MS29-O4 Insights into molecular spreading and bridging in chromosome condensation from the complex structure of Spo0J and *par*

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In the chromosome partitioning system (*par*ABS), the partition protein (ParB) and its regulatory protein (ParA) act cooperatively through *parS* DNA to facilitate chromosome segregation. ParB oligomer and *parS* interact together to form a high-order nucleoprotein that is required for the loading of the structural maintenance of chromosomes proteins onto the chromosome for chromosomal DNA condensation. Spo0J is a member of ParB superfamily. The binding of *par*S and Spo0J from *H. pylori* (*Hp*Spo0J) was characterized. The *Hp*Spo0J-parS complex structure was determined by Se-MAD method. The overall structure of *Hp*Spo0J is in an elongated shape including a flexible N-terminal domain for protein-protein interaction and a conserved DNA-binding domain for *par*S binding. A structure model for molecular spreading and bridging in chromosome condensation is proposed.

Keywords: Chromosome partitioning system, parABS

MS29-O5 Crystal-Packing and Spin-CrossOver in some Molecular Solids. Trends and new Features.

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One of the key-stones of modern science is the ability to determine the crystal structures of materials. To this end, diffraction techniques are in constant improvement always pushing the frontiers of investigation. For example, if focusing only on the **spin crossover (SCO)** molecular material field [1], recent X-ray diffraction developments permit to investigate local structures in materials that are not strictly crystalline, structural modifications at the picoseconds time scale or crystal structures under external perturbations as pressure or light irradiation [2-4]. As a result **a very fine description of the structure-properties relationships in molecular SCO solids can be achieved**. [5, 6].

In this context, we will present a multi-scale description of the SCO mechanism in molecular solids (Fig. 1) based on the **crystal-packing analysis** and focusing on **structural movies** showing the sample breathing of the **intermolecular interactions** and on the full determination of (pressure-temperature-light) **phase diagrams**. In addition, recent X-Ray diffraction on powders has revealed a potential **structural fatigability** upon cycling in a SCO compound. This fatigability, connected with some properties of the crystal-packing, will also be discussed [7].

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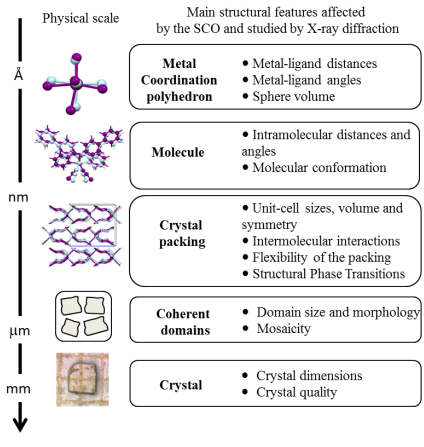

Figure 1. Physical scales and the related modifications due to the spin crossover in a molecular crystal (adapted from ref [6])

Keywords: X-ray diffraction, structure-properties relationship, spin-crossover, iron, molecular materials

MS30 Hydrogen bonding from theory to applications

Chairs: László Fábián, Nikoletta Bathori

MS30-O1 Molecular Cups and Capsules Through Hydrogen Bonding

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An exciting research challenge in crystal engineering and supramolecular chemistry is to design, synthesize, and characterize nano-sized architectures with applications in biology, chemistry, and materials science.[1] Predicting and designing non-covalently bound supramolecular complexes and assemblies is difficult because of the weakness of the interactions involved, thus the resulting superstructure is often a compromise between the geometrical constraints of the building blocks and the competing weak intermolecular interactions.[2]

Our research interest has been focused on the studies of weak non-covalent intermolecular, viz. supramolecular interactions as the driving force in self-assembly and molecular recognition, especially in the solid state by single crystal X-ray diffraction. The lecture will highlight some of our recent studies on a new family of macrocyclic host molecules, derived from well-known resorcinarenes, namely tetra-N- alkylammonium resorcinare salts (Fig. 1a), NARXs.3 The NARXs exhibit a rich host- guest chemistry and self-assembling properties, exemplified by an inclusion complex3a (Fig. 1b), a deep cavity cavitand based on hydrogen and halogen bonding3d (Fig. 1c) and the first halogen bonded dimeric resorcinare capsule3i (Fig. 1d).

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