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Crystallography of Molecular Switches under Constrains (T, P, hv): The multiscale approach of the Spin Crossover Phenomenon.

M. Marchivie^{1*}, P. Rosa¹, E. Tailleur¹, G. Chastanet¹, J.P. Itié², and P. Guionneau¹

¹ CNRS, Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France

² Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette Cedex, France

Molecular switches are molecules that can be reversibly switched between at least two different states using environmental stimuli as temperature, pressure, light, magnetic or electric field, but also change in chemical environment such as pH variation, solvent or water absorption and so on. Molecular switches has drawn attention of researchers according to their possibility to obtain a wide variety of functional material down to the molecular level and because of the quasi unlimited opportunities provided by synthesis of numerous new molecules. Among those molecular switches, Spin CrossOver (SCO) complexes have been widely explored by the scientific community for decades as they are often responsive to a wide number of the stimuli already cited above and present a very large panel of different switching behavior from very gradual conversions between the two state to very abrupt ones with or without hysteresis, stepwise or not etc... SCO phenomenon corresponds to a modification of the electronic state of a transition metal complex upon different constrains from a Low Spin (LS) state where most of the electrons are paired to a High Spin (HS) state where several electrons become unpaired. It results in changes of numerous physical characteristics such as magnetic, dielectric, optical and mechanical properties associated to usually strong thermodynamic and structural variations.

As a consequence, even if SCO originates at the atomic scale, the simple consideration of the transformations that occur following the SCO at this scale or in its close vicinity does not allow anyone to truly understand, anticipate and thus take advantage of what happens at the scale of the material, and even less at the device one.

As the fruit of years of work and experience on this phenomenon, we have formalized the concept of the multiscale understanding of SCO by showing how the initial impressive atomic modification propagates on all the physical scales of the solid (Figure 1). It lead to the description of the phenomenon in terms of structure-properties relationships that fit together, like Russian dolls, and propagate according to a kind of domino effect¹. The concept appears well illustrated, for example, by the volume modification, always the same at the

atomic level but drastically different and adaptable, in amplitude and sense, at any other physical scale.

The purpose of this conference is then a short travel through the structure – properties relationships of SCO materials at different scale and upon different stimuli. A particular attention will be paid to the role structural considerations in the chemical design of optimized of photo-active switching materials. Finally, as polymorphism plays a crucial role in SCO behaviors the question of establishment of the full P/T phase diagrams² will be discussed through the very subtle investigation of SCO complexes under pressure.

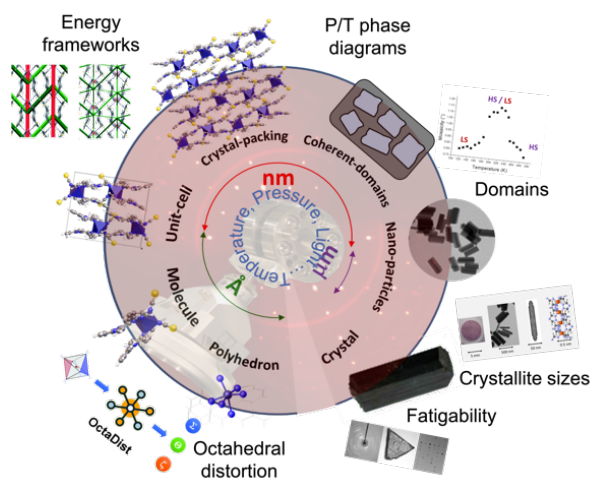


Figure 1 : The multiscale approach of spin crossover molecular switches.

1. P. Guionneau, M. Marchivie & G. Chastanet *Chem. – A Eur. J.* **2021**, *27*, 1483–1486
2. E. Tailleur, M. Marchivie, J.-P. Itié, P. Rosa, N. Daro & P. Guionneau *Chem. - A Eur. J.* **2018**, *24*, 14495–14499