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First principles design of new multiferroic materials

WCPM/CSC joint seminar

Nicholas Bristowe
Physical Sciences, University of Kent

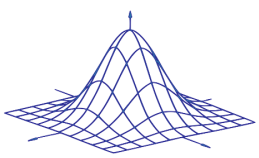
Monday, 15 May, 1 p.m.
D2.02 Seminar room, Engineering

Abstract: Multiferroics are highly sought for their ability to exhibit multiple ferroic properties, ideally ferroelectricity and ferromagnetism. Their ability to combine charge and magnetic polarisation in the same material has tremendous potential for application in technological devices in which magnetic spin can be manipulated and controlled through applied electric fields, and charges through applied magnetic fields. Indeed, multiferroics have been been proposed as the basis for the "ultimate memory device", which would be simultaneously fast, robust, nonvolatile and consume less energy. In addition, having spontaneous and switchable charge polarization and magnetism combined, multiferroics could enable four-state logic devices, and hence higher data densities. Multiferroic devices are, however, still far from being the "disruptive technology" originally envisioned, as they require materials that exhibit strong coupling between their ferroelectric and magnetic properties at ambient conditions. Even in oxide perovskites (ABO_3), known for their important magnetic and electronic properties, the simultaneous appearance of ferroelectricity and ferromagnetism is very rare. This is often because conventional ferroelectrics require cation displacements typically associated with empty d-orbitals, whereas ferromagnetism requires partially-filled d-orbitals. This dichotomy, and the inherent complexity of multiferroics, has somewhat stalled the design of new materials.

This talk will discuss how first principles calculations based on density functional theory (DFT), in combination with group theoretical analyses, are beginning to play an important role in the design of novel multiferroic materials. The strategy is based on creating unconventional ferroelectricity, called "improper ferroelectricity", in magnetic materials. Here the polar mode does not directly appear as a result of a certain type of chemical bonding, as in conventional "proper" ferroelectrics. It is instead no longer the primary order parameter involved in the ferroelectric phase transition but is itself driven by a (combination of) different non-polar mode(s). This occurs due to a specific anharmonic coupling between the modes. The requirements for improper ferroelectricity are therefore that i) the appropriate anharmonic coupling is allowed by symmetry, and ii) the primary non-polar modes are unstable and appears in the ground state. Whilst the concept of improper ferroelectricity is several decades old, developments in first principles calculations have only recently enabled the design of these two requirements in new materials. Furthermore, I will discuss how DFT simulations are beginning to uncover unusual anharmonic couplings for electrical control of not only spin, but also charge and orbital degrees of freedom.

A buffet lunch will be available from 12:45 pm.

More info: http://warwick.ac.uk/wcpm/seminars



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