## MS16-O4 Room temperature polarisation and magnetisation in a bulk layered perovskite by control of octahedral tilt distortions

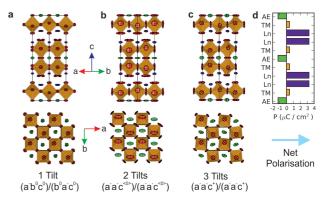
Michael J. Pitcher<sup>1</sup>, John B. Claridge<sup>1</sup>, Matthew J. Rosseinsky<sup>1</sup>

1. Department of Chemistry, University of Liverpool L69 7ZD, UK

## email: michael.pitcher@liv.ac.uk

Combining spontaneous, switchable polarisation and magnetisation into a single phase "multiferroic" material is a major challenge in materials chemistry. Such materials, with strongly coupled electric and magnetic polarisation, could provide the basis for low-energy high-density information storage devices but are unlikely to be viable unless they can operate at (or close to) ambient temperatures. The design and synthesis of multiferroic materials is difficult because the typical electronic requirements of polarisation (P) and magnetisation (M) are antagonistic: e.g. proper ferroelectrics such as PbZr<sub>1-x</sub>Ti<sub>x</sub>O3 require closed-shell s<sup>2</sup> and d<sup>0</sup> cations, while ferromagnetism at ambient temperatures requires a high concentration of open-shell cations.[1] Materials where both of these conditions are fulfilled above 300 K are very rare, and even in the leading example of BiFeO<sub>3</sub> – where P arising from the Bi<sup>3+</sup> sublattice is combined with long-range antiferromagnetic order of the Fe<sup>3+</sup> sublattice – the generation of an appreciable magnetisation and magnetoelectric coupling is challenging. [2] It is therefore important that new strategies for combining P and M at high temperatures are investigated. One basis for such a strategy is provided by recent theoretical work on "hybrid improper" ferroelectrics, which describes how specific combinations of octahedral tilt distortions in layered (AO)(ABO<sub>3</sub>)<sub>n</sub> perovskites may be used to break inversion symmetry.[3, 4] We have applied these structural principles to a carefully selected (AO)(ABO<sub>3</sub>)<sub>2</sub> parent phase with a strongly magnetic B-site sublattice, using chemical control to produce the desired polar distortion in a new series of compounds which order magnetically above room temperature.[5] In this series, electrical polarisation and spontaneous magnetisation are induced simultaneously by control of the same structural distortion (an octahedral tilt); these properties are therefore coupled (as demonstrated by a linear magnetoelectric response) and are shown to coexist at temperatures of up to 330 K across a range of compositions.[5]

- 1. N. A. Hill, J. Phys. Chem. B, 104, 6694-6709 (2000)
- 2. G. L. Yuan and S. W. Or, *J. Appl. Phys.*, **100**, 024109 (2006)
- 3. N. A. Benedek and C. J. Fennie, *Phys. Rev. Lett.*, **106**, 107204 (2011)
- 4. J. M. Rondinelli and C. J. Fennie, *Adv. Mater.*, **24**, 1961-1968 (2012)
- 5. M. J. Pitcher et. al., Science 347, 420-424 (2015)



**Figure 1.** Successive octahedral tilt distortions imposed on a family of Fe-based n=2 Ruddlesden-Popper phases by chemical substitution. (a-c) Refined crystal structures from neutron powder diffraction. (d) Layer-by-layer polarisation of the 3 tilt  $(a^*a^*c^*)/(a^*a^*c^*)$  structure.

**Keywords:** perovskite, polar, weak ferromagnetism, magnetoelectric