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Spin crossover, symmetry breaking and magnetoelectric coupling in Mn(III) systems

Elżbieta Trzop[a*], Vibe B. Jakobsen[b], Emiel Dobbelaaret [b], Conor T. Kelly[b], Laurence C. Gavin[b], Helge Mgller-Bunz[b], Shalinee Chikara[c], Xiaxin Ding[c], Franziska Weickert[c], Kane Esien[d], Solveig Felton[d], Jie-Xiang Yu[e], Hai-Ping Cheng[e], Vivien S. Zapf[c*], Michael Carpenter[f], Eric Collet[a*], and Grace G. Morgan[b*]

a. Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251 (France)
b. School of Chemistry, University College Dublin (Ireland)
c. National High Magnetic Field Lab, Los Alamos National Laboratory (USA)
d. Centre for Nanostructured Media, School of Mathematics and Physics - Belfast (UK)
e. Department of Physics, University of Florida - Gainesville (USA)
f. Department of Earth Sciences, University of Cambridge (UK)

* email : elzbieta.trzop@univ-rennes1.fr, vzapf@lanl.gov, eric.collet@univ-rennes1.fr, grace.morgan@ucd.ie

Switching in spin crossover materials is usually strongly coupled to structural degrees of freedom, with local bond-length changes of up to 0.2Å for metal–donor distances due to depopulation/population of anti-bonding orbitals. These local distortions at the molecular scale propagate macroscopically through elastic coupling, resulting in macroscopic changes that may involve symmetry breaking. To date, most research on such systems has been focused on temperature, light or pressure stimuli. An alternative, magnetic-field-driven spin-state bistability is definitely much less-explored [1,2].

Here we will present how magnetic-field-driven spin-state switching coupled to symmetry change allows for a new type of magneto-electric coupling. We will focus on the MnIII spin crossover in $[Mn^{III}L]BPh_4$ (L = (3,5-diBr-sal$_2$)323) [3,4]. The changes are driven from a low symmetry phase with high spin/low spin order towards a higher symmetry high spin phase, which remains stable once the magnetic field is switched off. The coupled spin state and symmetry changes are responsible for a change in electric polarization amplitude and direction, driven by the magnetic field. The detailed structural analysis and revealed symmetry breaking between polar space groups of thermally driven phase transition were a key tool to understand the ongoing processes.

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