## MS37-O2 Spin crossover materials: from molecular motion to switchable mechanical properties

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The spin crossover (SCO) phenomenon involves the switching of a transition metal complex between high spin (HS) and low spin (LS) states as a result of some perturbation to the species (for example changes in temperature or pressure, or as a result of light irradiation). Molecular species in the HS and LS states are distinguished by differences in their colour, magnetic moment and structure [1].

The strain associated with SCO has recently been demonstrated as an active component in actuating devices [2] and it is clear that mechanical properties play pivotal role in the switching phenomenon. Thus it is surprising that while the volumetric and morphological changes associated with the switching event are usually well characterised by traditional crystallographic methods, elastic moduli and their correlation with molecular structure have never been thoroughly analysed.

Single crystal X-ray diffraction techniques at elevated pressure and variable temperatures, complimented by spectroscopic and magnetic studies, have been used to probe the structure-properties relationship of a series of molecular $Fe^{II}$ derivatives. A range of fascinating pressure-induced behaviours has been observed providing unprecedented insight into the driving forces behind the dynamic solid state processes. Examples include negative linear compression that is structurally antagonistic to the requirements of SCO [3] and pressure-induced stepped SCO accompanied by symmetry breaking [4]. More importantly, these studies have for the first time allowed a systematic investigation into the relationship between crystal structure and mechanical properties for a family molecular SCO complexes.

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## MS37-O3 Understanding polymorph stability and phase transformations by combining ab-initio lattice dynamics, multi-temperature elastic scattering and inelastic scattering measurements

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The relative stability of polymorphic molecular crystals is not easy to assess, neither from experiment nor from ab-initio approaches. Despite recent advances in periodic DFT calculations, which have helped crystal structure prediction tremendously, it is still not possible to predict the relative stabilities at ambient conditions. In this contribution, we use models of thermal motion derived from ab-initio lattice dynamical calculations in refinements against X-ray diffraction data [1], and show how this can lead to an understanding of the different contributions of entropy and enthalpy to the free energies of the different polymorphic structures. We use the tetramorphic anti-tuberculosis drug pyrazinamide [2] as test case. Pyrazinamide undergoes several solid-state phase transformations as a function of temperature, and it is thus possible to construct a tentative phase diagram of the relative stabilities [3-4], which compare favourably to our modeling efforts. Additionally, inelastic X-ray and neutron diffraction measurements have been performed in order to further validate the resulting models.

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