Emergent helical dipole textures in quadruple perovskites

View on GitHub

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Project ID: 2228cd1393 (You will need this ID for your application)

Research Theme: Advanced Materials

UCL Lead department: London Centre for Nanotechnology (LCN)

Department Website

Lead Supervisor: David Bowler

Project Summary:

Ordering of magnetic dipoles in materials gives rise to many kinds of magnetic structures, from simple ferromagnetism to complex helices, that have found important applications with profound impacts in society. Electrical dipoles in dielectrics are normally associated with only simple alignment, but recent experiments at UCL have found helical order in the quadruple perovskite BiCuxMn7-xO12. This discovery has opened a completely new area for research and potential applications such as chiral optical devices that control the light-matter interaction in solid-state quantum information processing. You will use state-of-the-art density functional theory (DFT) codes, performing simulations to explore and understand the mechanisms behind helical order, working closely with experiments at ISIS and [Diamond] (www.diamond.ac.uk) to suggest routes to control and develop new materials and orderings. You will work with David Bowler (LCN), who leads the development of the large scale DFT code CONQUEST, and with Roger Johnson (CMMP), who leads the experimental work on BiCuxMn7-xO12. CONQUEST is a world-leading code, and has been applied to simulations with over 1,000,000 atoms (standard calculations address a few hundred atoms): it is uniquely capable of calculating complex orders. You will work to understand the phase diagram of BiCuxMn7-xO12, both pure and as it is doped with Cu. You will explore the different local dipole arrangements in the material, and use the modern theory of polarisation. These calculations will be at the very edge of what is possible with DFT, and will drive forward both large-scale DFT and our understanding of polarisation and dipole textures in dielectrics. We are looking for someone with a strong background in condensed matter physics and quantum mechanics, alongside good computational skills. Experience of high-performance computing (HPC) would be an advantage but is not necessary. A keen interest in understanding experimental techniques and working with experiment is essential.