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"Structure:function relationships in molecular spin-crossover complexes"

Spin-crossover (SCO) involves the rearrangement of electrons in a metal ion, from a high-spin to a low-spin state. Such transitions have a large impact on the physical properties of a solid material, including its magnetic moment, colour, dielectric constant and electrical resistance. Several practical applications of SCO switches have been demonstrated, including: display and memory devices, with switchable pixels of a SCO material; electrical and electroluminescent devices, employing changes in the electrical resistance of a SCO thin-film; and, in a temperature-sensitive MRI contrast agent. The design of new SCO materials with technologically useful properties is an important problem of crystal engineering.

We have proposed a relationship between molecular shape and the occurrence of cooperative (abrupt and hysteretic) SCO in molecular crystals.[1] On one hand, spin-crossover can be can be promoted by molecules that interdigitate in the crystal, to maximise mechanical coupling between the switching centres as they change their shape. On the other hand, if the structure difference between the high-spin and low-spin materials is too large, then spin-crossover cannot occur.

I will describe the data giving rise to these ideas, and recent experiments we have performed to test them.[2-4]

[1] M.A. Halcrow, *Chem. Soc. Rev.*, **2011**, *40*, 4119.

[2] L.J. Kershaw Cook, R. Mohammed, G. Sherborne, T.D. Roberts, S. Alvarez and M.A. Halcrow, *Coord. Chem. Rev.*, **2015**, *289–290*, 2.

[3] R. Kulmaczewski, H.J. Shepherd, O. Cespedes and M.A. Halcrow, *Inorg. Chem.*, **2014**, *53*, 9809.

[4] A. Santoro, L.J. Kershaw Cook, R. Kulmaczewski, S.A. Barrett, O. Cespedes and M.A. Halcrow, *Inorg. Chem.*, **2015**, *54*, 682.