



Project Title

Neutron Diffraction Studies of Inorganic Microcrystals

A PhD studentship is available in the group of [Professor J. Paul Attfield](#), University of Edinburgh, School of Chemistry, and is co-supervised by [Dr Pascal Manuel](#), UKRI STFC [ISIS Neutron and Muon Facility](#).

Project Summary

This project will explore and develop capabilities for neutron microcrystal diffraction to study functional inorganic materials. These are transition metal oxides and nitrides [1], which are major classes of materials with many important properties such as high-T_c superconductivity, ferroelectricity, CMR (colossal magnetoresistance) and spintronics, multiferroicity, and ionic conductivity for oxides, while nitrides find applications as superconductors, semiconductors, photovoltaics, hard ceramic coatings, ferroelectrics, luminescent materials, and permanent magnets.

Neutron diffraction is essential for studying the structures of such materials, making use of the strong scattering from O/N atoms and the large contrasts between many metals e.g. Fe/Co, as well as magnetic scattering from spin-ordered materials. Experiments traditionally use relatively large single crystals (edge length 1-10 mm) or polycrystalline powders typically consisting of 0.1 – 10 μm grains

The high photon fluxes available at modern synchrotrons have enabled single crystal X-ray experiments to bridge the gap between traditional crystal and powder regimes, enabling a single grain in a powder to be analysed as a single crystal [2]. Development of new high flux pulsed neutron sources such as ESS and the proposed ISIS-II makes it timely to explore and extend the limits of microcrystal neutron diffraction. This project will explore and develop capabilities for neutron microcrystal diffraction using the WISH [3] and the future WISH-II [4] diffractometers at ISIS [3].

The student will be based in Edinburgh during Years 1 and 2, and at the ISIS facility during Year 3.

References

[1] Weidemann, M.; Werhahn, D.; Mayer, C.; Klaeger, S.; Ritter, C.; Manuel, P.; Attfield, J. P.; Kloss, Simon D. *Nature Chem.*, DOI 10.1038/s41557-024-01558-1 (2024).

[2] M. Senn, J.P. Wright and J.P. Attfield. *Nature* 481, 173 – 176 (2012).

[3] <https://www.isis.stfc.ac.uk/Pages/wish.aspx>

[4] <https://www.isis.stfc.ac.uk/Pages/WISH-II.aspx>

Funding Notes

The studentship is fully funded for 42 months by the University of Edinburgh and STFC, and covers tuition fees and an annual stipend at the UKRI rate, for 2024-25 this is £19,237 per annum, for a candidate satisfying EPSRC residency criteria., see:

<https://www.ukri.org/wp-content/uploads/2024/04/UKRI-020424-TrainingGrantTermsConditionsApril2024.pdf>

How to apply

In the first instance, the initial application of cover letter and CV should be directed to Professor J P Attfield, email: j.p.attfield@ed.ac.uk

The position will remain open until filled. A closing date may be added at a later date. The student must start by 1/10/2025.

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IMPORTANT

Before Submitting your cover letter and CV, please complete the online EDI Form, see:

[School of Chemistry Equality, Diversity and Inclusion Form, entry 2025-26.](#)

The form will automatically generate a unique 'Response ID number' that you must include in your cover letter.

Equality and Diversity

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality.

The University has a range of initiatives to support a family friendly working environment.

For further information, please see our University Initiatives website:

<https://equality-diversity.ed.ac.uk/inclusion/family-and-carer>