SCIENCE LONDON ROADSHOW 24TH SEPTEMBER 2024

Dr Neal Skipper - University College London
"*Neutron Scattering Studies of Molecular Liquids: Strong Structures from Weak Interactions* "

Weak intermolecular interactions, such as those involving mildly polar and aromatic groups, play a key role in many important natural and technological processes, but are extremely challenging to understand and observe directly. Neutron scattering studies of molecular liquids and solutions are helping to unveil the complex world of weak interactions, and point to strength through cooperativity.

Dr Keenan Smith - University College London
"*Neutron scattering to probe nanostructure and dynamics of emerging electrolytes*"

The transition to a carbon neutral society is dependent on the growing use of renewable electrical energy, made possible by electrochemical energy storage and conversion devices, such as batteries, fuel cells and supercapacitors. Electrolytes play a key role in these devices, providing the environment for facile charge transport, ultimately permitting advances in energy and power density, durability and safety. Small angle neutron scattering (SANS) can offer a unique perspective across the nano-/micro- structure on the molecular aggregates, percolation networks, and domain sizes formed within electrolyte structures. Quasi-elastic neutron scattering (QENS) which simultaneously acquires spatial and temporal information on molecular relaxations and motions is unique in its ability to understand the charge transport mechanism in such electrolytes. Combining SANS and QENS, alongside macroscale property investigation, provides the ability to bridge the knowledge gap between microscopic and macroscopic structure-property relationships. Herein, recent studies using neutron scattering to elucidate fundamental structural and dynamical features of novel electrolyte systems will be discussed and the learnings applied to improved design of such materials.

Mr Daniel Bradley - ISIS/ University of Nottingham
"*One Potential Set to Rule Them All: Multi-composition EPSR simulations of the structure of strontium doped bioactive phosphate glasses*"-

The process-structure-property interrelationship of glass is vital for fully understanding the interaction of cation substitution and its effect on bio-phosphates, but despite many structural studies, little is known about this effect. Dissolve is a next generational software being developed at the ISIS Neutron and Muon Source, for the interpretation of total scattering data by empirical potential generation. Multi-Composition Empirical Potential Structure Refinement (MC-EPSR) is a technique which refines one set of these potentials across a series of similar glasses to allow further constraints on the fitting. This has then been used to extract reliable partial correlation functions for each glass and generated models that have been analysed, revealing the medium range structure and modifier-modifier interactions that may give rise to mixed modifier effects. In this study, a series of binary and multi-component phosphate glasses have been analysed where CaO has be substituted for SrO (40P2O5.(16-x)CaO.20Na2O.24MgO.xSrO). The biocompatibility and full absorbability of phosphate glasses has meant that they have gained lots of attention for their use in biomedical applications. Their desirable characteristics make them suitable for use in hard and soft tissue engineering, bone fracture fixation and dental repair, and controlled delivery of therapeutic ions.

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Dr Donna Arnold - University of Kent

"*Exploring structure-property correlations in the frustrated layered material, $Mn_2Mo_3O_8$*"

Multiferroic materials continue to attract extensive attention within the literature due to potential application in lower energy consuming devices. These materials exhibit both ferroelectric and magnetic ordering in a single phase. In type 1 materials these two components are independent. In contrast, in type 2 materials ferroelectricity arises as a result of complex magnetic ordering related to geometric frustration. This has the benefit of strong magnetoelectric coupling, essential for efficient device design, but with the disadvantage that ordering occurs at very low temperatures which is not desirable.

We have been investigating structure-property correlations in complex layered materials with the aim of elucidating the role of magnetic topography in controlling magnetic order and transition temperature. Of interest is the polar hexagonal (S = 5/2) layered oxide $Mn_2Mo_3O_8$ which crystallises in the $P6_3mc$ space group and exhibits strong linear magnetoelectric coupling. Along the lattice c-direction, $Mn_2Mo_3O_8$ ($a = b$ = 5.80 Å, c = 10.24 Å) is composed of stacked honeycomb-like Mn-O layers separated by trimerized Mo_3O_{13} sheets. In the ab-plane, the honeycomb layer contains a 1:1 ratio of alternating corner-sharing MnO_4 tetrahedra (Mn1) and MnO_6 octahedra (Mn2), giving rise to honeycomb connectivity. This gives rise to an easy-axis-type ferrimagnetic ground state below T_c = 41 K[1]. However, a full understanding of the structural and magnetic behaviour of $Mn_2Mo_3O_8$, including when the honeycomb lattice is doped with other 3d transition metals, remains limited [2,3].

We will report the structure (including neutron diffraction) and roperties of $Mn_2Mo_3O_8$ and $MnAMo_3O_8$ materials (where A^{2+} = Fe^{2+}, Co^{2+} and Zn^{2+}). We will discuss the role of site preference of cations (octahedral vs tetrahedral) and provide new insight into the magentic behaviour of these materials.

Dr Sarah Rogers - ISIS

"*40 Years of ISIS (Neutron) Science Highlights*"

40 years of neutrons at the ISIS Neutron and Muon Source has led to a large, diverse and exciting range of science being produced. As part of the year of celebration of the 40th anniversary of neutron production at ISIS, I was tasked with compiling a list of our science highlights. This has been a challenging but incredibly enjoyable job and during this 20 minute talk, I will attempt to give a flavour of the broad range of science that we, along with our fantastic collaborators, have produced. The highlights will cover the science themes of quantum science, life science, materials and engineering and energy and environment and will show collaborations with both our academic and industrial partners.

Science and Technology Facilities Council
ISIS Neutron and Muon Source

40 Years of ISIS Neutron and Muon Source

IMPERIAL
Department of Materials

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Mr Edward Stuckey – ISIS / Royal Holloway University of London
“Carbon double-bond dependent removal of organic films at the aerosol mineral-water interface by ozone: a novel investigation for atmospheric sciences.”

Abstract: Buried interfaces such as the mineral-water interface remain difficult to investigate experimentally owing to limitations of most surface measurement techniques. The penetrative nature of neutrons allows us to access this interface and neutron reflectometry has allowed us to measure in-situ reactions of organic material at the mineral water interface, replicating atmospheric reactions. Here, we react three lipid bilayers on a quartz surface with aqueous ozone, each with a different number of carbon-carbon double bonds, and determine how the number of unsaturated carbon-carbon double bonds may change the amount of material removed from the interface by reaction with ozone. The high flux of modern neutron instruments has allowed us to produce a high time resolution representation of how the structures of these bilayers are transformed with time. We apply the measurements taken here to light scattering models to show how an aerosol containing an organic film at the mineral-water interface may have its optical properties altered throughout its lifetime in the atmosphere which may ultimately have climatic impacts.

Dr Mona Sarter – ISIS
Data analysis of dynamics in protein solutions using QENS-New insights from polarised neutrons”

Protein dynamics play a vital role in biology. Quasi elastic neutron scattering is an ideal method to access these dynamics. Normally data analysis is performed based on the assumption that the scattering spectrum is incoherent. In order to be observe the full range of protein dynamics it is necessary to perform the experiments in solution. This solution is usually a fully deuterated buffer, while the protein remains protonated. It is generally assumed that while the buffer leads to a coherent contribution, this can be taken into account during data analysis by subtracting the buffer contribution from the sample spectrum. Up until recently there was no way to experimentally verify this assumption. Polarised QENS experiments on LET allow for the coherent and incoherent contributions to be separated. By comparing the results from the polarised QENS experiment and the standard analysis method from unpolarised QENS it was possible to experimentally check this assumption. This has shown that the pure incoherent spectrum obtained from polarisation analysis does not match the results for normal QENS. The implications of this will be discussed.

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Dr Fabrizia Foglia – UCL

“Neutrons for a sustainable society”

Despite the widespread use (e.g. in healthcare, energy and water treatment applications) and the continued development of new materials and solutions for their implementation in advanced devices, improving membrane performance and durability remains a non-trivial problem. In large part this is due to the lack of a detailed understanding of the dynamics of the permeant confined within the membrane structures, that are typically multi-scale in terms of correlation lengths and relaxation timescales for the different processes involved. It is therefore difficult to disentangle individual contributions to the various motions and their involvement in the membrane structure-dynamics correlation, especially in situ and under operando conditions.

Neutron scattering is ideal for this type of study because it allows a unique view of structures of soft condensed matter systems. The nature of neutron-matter interaction provides a non-destructive approach, making it a perfect tool to investigate structurally delicate membrane structure-dynamics properties as well as biological systems. Cold neutrons, with wavelengths of a few Å and energies from μeV to several meV, allow investigations and correlations of structure on the Å- to nano-scale combined with molecular motions on a nano- to pico-second time regimes. Furthermore, because of the difference in neutron scattering cross section between H and D, isotopic contrast experiments can be used to highlight different spatial/dynamic regions under varied chemical and physical conditions.

Here we present our journey using advanced neutron scattering techniques to shed light on the structure-dynamical interplay, while developing a new understanding by correlating energy, time and space to resolve structure to function interplay. We apply this approach not only to guide the design of new materials with improved performance characteristics but also to enhance our understanding and improve the recyclability of materials.

Dr Paul Collier and Mr Jonathan Booth - Johnson Matthey

“JM's collaboration with ISIS - from the past to the future”

This presentation explores the fruitful collaboration between Johnson Matthey (JM) and the ISIS Neutron and Muon Source, highlighting the significant advancements achieved through this partnership. The talk begins with an introduction to JM and the strategic importance of its collaboration with ISIS, emphasising the mutual benefits for both industry and scientific research.
Specific examples of JM-ISIS collaborative projects are discussed, including NH3 selective catalytic reduction (SCR), neutron reflectometry for hydrogen fuel cell nanostructures, and the use of inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS) for zeolite research. The talk also highlights personal experiences and future collaborations, showcasing the impact of neutron techniques on JM's research and development.
Through this presentation, attendees will gain insights into the close relationship between JM and ISIS, the collaborative research projects, and the significant contributions of various individuals and teams to this partnership. The talk aims to inspire continued collaboration and innovation to address the world's sustainability challenges."

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Dr Graham Appleby - ISIS

"Industrial Engagement at ISIS Neutron and Muon Source"

Traditionally used by academic researchers, ISIS also provide commercial advantages to those companies which are aware of the unique benefits of neutron and muon techniques for their research and innovation. The advanced characterisation techniques offered at ISIS are powerful tools for multi-scale material and process characterisation down to atomic detail. As such, they are useful for a wide range of industry sectors for developing new advanced materials, new innovative products, and more efficient manufacturing processes. As neutron sources become more advanced and expensive, there is an increasing need to demonstrate the impact of the public investment to funding stakeholders, and both the societal and the economic impact are an important part of this.

Recent industrial partnerships at ISIS result in high quality case-studies which illustrate the impact of neutron scattering techniques to societal challenges, and the economic impact data provided by commercial users have formed the basis for assessment of ISIS contribution to the UK's economy. This presentation will present societally interesting examples of industrial measurements at ISIS and discuss the resulting impact of these to the UK's economy.

Miss Corrin Blake – UCL/ISIS

"Developing model membranes to characterise the effects of antimicrobials on the Gram-negative bacterial outer membrane"

Antibiotic resistance is a major threat to global health and socioeconomics. Gram negative (GN) bacteria are recognized as the primary source of antibiotic-resistant strains, and understanding the mechanisms behind this resistance is crucial for developing new antibiotics. The structure of the GN bacterial cell envelope, which includes a unique outer membrane made up of an asymmetric bilayer of lipopolysaccharide (LPS) and phospholipids, is largely responsible for their antibiotic resistance. LPS is a critical target for the development of novel antibiotics, and a better understanding of its structure, behaviour and interactions is needed. Model membranes offer a controlled and tuneable platform for studying bacterial structure, which is compatible with advanced characterised techniques. Neutron Reflectometry (NR) is a powerful tool which allows both the surface and cross-sectional structure of model membranes to be characterised at the nanoscale. Furthermore NR provides real time measurements of antibiotic-membrane interactions, in turn allowing for a deeper mechanistic understanding of such interactions to be obtained.

Miss Jing Ming - Queen Mary University of London

"Defect Clustering and Vacancy Ordering in Gadolinium doped Ceria"

Lanthanide-doped cerias exhibit fast oxide ion conduction, making it an effective electrolyte for solid oxide fuel cells operating at intermediate temperatures (ca. 500-700 °C).1Among all the lanthanides, ceria doped with gadolinium (GDC, Ce1-xGdxO2-x/2) offers the best conductivity systems and has already been adopted commercially.2This high ionic conductivity arises from the creation of high concentrations of oxide ion vacancies along with 3-dimensional conduction pathways within the cubic fluorite structure when Ce4+ substituted by Gd3+. However, a lack of homogeneity or disruptions in local atomic arrangements in these systems, can impede O2- ion diffusion, potentially suppressing ionic conductivity.

To address the structural complexity, recent advancements in neutron total scattering data analysis now allow for a detailed atomic arrangement through the combination of Bragg and diffuse scattering, providing a more complete picture of both long-range and short-range structures, respectively.

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Mr Chenyang Liao - Imperial College London
"Combining neutron with electrochemistry to study protonic diffusion in fuel cells"

Proton conducting fuel cells captured great research interests based on its lower operating temperature. However, tracing and measuring the proton dynamics are challenging to most techniques due to protons' low atomic mass and rapid motions. To study the proton dynamics, Quasi-elastic neutron scattering (QENS) is regarded as the suitable technique due to its proton-sensitivity and the ability to locate dynamics with short time and length scale. Nevertheless, as QENS measures relatively localised diffusion, the difference of the measuring scale makes it hard to compare directly with the proton conductivity measured by conventional electrochemical methods such as Impedance Spectroscopy (EIS). In this talk, we wish to present our idea of combining neutron techniques with electrochemical methods. By estimating the concentration of protons from neutron techniques and applying the Nernst-Einstein equation, we could link the localised and long-range proton diffusion coefficients with proton conductivity, thus estimate the conductivity which could not be measured easily. This methodology could be beneficial to overcome the limitations of EIS: Hard to probe protons exclusively, and high frequency is required to monitor fast proton dynamics.

Dr Isaac Abrahams - Queen Mary University of London
"*Down to the Local: A total neutron scattering approach to revealing local structure* "

Solid electrolytes, are remarkable materials that show fast ionic conduction in the solid state in the absence of significant electronic conductivity. They have found use in systems such as batteries fuel cells and sensors. Their crystal structures are typically made up of an immobile sublattice in which the mobile ions are disordered. Until fairly recently, analysis of local structure in such partially disordered systems relied on careful examination of average structural models, derived from diffraction data, to speculate on local coordination environments, in some cases supported by local structural probes such as solid-state NMR and EXAFS as well as computational modelling. However, recent developments in reverse Monte Carlo (RMC) analysis of total neutron scattering data have allowed for a more detailed analysis of local structure based on physical data using a combination of Bragg and diffuse scattering. The former is associated with the long-range order while the latter arises from short-range order. The large box approach of RMC modelling uniquely allows for examination of the resulting model for local vacancy ordering as well as preferred vacancy association and dopant clustering. Examples of the application of this technique in the analysis of local structure in solid electrolytes will be presented.

Professor Catrin Davis - Imperial College London
"Qualification of Additively Manufactured Components through Neutron Diffraction Measurements".

Laser powder bed fusion (LPBF) is an additive manufacturing process for creating intricate components from metal powders. However, this process is notorious for generating high residual stresses that can cause part distortion and may even cause part cracking during or after the build process. Characterising the residual stress profile in LPBF components is essential to certify their integrity and models that simulate the LPBF process are required to optimise the build and post processing of the component. Neutron diffraction measurements will be presented that have enabled finite element models to be developed and validated to predict the residual stress distribution in LPBF components in their as-built state and subsequently post stress-relaxation heat treatments, removal from the base plate and post build machining.

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Dr Ruiyao Zhang – ISIS

"Introduction to Neutron Imaging at IMAT: Radiography, Tomography and Strain Mapping"

Neutron imaging at IMAT, part of the ISIS neutron source at Rutherford Appleton Laboratory, is a powerful tool for materials science, offering radiography, tomography, and strain mapping. Radiography generates 2D images by measuring neutron attenuation, while tomography reconstructs 3D images from multiple projections. Strain mapping through neutron diffraction measures internal strain, crucial for assessing material performance. Unlike X-rays, neutron imaging excels at visualizing light elements like hydrogen and lithium and penetrates dense materials effectively. Its ability to distinguish isotopes provides unique insights into material composition. This makes IMAT valuable for a range of applications, including industrial non-destructive testing and analysing cultural heritage artifacts. IMAT has been used for studies such as defect detections in critical components of aero engines and fusion reactors, metallurgy of historical artifacts, and battery performance.

Dr Adam Berlie (ISIS)

"*Using Muons To Study Heterogeneous Catalysts"*

Understanding the fundamentals behind how catalysts work it's important in improving their catalytic behaviour. This work shows results from recent experiments to understand how muons can help probe the catalytic mechanisms within Cu doped SSZ13.

Dr Anthony Philips - Queen Mary University of London

"*Designing materials for solid-state cooling*"

Barocaloric cooling is a rapidly developing technology that takes advantage of solid-solid phase transitions with large entropy changes. By applying and releasing pressure, a barocaloric material can be cycled between high- and low-entropy phases – analogous to the vapour and liquid phases in traditional vapour-compression refrigeration – producing an efficient, environmentally friendly cooling cycle.

The barocaloric effect has now been observed among many different materials families, including alloys, molecular, ionic, and framework materials, each of which has a different molecular mechanism for the phase change. Some general design principles are well established within particular materials classes. For instance, the rotational degrees of freedom of approximately spherical molecules or molecular ions, or the torsional degrees of freedom of long alkyl chains, often freeze at low temperatures but unlock at high temperatures, producing a high-entropy phase transition.

However, optimising the technologically relevant properties of barocaloric materials – for instance, the phase transition temperature, adiabatic temperature change, or thermal conductivity – will require us to move beyond these general heuristics to a quantitative understanding of the entropy change. In other words, we need to understand in detail the molecular dynamics and how they contribute to the entropy. This requires a combination of experimental and computational techniques among which neutron scattering is pivotal, due to its sensitivity to both the geometry and dynamics of molecular motion.

I will compare the behaviour of a variety of materials my group has studied over the past few years. I will show that a combination of neutron scattering techniques supported by atomistic modelling is capable both of reproducing the experimentally observed entropy changes and of guiding the development of novel barocaloric materials.

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Dr Roger Eccleston - ISIS –Director

"*The Development Road Map for the ISIS Pulsed Neutron and Muon Source:* "

The ISIS Pulsed Neutron and Muon Source has been operating for nearly 40 years. Through continuous development and significant upgrades, including the addition of a second target station, ISIS has continued to provide world-leading capability to a thriving international user base and deliver world-leading productivity.

The next wave of development of the instrument suite, the Endeavour Programme, which involves five significant instrument upgrades and the construction of four new instruments, is now underway and will be completed within ten years. A further wave of instrument development is proposed which will maximize the capacity and optimize capability.

Throughout 2021 and 2023 the synchrotron and high power target station (Target Station 1) underwent a significant refurbishment to improve performance and serviceability. This extensive project is now complete and both target stations are fully operational. The ISIS Accelerator Strategy focuses on maximizing the performance of the source in terms for both beam current and reliability.

A feasibility study for a MW class source to replace ISIS, ISIS-II, is in progress, which includes a detailed analysis of technical options and the scientific specification.

An overview of plans for the future development of ISIS will be presented, including the Endeavor Programme and ISIS-II