Oral Contributions

[MS35-05] Structural chemistry and magnetism of transition metal oxyselenides $Ln_2O_2Fe_2OSe_2$

Emma E. McCabe,[a] Chris Stock,[b] Efrain E. Rodriguez,[c] Andrew S. Wills,[d] Mark A. Green,[a] John S. O. Evans[e]

[a] *School of Physical Sciences, University of Kent, Canterbury, CT2 7NH, UK*
[b] *School of Physics and Astronomy, University of Edinburgh, JCM Building, Mayfield Road, Edinburgh, EH9 3JZ, UK*
[c] *Department of Chemistry and Biochemistry, 0107 Chemistry Building, University of Maryland, College Park, Maryland 20742+4454, USA*
[d] *Department of Chemistry -University College London -20 Gordon Street -London -WC1H 0AJ, UK*
[e] *School of Chemistry, Durham University, South Road, Durham, DH1 3LE*
Email: e.e.mccabe@kent.ac.uk

The layered transition metal oxyselenides Ln2O2M2OSe2 (Ln= lanthanide cation, M = Mn, Fe, Co) are currently of considerable interest due to the unusual M2+ coordination environment, which gives rise to complex magnetic behaviour. [1] The manganese analogue orders magnetically at 168 K with Mn2+ moments perpendicular to the Mn2O layers, with nearest-neighbour interactions dominating.[1a] The more electronegative cobalt analogue is reported to adopt a magnetic structure with Co2+ moments in the Co2O planes, orthogonal to one another below 220 K.[1a, 2] The iron analogue is intermediate between these two and there is some controversy in the literature regarding the its magnetism, with two magnetic structures proposed.[3] We present here an investigation using neutron powder diffraction (NPD) and inelastic neutron scattering (INS) data to understand the magnetic behaviour of Ln2O2Fe2OSe2 (Ln= La, Ce, Pr and Nd). We consider the symmetry of both proposed models, their fit to the diffraction data and modelling of microstructural effects in these magnetic refinements. Analysis of INS data can give estimates of the strengths of magnetic exchange interactions.[4] In addition, the structural role (including both size and electronic effects) of the Ln3+ cations is investigated, alongside their magnetic behaviour.[5]

Phys. Rev. B 2010, 82 (21).

[1] (a) Free, D. G.; Withers, N . D.; Hickey, P. J.;
Evans, J. S. O., Chem. Mater. 2011, 23; (b) Ni, N.; Climent-Pascal, E.; Jia, S.; Huang, Q.; Cava, R. J.,
[2] **Fuwa, Y.; Endo, T.; Wakeshima, M.; Hinatsu, Y.; Ohoyama, K., J. Am. Chem. Soc. 2010, 132, 18020-18022.**
[3] (a) Free, D. G.; Evans, J. S. O., Phys. Rev. B 2010, 81, 214433; (b) Fuwa, Y.; Wakeshima, M.; Hinatsu, Y., J. Phys. Condens. Matter 2010, 22; (c) Ni, N.; Jia, S.; Huang, Q.; Climent-Pascual, E.; Cava, R. J., Phys. Rev. B 2011, 83, 224403; (d) Zhao, L. L.; Wu, S.; Wang, J. K.; Hodges, J. P.; Broholm, C.; Morosan, E., Phys. Rev. B 2013, 87, 020406(R).
[4] McCabe, E. E.; Stock, C.; Rodrigues, E. E.; Green,
M. A.; Wills, A. S.; Evans, J. S. O., in preparation 2013.
[5] *McCabe, E. E.; Manuel, P.; Chapon, L.; Evans, J.*
S. O., in preparation 2013.

Keywords: magnetic neutron scattering, structural phase transitions, Rietveld structural analysis