

Wed 15 June, 2pm [Alex Gibbs](#)
(Ingram Lecture [\(STFC\)](#)
Theatre)

Why crystal structure matters:
Emergence of magnetism and
electronic properties of transition
metal oxides

Transition metal oxides are a versatile playground for physicists, chemists and material scientists, displaying a wide variety of intriguing physical phenomena such as superconductivity, colossal magnetoresistance, multiferroicity and complex magnetism. This emergence of new phases with interlinked electrical, magnetic and structural properties often has its origins in the fine balance between charge, spin and orbital degrees of freedom. Some well-known examples in which structure plays a particularly crucial role are the proposed quantum spin liquid state in $\text{Ba}_3\text{CuSb}_2\text{O}_9$ [1] and the possible realisation of the Kitaev model in iridates [2]. Intriguingly, the effective Hamiltonians emerging in transition metal oxides have been shown to have relevance to other fields of physics with, for example, links to cosmology and high energy physics.

The structure of a transition metal oxide compound, which crucially determines the allowed symmetries, can be seen as the very fabric out of which these new electronic phases emerge. However it is the determination of this critical 'detail' – the crystal structure – which is too often taken as given and rarely questioned, with errors easily being overlooked. High resolution structural studies are key to elucidating the symmetry underlying the mechanisms which give rise to many important materials properties. In my talk I will present a few key examples exemplifying this interplay between structure and properties. Neutron diffraction in particular is the gold standard for structural investigations of transition metal oxides, in part due to its superior sensitivity to oxygen positions, which are often key to the electronic and magnetic properties of these materials. The ISIS neutron source at the STFC Rutherford Appleton Laboratory in Oxfordshire is a world leading facility in this area. I will introduce some of its outstanding capabilities with a particular focus on high resolution structure determination using the phase transitions in multiferroic YMnO_3 [3], and more recently complex magnetism in the hexagonal perovskites $\text{Ba}_2\text{CuTeO}_6$ and $\text{Ba}_2\text{NiTeO}_6$ and electronic and magnetic properties of platinum group metal-based oxides as examples.

While neutron diffraction is often seen as a mature technique, exciting new developments pushing the limits of our capabilities are continuously taking place. At the end of my talk I will discuss some of the new capabilities of the next generation of instruments currently being developed which will become available to the community in the near future.

[1] S. Nakatsuji, K. Kuga, K. Kimura *et al.*, Science 336, 559 (2012)

- [2] T. Takayama, A. Kato, R. Dinnebier *et al.*, Phys. Rev. Lett. 114, 077202 (2015)
- [3] A.S. Gibbs, K. S. Knight and P. Lightfoot., Phys. Rev. B, 83, 094111 (2011)