain number of recent preliminary results, this project deals with measurement and real time imaging of the behavior of SCO single crystals and bistable molecular composites made of cooperative SCO crystals embedded in polymers. The idea is to monitor the thermally and photo-induced phase transitions of the crystals along their transformations on the one hand, as well when they are operating (during their luminescence), on the other hand, in particular when they are subject to external stimuli, such as electric field, light, mechanical strain etc.

In this thesis, we will first use strongly cooperative SCO systems, presenting an enhanced thermo-chromic contrast between the low-spin and the high-spin states, involving appropriate fluorescent ligands. Among the pursued objectives, we quote: (i) the reversible switching control of SCO part, such as the transition temperature, the width of the thermal hysteresis; (ii) the control and the real time observation of the elastic properties of these materials inside their bistable region (the thermal hysteresis) allowing to generate memory effects, either through photo-thermal effects (laser spot well focused on the crystal's surface) or by an electric field; (iii) tuning and imaging while operating the fluorescence emission and its switching inside the thermal hysteresis as a function of the nature of the used organic fluorophore ; (iv) understanding, modelling and predicting through high performance simulations on 3D systems (based on CUDA programming), the required physical mechanisms in order to propose innovative solutions towards obtaining multi-functional SCO systems with tailored physical properties.