



Royal Holloway
University of London
Egham, Surrey
TW20 0EX

DFT Methods for Complex magnetic Systems

A fully-funded three-year PhD studentship is available at Royal Holloway, University of London starting in October 2015, and is open to applicants from the European Economic Area.

This is a joint project with the ISIS spallation neutron source at the Rutherford Appleton Laboratory, Oxfordshire, with the aim of using and developing electronic structure calculation methods for the study of advanced materials with complex magnetic structures.

Magnetic structure is fundamental to understanding the quantum solid state, and magnetic materials are the functional component of many present and future technologies. Examples such as multiferroics, high-temperature superconductors, thermoelectrics and spin-ice pyrochlores are at the cutting edge of condensed-matter physics research. Their magnetic ground states are frequently complex, featuring spin spirals, antiferromagnetic and ferrimagnetic order, charge and spin density waves, and geometrically frustrated antiferromagnetism.

The first goal of this project is to advance the state-of-the-art in methods for DFT electronic structure modelling for complex magnetic systems, using random search methods to map the landscape of magnetic ground states. The main code development platform will be the CASTEP electronic structure and materials modelling code, used by over 100 UK and worldwide research groups. CASTEP is one of the most-used codes on UK national high-performance computing (HPC) facilities including ARCHER and the project will be associated with the UK Car-Parrinello HPC consortium. There will also be collaborations with CASTEP developers and researchers at University College London, Oxford and York universities.

The second part of project will be to apply the newly developed methods to simulate magnetic ordering in spin-ice pyrochlores and other magnetic materials studied using neutron scattering at the ISIS facility, working closely with ISIS scientists and users.

The successful candidate should have a degree in physics, at the equivalent level to a UK MSci. A strong education in condensed matter physics, quantum mechanics and electronic structure of solids would be an advantage as will excellent computer programming skills.

Royal Holloway is based in an attractive leafy campus close to London

<http://www.rhul.ac.uk/physics/prospectivestudents/home.aspx>.

Applications must be made using the Royal Holloway web site

<http://www.rhul.ac.uk/studyhere/postgraduate/applying/home.aspx>

For further details, please contact Professor Keith Refson (Keith.Refson@rhul.ac.uk).