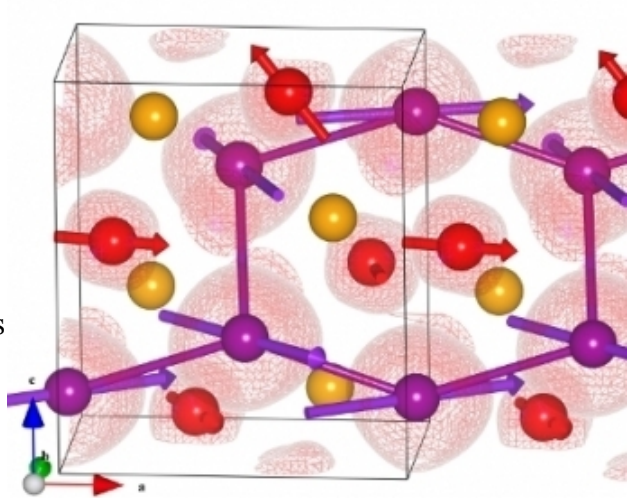
PhD Project for October 2018

Physics of magnets and the arrangements of atoms comprising them: theory of magnetic -compositional correlation.

There are opportunities for post-graduate research available in the Warwick Theory Group on a theoretical/computational PhD project on the modelling of magnetic materials. The project will involve condensed matter physics theory, high performance computing and collaboration with leading groups in this area in the EU, USA and Japan. We are looking for candidates with a strong interest and aptitude for theoretical development and scientific computing.

Permanent magnets are pervasive in both established and developing technologies and are found in motors and generators, transducers, magnetomechanical devices and magnetic field and imaging systems. They are also both fascinating and challenging in terms of their fundamental materials physics. At the Universities of Warwick and Birmingham we have an integrated theory/experiment research programme to uncover key design principles and are looking for postgraduate students to participate. On the theory side of our EPSRC-funded PRETAMAG project ("Investigations of the Physics underlying the principles of design of Rare Earth Transition metAl permanent MAGnets") [1] there is a postgraduate research project to help develop the theory for how atoms arrange themselves over the crystalline sites in a permanent magnetic material such as impurity-doped $SmCo_5$.



We want to understand what elements can substitute into the magnet and if so what effects on the magnetic properties are likely to occur. We can then work closely with experimentalists and study promising materials in more detail. We will assess short- and long- range compositional order. This work will have wider impact too. The development will be applicable to many other materials, e.g. high entropy alloys [2], new solid state cooling materials [3] and thermoelectrics, all cases where properties can be optimised by compositional tuning.

Our PRETAMAG joint theory/experimental project provides some excellent opportunities for postgraduate students. We already have four PhD students involved, two working on the theory side and two on experiment and we are keen to strengthen the team further. The students benefit from working in a diverse team which comprises:

[Ab-initio theory/computational modelling] J. B. Staunton, C. Patrick (Warwick), M. Lueders, L. Petit and Z. Szotek (STFC, Daresbury).

[Sample synthesis and experimental work] G. Balakrishnan, R.S. Edwards, M.R. Lees, S. Kumar (Warwick). M. Laver and A. Walton (Materials and Metallurgy, Birmingham).

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References:

[1] See information at https://www2.warwick.ac.uk/fac/sci/physics/research/theory/research/electrstr

[2]'Statistical physics of multicomponent alloys using KKR-CPA' by Suffian N. Khan, J. B. Staunton, and G. M. Stocks, Phys. Rev. B **93**, 054206, (2016).

[3] 'Frustrated magnetism and caloric effects in Mn-based antiperovskite nitrides: Ab initio theory' by J. Zemen, E. Mendive-Tapia, Z. Gercsi, R. Banerjee, J. B. Staunton, and K. G. Sandeman, Phys. Rev. B 95, 184438, (2017).