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Structure–property relationships in multiferroic metal–formate frameworks under pressure

Ines Emily Collings[1], Maxim Bykov[2], Elena Bykova[3], Rudra Sekhar Manna[4], Alexander Tsirlin[4], Sylvain Petitgirard[2], Michael Hanfland[1], Sander van Smaalen[5], Natalia Dubrovinskaia[5], Leonid Dubrovinsky[2]

[1]European Synchrotron Radiation Facility, Grenoble, France, [2]Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany, [3]Deutsches Elektronen-Synchrotron, Hamburg, Germany, [4]Institute of Physics, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany, [5]Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany

E-mail: ines.collings@esrf.fr

Dense metal–organic frameworks (MOFs) show promise for a new class of multiferroic materials [1], which have technological importance in sophisticated multistate memory devices. MOFs offer attractive perspectives as intrinsic multiferroic systems due to the large chemical and structural diversity that can be varied through the metal ion, ligand, and organic counterion. In particular, the MOF families of AM(HCOO)3, where M = Mn–Cu, and A = alkylammonium cation, have shown multiferroic properties at certain compositions upon cooling, and rely on hydrogen bonding interactions for the coupling of ferroic parameters [2]. The chemical and structural diversity of MOFs would allow the ferroic parameters and their coupling to be readily tuned. However, a much greater understanding of the structure–property relationships is needed in order to design improved multiferroic MOFs.

To investigate the effect of structural modifications on the magnetic and electric properties in MOFs, we study two MOF families as a function of pressure: [NH4][M(HCOO)3] and [(CH3)2NH2][M(HCOO)3] where M = Fe, Ni. High-pressure single-crystal X-ray diffraction measurements were performed to follow the structural transformations upon compression, and thus estimate the evolution of structural polarity [3]. Structural studies are complemented with high-pressure magnetisation measurements to investigate the effect of compression and the high-pressure phase transitions on the magnetic properties of the MOFs. These data allow us to derive structure–property relationships for a wide range of AM(HCOO)3 atomic configurations, and determine how chemical pressure should be used to improve the ferroic properties of the MOFs.

[1] G. Rogez, N. Viart, and M. Drillon, (2010) Angew. Chem. Int. Ed., 49, 1921–1923.
[2] Y. Tian et al., (2014) Sci. Rep., 4, 6062.
[3] I. E. Collings et al., (2016) CrystEngComm, 18, 8849–8857.

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