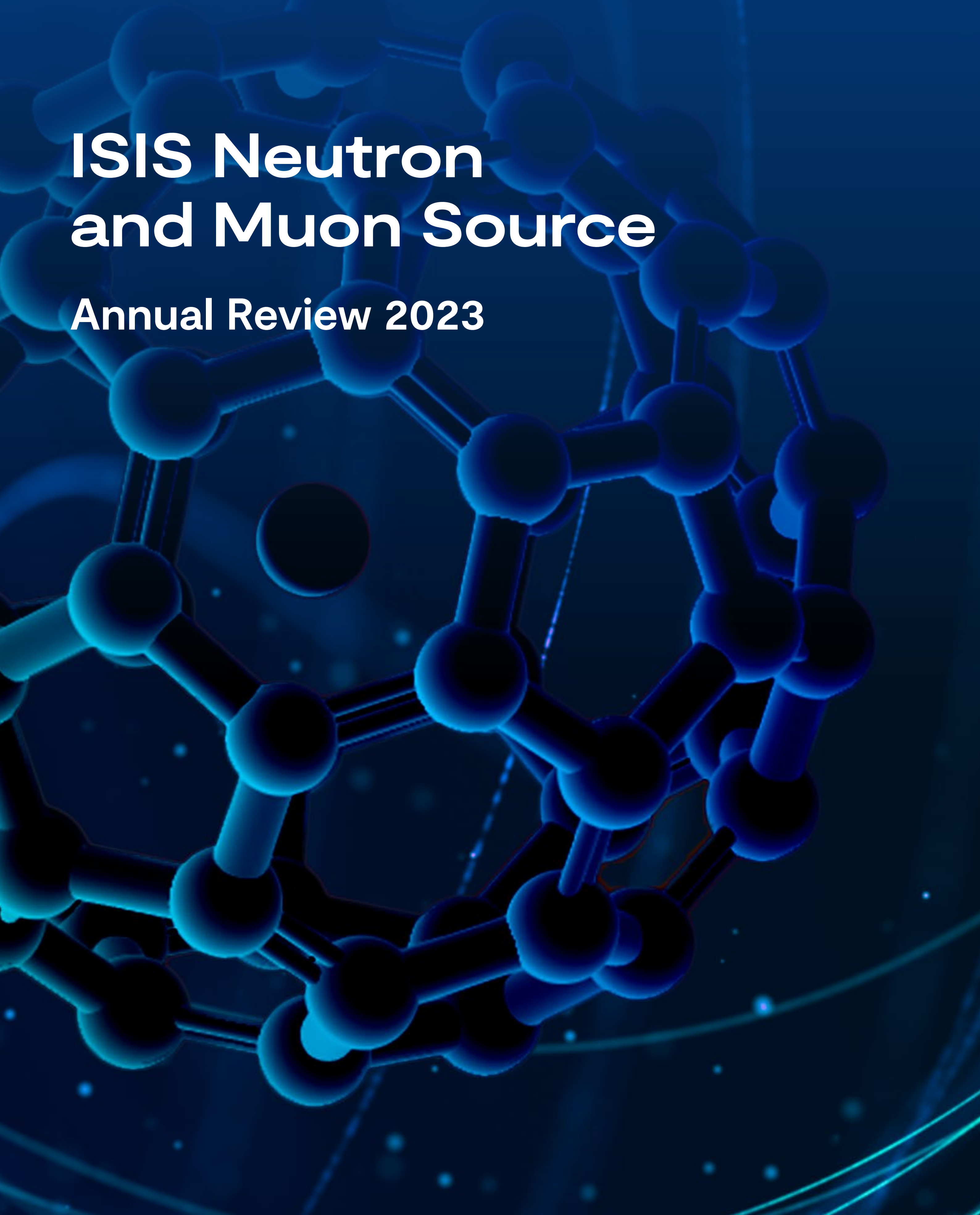
Science and Technology Facilities Council

ISIS Neutron and Muon Source

Annual Review 2023



Our mission

Our aim is to enable research that advances knowledge and improves lives. We support a large and diverse user community that uses neutrons and muons to address global challenges and answer fundamental questions across a broad range of sciences. ISIS brings together national and international academics and industrialists to advance these challenges by taking advantage of the unique insights that neutrons and muons provide. The ability of our instruments to investigate the structure and dynamics of materials with unprecedented detail helps to ensure that the UK remains at the forefront of global materials research.

Contents

Foreword

"Success supposes endeavour. Your time has been properly and delicately spent, if you have been endeavouring for the last four years". So said Mr Knightley in Jane Austen's *Emma*. At ISIS, we have been endeavouring for much longer than four years and, following the funding announcement in May, we will be Endeavouring for the next ten years. The funding for Endeavour is a critically important step in the development of ISIS, enabling us to build four new instruments and significantly upgrade five of our existing instrument suite. The new instruments and upgrades represent considerable increases in capability and will open up new scientific opportunities. The new instruments will also enhance capacity at a time when access to neutron facilities, particularly in Europe, continues to be under pressure.

The announcement of Endeavour funding almost coincided with the 15th anniversary of first neutrons on Target Station 2. Target Station 2 has been vitally important to the development of ISIS, supporting an increase in the size and diversity of the science programme offering world-class capability and capacity to our partners in the user community.

Another important anniversary is on the horizon. ISIS produced its first neutrons on 16 December 1984 - a milestone we intend to celebrate throughout 2024 through a variety of events and activities. Our celebrations will look back on 40 years of development, operation and outstanding science and will also look forward to the next 40 years.

Alongside Endeavour, the ISIS-II project represents the long-term development of ISIS to a megawatt-class facility as we look further into the future. After the Endeavour programme is completed, ISIS will still have three vacant beam ports. There are many ideas emerging about how these ports can be utilised and ways in which current instruments can be upgraded to realise significant performance improvements. All the science groups have drafted Instrument Development Plans that lay out ideas for the further development of the ISIS instrument suite. They demonstrate a high level of ambition and innovation and over the coming months, we will be initiating a project to take the best of these ideas forward to consultation with the user community and thereafter a case for funding.

The international reputation of ISIS continues to shine. Amidst new agreements including those with The Netherlands and Japan, we are working closely with colleagues in Canada, Brazil, Indonesia, Malaysia, and Switzerland, following funding from the UK International Science Partnerships Fund. ISIS's reach, impact and influence are truly international, something we can be immensely proud of.

Operationally, the year has had some challenges as Target Station 1 has been brought back into operation following a major refurbishment. Resuming operations following the biggest intervention on Target Station 1 since ISIS was built has been a major achievement. This was the result of an enormous amount of hard work and the kind of exceptional team working that has been the foundation for ISIS's success for the last 39 years.

The scientific programme on both target stations has been excellent, and you will find some examples of outstanding research within the pages of this report.

Roger Eccleston
Director of ISIS Neutron and Muon Source

Image left: Roger Eccleston giving a staff talk on 10 May 2022.

Even during the planned long shutdown of Target Station 1, ISIS staff and users delivered a vibrant research programme.

Operations

5 cycles

3476 hours of beam on target

131 mAh of beam delivered

84% average availability

Experiments

1283 proposals submitted
(Including from 126 new Principal Investigators)

35 countries represented in proposals

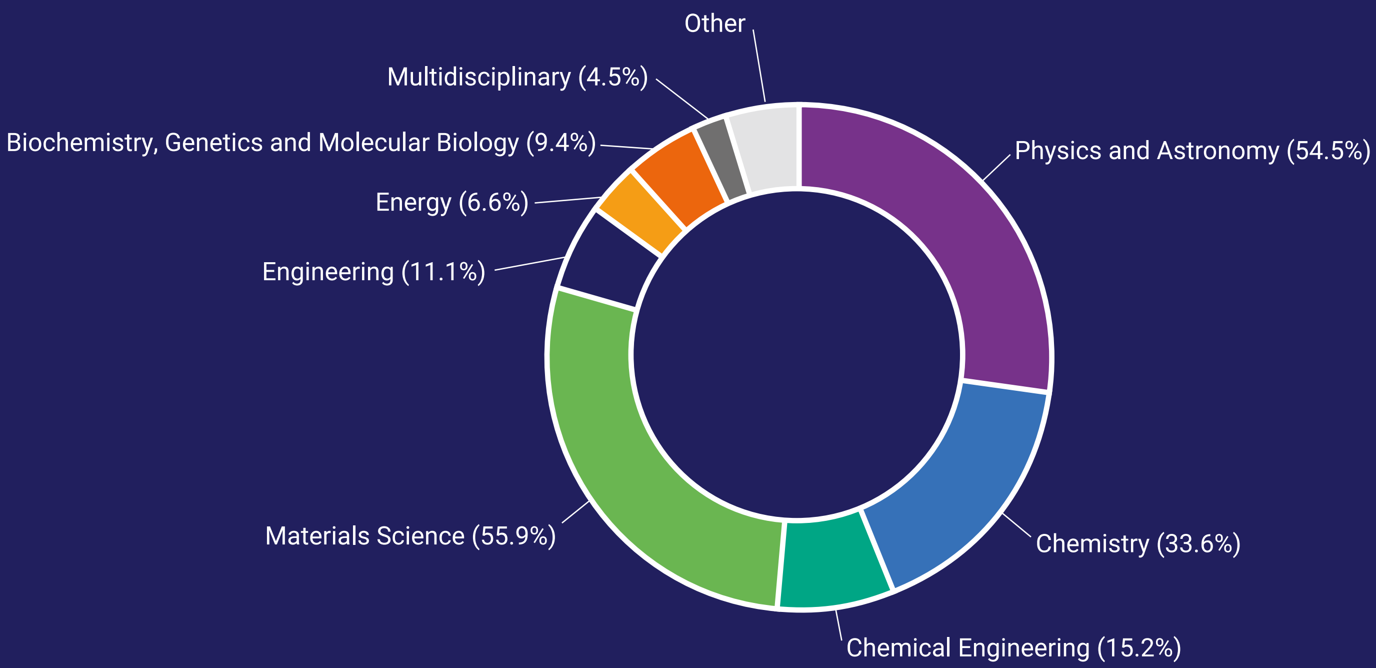
2347 beam days allocated

509 scheduled experiments

1130 unique users

Publication share by subject area

Note that a publication can be mapped to multiple Subject Areas.



Publications

549 publications

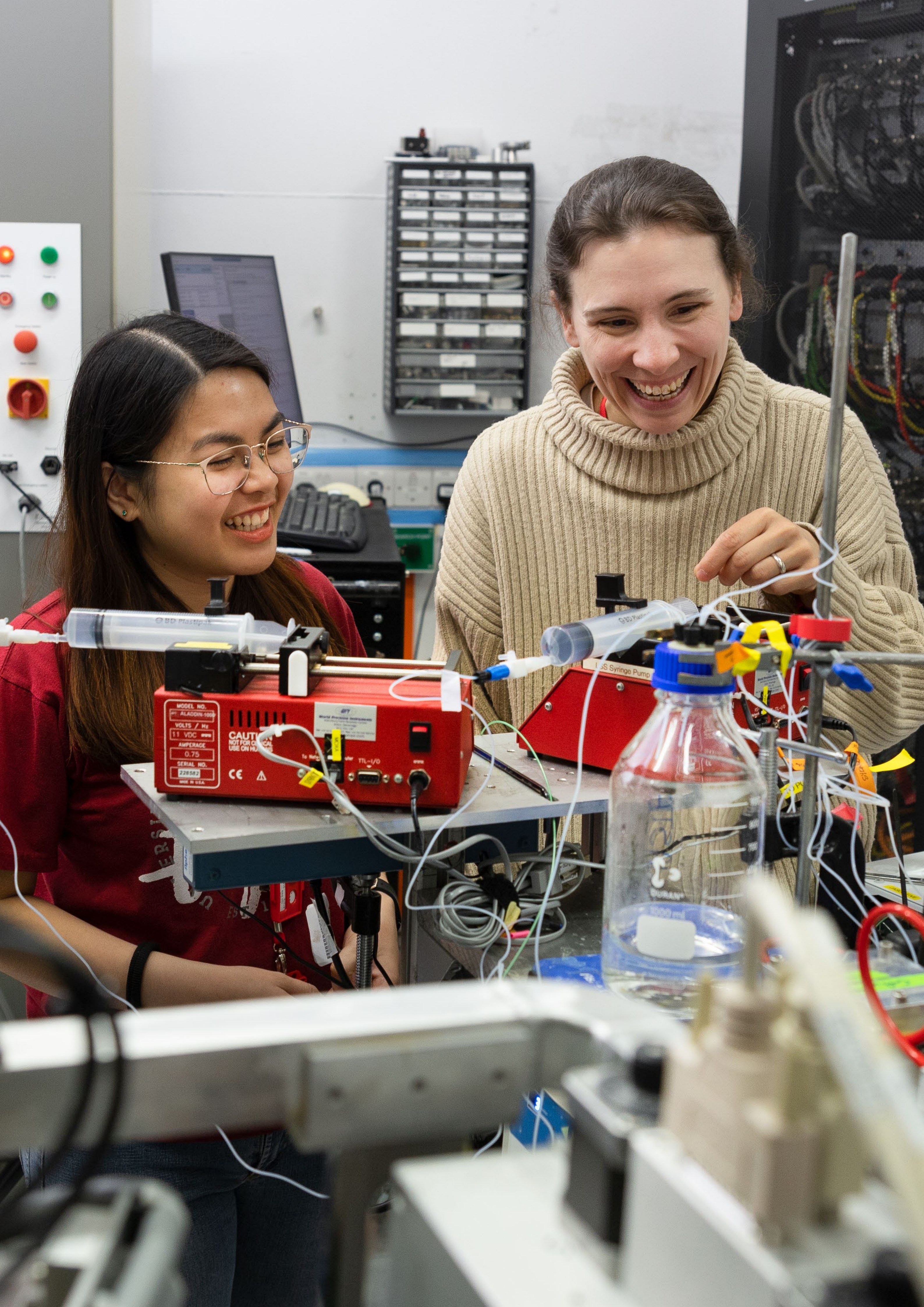
2700 authors

80% international collaborations

5.5% industrial collaborations

Link to publications

bit.ly/3RV6YGv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Delivering a world-leading science programme

The research conducted at ISIS throughout 2023 showcases the breadth, depth and quality of the science that is delivered. We have welcomed new and returning scientists and supported them to enable outstanding contributions in science and industry, including quantum materials, clean energy, manufacturing and healthcare.

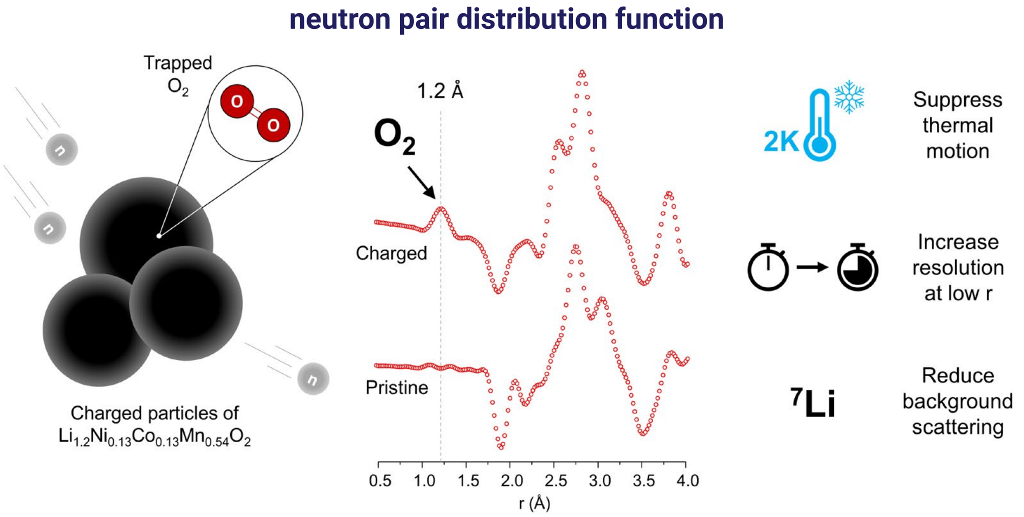
Image left: Debbie Nicdao and Vesa Halipi from Chalmers University of Technology in Sweden set up an experiment on Offspec to study the fusion mechanisms of asymmetric lipid vesicles and membranes mimicking the cell wall and endosome.

A revelatory new pathway to increase the energy density of lithium-ion batteries

Efficient energy storage systems require reliable and efficient high-energy battery systems with long cycle-life and low cost. The enormous commercial success of lithium-ion batteries has paved the way for compact and clean energy storage by powering portable electronic devices and electric vehicles (EVs). Looking for a way to increase the energy density of Li-ion batteries, neutron and X-ray techniques were employed to detect molecular O_2 trapped inside a cathode material. These neutron scattering experiments represent the first time trapped O_2 has been observed by a structural technique.

The drive for reducing greenhouse gas emissions to achieve net zero has created huge demands for the electrification of transport and energy storage, which have in turn become vital areas of research. Harvesting energy from renewable but intermittent energy sources has become intrinsic to the transition to greener energy. Lithium-rich cathode materials represent a potential route towards increasing the energy density of lithium-ion batteries, which can be used for applications in EVs, aviation and portable electronics. They can store more charge than conventional cathode materials by involving oxygen in the energy storage reaction; however, they suffer from voltage and capacity loss with cycling which must be addressed before they can be commercialised.

Characterising the nature of oxidised oxygen and tying it to the structural changes in these materials continues to attract considerable research attention. A team of researchers from the University of Oxford, ISIS, and Diamond Light Source have examined the local atomic structure of a commercially relevant lithium-rich cathode material by using neutron total scattering. Pair distribution function (PDF) analysis of total scattering offers information about the short range structure. The Polaris instrument at ISIS was used to collect data from a ^{7}Li-enriched material at temperatures close to absolute zero, to reduce the influence of background absorption and thermal motion. Under these conditions, the team were able to detect the presence of O_2 molecules trapped inside the crystal structure of the cathode. The study also identified nickel as the species responsible for out-of-plane migration, which has been a longstanding unanswered question for the field. With this revelatory understanding, the team demonstrated that large, uniform cathode particles which exhibit less surface O_2 loss and more trapped O_2, reveal greater energy efficiencies as a result. This opens up a new pathway towards higher performance energy storage materials for a net-zero world.



First direct structural evidence of O_2 in Li-rich cathode materials observed using neutron pair distribution function (PDF).

Instrument: Polaris

Related publication: Detection of trapped molecular O_2 in a charged Li-rich cathode by neutron PDF, *Energy & Environment Science*, 15, (2022), 376-383.

DOI: 10.1039/D1EE02237G

Funding: Henry Royce Institute

Authors: RA House, PG Bruce (University of Oxford, Henry Royce Institute, The Faraday Institution), HY Playford, R Smith (ISIS), J Holter, I Griffiths (University of Oxford) and KJ Zhou (Diamond Light Source)

Looking inside a fridge that cools to ultra-low temperatures

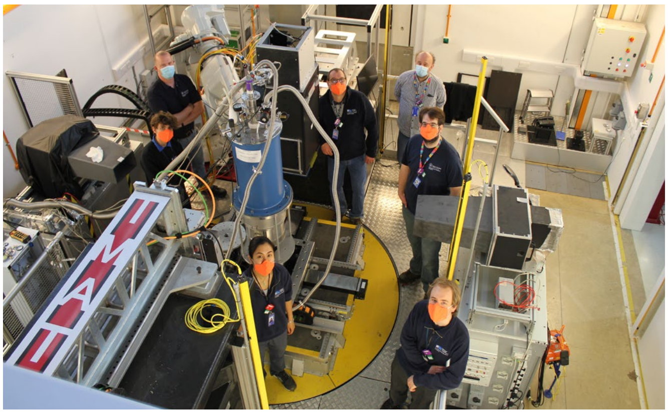
Over 100 experiments each year at ISIS require ultra-low temperatures below 1 K, or -272°C. These experimental conditions are extremely challenging to create; even a neutron beam can make the sample too hot. To create these ultra-low temperature environments, the Cryogenics Group use dilution fridges and neutron imaging measurements of the fridges provided valuable insight and some surprises!

This publication was amongst the Top 100 most downloaded Physics papers from Scientific Reports in 2022.

Dilution fridges rely on quantum mechanical effects that occur when two isotopes of helium are mixed. Diluting a mixture of helium-4 with the much rarer isotope, helium-3, can achieve cooling due to the heat of mixing of the two isotopes. This cooling occurs when helium-3 flows from an almost pure helium-3 phase to a lower purity 'dilute' phase. Neutrons are an ideal probe of this phenomenon, since they do not interact strongly with the metal components surrounding a fridge, nor the helium-4, but they are extremely sensitive to helium-3. So, to gain a new insight into the real movement of helium during the cooling, and inform the development of new dilution fridges, the ISIS Cryogenics Group looked to one of the facility's own instruments: IMAT.

The team took neutron imaging measurements of the dilution fridge under both continuous circulation and 'single shot' conditions. They were able to see the change in helium-3 concentration over time and at different temperatures. They found that the movement of helium during the continuous cycle operation was consistent with the accepted theory. They also looked at what happened when the fridge was operated incorrectly, causing it to fail. This revealed some surprises, as the effect of the failure was not what they expected.

Although these dilution fridges are in widespread use across the world, this insight into their operation is unique and provides a valuable resource. The method will also allow the development of atypical dilution fridges for space applications, diagnosis of other common dilution fridge fault modes, and be used for the training and instruction of the next generation of cryogenic technicians.



The ISIS Cryogenics Group at IMAT.

> **By altering the ratio of helium-3 to helium-4 in the dilution fridge mixture, we were able to simulate what would happen if helium-3 were to be lost… a low temperature physicist's worst nightmare! Interestingly, we found that whilst on the outside the fridge appeared to be working (albeit somewhat poorly), IMAT was able to reveal that the internal situation was far from ideal, with the boundary between the two phases seemingly absent from the mixing chamber.**
>
> Dr Chris Lawson – ULT & HMF Group Leader

Hamster Productions created a fantastic video for us named 'Cold Snap' using stop-motion where a LEGO figure was used to demonstrate neutron imaging. Access via the QR code here!

youtube.com/watch?v=P40NPahQPYA

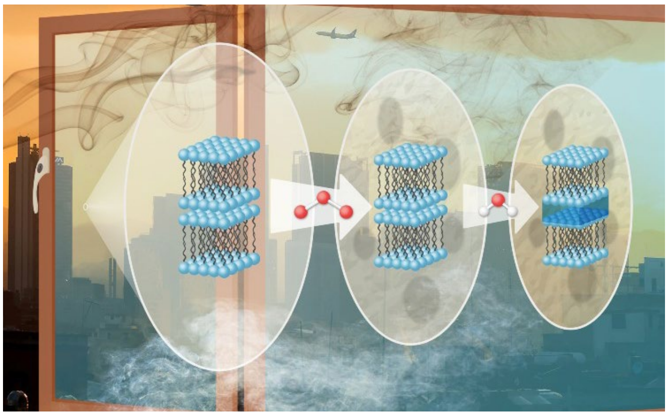
Instrument: IMAT
Related publication: Neutron imaging of an operational dilution refrigerator, *Scientific Reports*, 12, (2022), 1130.
DOI: 10.1038/s41598-022-05025-0
Funding: STFC
Authors: CR Lawson, AT Jones, W Kockelmann, SJ Horney and O Kirichek (ISIS)

Grimy windows could be harbouring toxic pollutants

Organic emissions, such as fatty acids from cooking, can get stuck to surfaces where they can trap toxins for long periods of time. Neutron reflectometry experiments have provided insight into the structure and composition of these organic surfactant films, improving our understanding of the behaviour of toxic pollutants and the implications for the climate and air pollution.

Fatty acids emitted during cooking are not easily broken down in the atmosphere. That means that when they hit a solid surface such as a window, they can form a self-organised thin film that builds up over time and will only be very slowly broken down by other chemicals in the atmosphere. During this process, the film becomes rougher and absorbs more water from the humidity in the air. In addition, toxic pollutants can become trapped underneath this persistent crust and are then protected from breakdown in the atmosphere.

For this study, which featured on the inside front cover of *Environmental Science*: *Atmospheres*, the team studied laboratory 'proxies', or models of 'real world' samples. These were spun into super-thin films of pollution, just a few tens of nanometres in thickness. Using the Inter beamline at ISIS, as well as experiments at Diamond Light Source and the Institut Laue-Langevin, the team studied the nano-scale composition of the films and the changes in their surface structures. By changing the humidity and amount of ozone, which is a key pollutant indoors and outdoors, the researchers were also able to mimic the behaviour of the films over time.



© University of Birmingham.

They found that the self-organised arrangement within the films of repeating molecular sheets, known as a lamellar phase, made it difficult for smaller molecules such as ozone to access the reactive parts of the fatty acids within these structures. Once deposited and exposed to ozone, the surfaces of the films became less smooth and increasingly likely to take up water, an effect which also has implications for the formation of cloud droplets and lifetime of aerosols in the atmosphere.

Awarded amongst the Best Papers from 2022 published in the Environmental Science journals of the Royal Society of Chemistry (RSC) for providing 'important insight into how details of molecular structure and emergent morphology may have a strong influence on the environmental persistence of compounds, bridging fundamental physical chemistry and environmental chemistry.'

> **I am very pleased that the importance of this study has been recognised. It demonstrates very nicely how neutron reflectometry can yield a wealth of structural information at the nanoscale and thus contribute to a deeper understanding of atmospherically relevant processes.**
>
> Maximilian Skoda,
> Deputy Group Leader for Reflectometry at ISIS

Instrument: Inter

Related publication: The evolution of surface structure during simulated atmospheric ageing of nano-scale coatings of an organic surfactant aerosol proxy, *Environmental Science: Atmospheres*, 2, (2022), 964-977.

DOI: 10.1039/D2EA00011C

Funding: NERC

Authors: A Milsom (University of Birmingham), A Squires (University of Bath), MWA Skoda (ISIS), P Gutfreund (Institut Laue-Langevin), E Mason (University of Bath, Diamond Light Source), NJ Terill (Diamond Light Source) and C Pfrang (University of Bath, University of Reading)

Using neutrons to understand atmospheric aerosols and their impact on air pollution, health and modern climate change

A new approach of studying the behaviour of surface films covering particles from the atmosphere has been developed by scientists. The technique offers a fresh perspective on the way that pollutants behave and break down in 'real' atmospheric conditions compared to the laboratory.

All cloud droplets start as a particle in the atmosphere. Pollution leads to these atmospheric particles being covered in a thin film, with the thickness and lifetime of these films determining how much of an effect they have on cloud formation and the climate. The effect of pollutants on the atmosphere is still not fully understood and although model systems have been used as a predictor, they are still a long way from representing what happens in the real world. To bridge that gap, Professor Martin King from Royal Holloway, University of London and his team studied atmospheric pollutant particles taken from real-world environments. Unlike model systems, these samples contained different mixtures of molecules, depending on where they came from.

The group used neutron reflectometry to study samples from Antarctica, a remote Atlantic Island near Canada, and UK rural and urban areas. They used the hydroxyl radical (one of the most reactive molecules found in the atmosphere) and followed its reaction with the natural thin films as a function of time. Once they had measured both the film thickness and the way the film reacts with the OH radical, they could input these data into a multi-layer model.

Using this model, they were able to show that the atmospheric particles remain in the atmosphere for long enough that they need inclusion in meteorological models. Their work highlights key differences between the way pollutants behave and break down in 'real' atmospheric conditions compared to the way they behave in the laboratory.

Professor King and his collaborators from the University of Birmingham, University of Uppsala, ISIS, Laser Science Facility and British Antarctic Survey continue to investigate the impact of atmospheric pollutants on our health and the climate. This work demonstrates how ISIS provides unique capabilities that bridge the gap between highly controlled laboratory experiments and field research in the very important area of atmospheric science.

Illustration from front cover of *Environmental Science: Atmospheres*, 2, (2022), designed by Helen Towrie.

ISIS Impact Awards 2023

2023 Society Impact Award Winner: Martin King, Royal Holloway, University of London

Awarded for his work investigating real-world atmospheric pollutants using neutron reflectometry.

Instrument: Inter

Related publication: Measurement of gas-phase OH radical oxidation and film thickness of organic films at the air-water interface using material extracted from urban, remote and wood smoke aerosol, *Environmental Science: Atmospheres*, 2, (2022), 574-590

DOI: 10.1039/D2EA00013J

Funding: STFC and NERC

Authors: RH Shephed (Central Laser Facility, Royal Holloway, University of London), MD King (Royal Holloway University of London), AR Rennie (Uppsala University), AD Ward (Central Laser Facility), MM Frey, N Brough, J Eveson, S Del Vento (British Antarctic Survey, NERC), A Milsom, C Pfrang (University of Birmingham), MWA Skoda (ISIS) and RJL Welbourn (University of Birmingham)

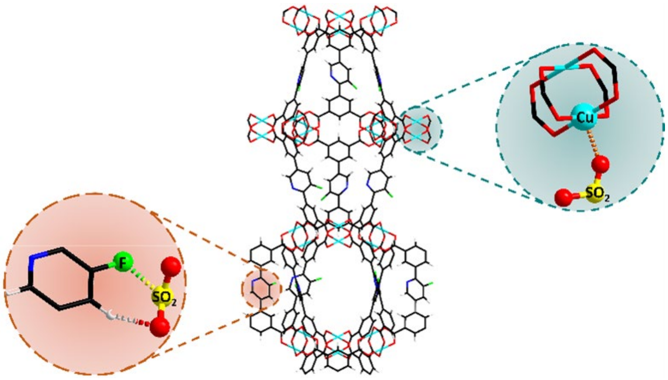
Designing porous materials for selective and reversible gas storage

Porous materials, such as metal-organic frameworks (MOFs), have the potential to be used across many industries for their ability to selectively adsorb and store gas molecules. A research collaboration led by Professor Martin Schröder and Professor Sihai Yang from the University of Manchester, has used neutron scattering to understand how changes in chemical structure impact a MOF's gas selectivity.

As well as capturing gases when they are produced, MOFs can also be used to capture unwanted gases from mixed streams. One example is sulphur dioxide, SO_2, which is produced during the combustion of fossil fuels. An advantage of using a MOF to capture SO_2 in this process is that the adsorption is reversible, unlike current methods that produce large quantities of solid waste and wastewater.

In one study, the researchers carried out a comprehensive investigation of a series of Cu(II)-carboxylate-based MOFs with different pore sizes and various functional groups. Using neutron studies to compare MFM-190(F) with MFM-126, the researchers could attribute higher adsorption performance of MFM-190(F) to open Cu(II) sites - the strongest adsorption sites for SO_2.

Through this and other studies, and their other work using neutron and X-ray scattering, the Manchester group have been able to make significant progress in the understanding of how pore geometry and chemistry links to gas adsorption. By understanding what influences selectivity and reversibility, their work will inform the design of future materials that will act as energy-efficient gas separators.



View of the SO_2 binding sites derived from open Cu(II) sites and organic functional groups in the pore of MFM-190(F).

> **The studies enabled by scientists at ISIS and the Diamond Light Source have been essential in establishing and defining a real understanding of how our new materials function. Interdisciplinary and collaborative research is essential in driving real understanding of structure-property-function relationships.**
>
> Professor Martin Schröder, University of Manchester

Instruments: Tosca, WISH

Related publication: Adsorption of sulfur dioxide in Cu(II)-carboxylate framework materials: the role of ligand functionalization and open metal sites, *Journal of the American Chemical Society,* 144, (2022), 13196–13204.

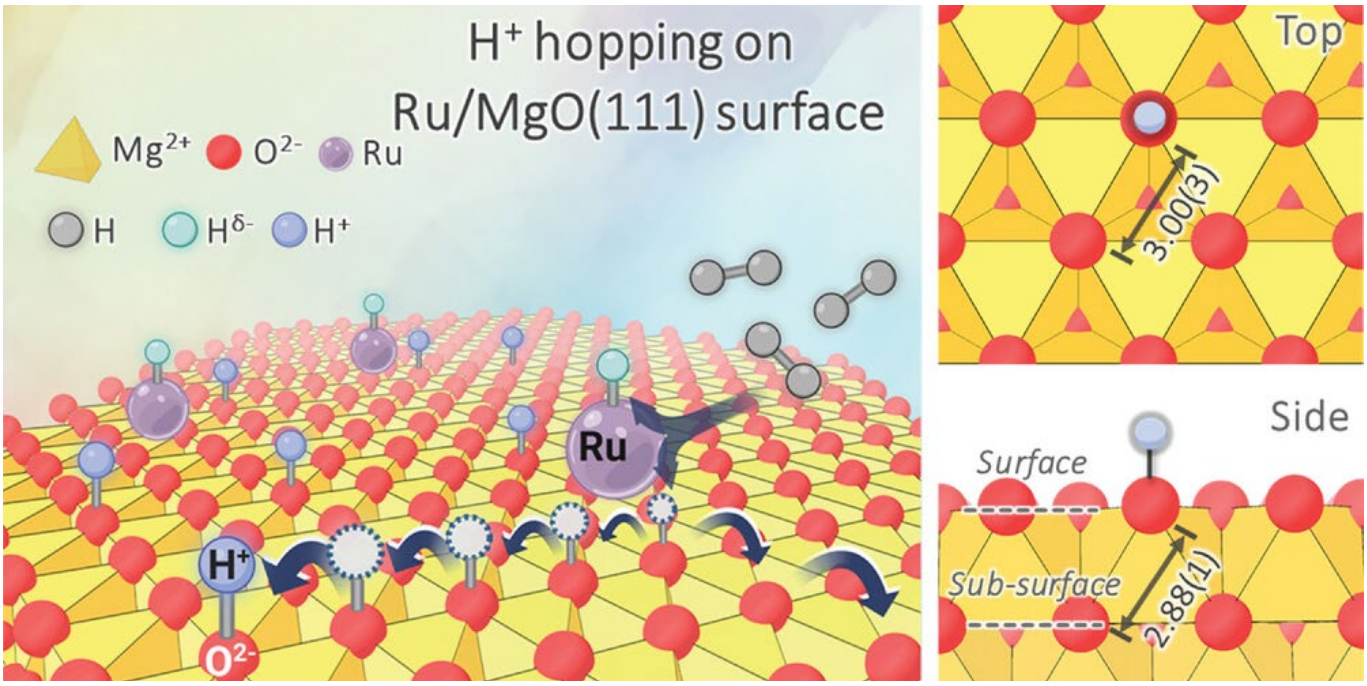
DOI: 10.1021/jacs.2c03280

Funding: EPSRC, ERC, Royal Society and University of Manchester

Authors: W Li, J Li, TD Duong, SA Sapchenko, X Han, JD Humby, GFS Whitehead, IJ Victórica-Yrezábal M Schröder, S Yang (University of Manchester), I da Silva, P Manuel (ISIS), MD Frogley and G Cinque (Diamond Light Source)

Introducing polarity increases proton diffusion

Quasi-elastic neutron scattering has revealed an exceptional proton diffusion rate on the surface of a catalytic material. The experiments required the expertise of the ISIS Pressure and Furnace Group, who designed a specialist sample can for high temperatures and pressures, as well as *in situ* gas handling.



The proposed mechanism for hydrogen spillover over the Ru/MgO(111) material. Ru: purple; Mg: yellow; O: red; molecular H: grey; Hydridic H ($H^{\delta-}$): green; and proton (H^+): blue.

Hydrogen diffusion is crucial to many chemical processes, including industrial catalysis and fuel cells. However, the dynamics of hydrogen migration over catalyst surfaces still remains unclear and extremely difficult to observe experimentally on atomic length scales. This is especially true for light molecules with a limited number of electrons, such as hydrogen. It is, therefore, important to investigate the diffusion of hydrogen over the surface of metal oxide materials using high-resolution equipment capable of detecting the dynamics of such a light element under realistic conditions. One proposed mechanism for this diffusion on surfaces is where surface-activated hydrogen atoms migrate from a hydrogen-rich metal cluster(s) to the surface of a catalyst support, a process known as hydrogen spillover. Neutron experiments are extremely useful when investigating these mechanisms, as the dynamics of migration of small atoms such as hydrogen are hard to observe on the atomic scale using other techniques. A collaboration between researchers at ISIS, the University of Oxford and East China University of Science and Technology, used quasi-elastic neutron scattering (QENS) to study the hydrogen diffusion rate on a ruthenium (Ru)-doped magnesium oxide catalyst, comparing polar MgO(111) surface to the nonpolar MgO(110) surface.

The QENS revealed rapid proton diffusion on the polar facet, which was an order of magnitude greater than typical proton-conducting oxides. They believe this is due to the unique layered arrangement of Mg^{2+} and O^{2-} anions in MgO(111), with the terminal oxygen anions facilitating fast H^+ transport via a proton hopping mechanism. This insight will feed into the future design of efficient catalysts for processes that rely on hydrogen diffusion.

Instrument: Osiris

Related publication: Exceptional hydrogen diffusion rate over Ru nanoparticle-doped polar MgO(111) surface, *Small Methods*, 7, (2022), 2201200

DOI: 10.1002/smtd.202201200

Funding: National Natural Science Foundation of China

Authors: T Yoskamtorn, J Mo, S Wu (University of Oxford), L Chen, XP Wu, SCE Tsang (East China University of Science and Technology), S Mukhopadhyay and A Hawkins (ISIS)

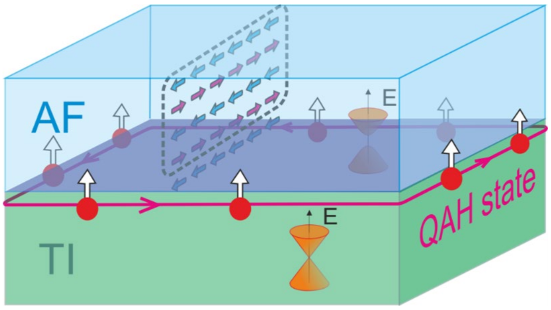
The value of using a full toolbox of techniques for evaluating quantum materials

For many years, scientists have been searching for materials that can be used to conduct electricity with minimal resistance and drastically increase energy efficiency. By using the combination of polarised neutron reflectometry, X-ray spectroscopy and magneto-transport, researchers been able to characterise individual layers of a potential candidate for building future quantum computers.

Novel conducting materials are potential candidates for building quantum computing devices. Recently, some materials have been shown to exhibit a phenomenon known as the quantum anomalous Hall (QAH) effect. In this QAH state, materials show properties that are suitable for energy efficient devices, as well as the complex magnetism needed for spintronic applications. However, to achieve this state, magnetic order must be present in a topological insulator, something that is hard to achieve. When it has been completed, it usually results in either reducing the QAH effect or causing it to only appear at lower temperatures.

It has been suggested that such a system can be created by placing an antiferromagnetic layer on top of the topological insulator (TI). Having this interface with a magnetically ordered system could induce a magnetic ordering in the TI as well. To understand whether this was the case, a group of researchers used magneto-transport alongside polarised neutron reflectometry on the Polref instrument at ISIS, and X-ray spectroscopy on the I06 beamline at Diamond Light Source. In doing so, they were able to study the layers individually and find out whether magnetisation was being induced, and/or whether the magnetic constituents were migrating between the layers. Extracting the relevant information from these data would not have been possible without being able to deploy the capability of the SCD SCARF cluster, which allowed the team to fully explore and quantify the data.

Only by using this combination of techniques were they able to show that, in this system, there was no magnetism induced in the TI layer. This explains why the QAH effect had not been observed, even though it was expected to be present.



Schematic of a QAH effect system based on a topological insulator and an antiferromagnet.

> **Our work delivers a robust method to evaluate candidate materials and single out the best possible materials system, which then can be the cornerstone of real-world applications. Fortunately for our team of scientists, we have world-class neutron and X-ray sources available at the same location. By combining both techniques, we could show how large-scale facilities contribute to the development of novel, complex materials that can address present day challenges and shape our future.**
>
> Dr Dirk Backes, lead author and beamline scientist at Diamond Light Source

Instrument: PolRef

Related publication: Critical analysis of proximity-induced magnetism in MnTe/Bi_2Te_3 heterostructures, *Physical Review Materials*, 6, (2022), 053402

DOI: 10.1103/PhysRevMaterials.6.053402

Funding: National Key R&D Program of China, National Natural Science Foundation of China, Major Project of Shanghai Municipal Science and Technology, Shanghai Sailing Program, Strategic Priority Research Program of Chinese Academy of Sciences, EPSRC (Engineering and Physical Sciences Research Council), Oxford-Shanghai Tech collaboration.

Authors: G Awana (Loughborough University), R Fujita, T Hesjedal (University of Oxford), A Frisk, P Olalde-Velasco, SS Dhesi, G van der Laan, D Backes (Diamond Light Source), P Chen, Q Yao, XF Kou, SL Zhang (Shanghai Tech University), AJ Caruana, CJ Kinane, S Langridge (ISIS) and NJ Steinke (Institut Laue-Langevin)

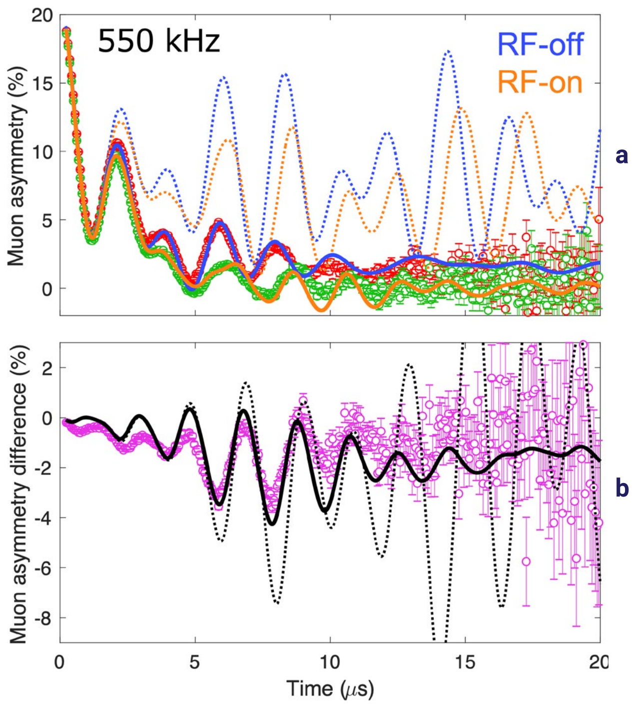
Using muon spin relaxation with radio-frequency manipulation

Entanglement is a primary feature of quantum mechanics, and the preparation, manipulation and measurement of entangled quantum states lies at the heart of emerging quantum technologies. New methodology using muon spin relaxation to manipulate the populations of entangled quantum states is paving the way to understanding complex systems.

There are numerous methods for creating entangled states, where the manipulation can be enabled by electromagnetic pumping at a frequency corresponding to the interval between the energy levels. One such entangled state often occurs when a positively charged, 100% spin-polarised muon, μ^+, is implanted into a material containing fluorine.

Manipulating the entangled state populations is enabled via the application of continuous, radio-frequency (RF) electromagnetic excitation fields. Led by Professor Sean Giblin of Cardiff University, a team of researchers from ISIS, Universities of Cardiff and Durham, TRIUMF and Boston College employed a dual experimental and computational approach to probe, manipulate, and model the populations of entangled quantum states in a system of spins, which were excited with continuous RF fields. Muon spin relaxation (μ^+SR) was used to measure oscillations of the μ^+ spin polarisation, which are characteristic of the energy level structure of the spin states in single-crystal $LiY_{0.95}Ho_{0.05}F_4$, and changes in the oscillations were observed on application of the RF fields.

To model these changes, the team were able to describe the system mathematically and demonstrated that this can represent the experimentally observed μ^+ spin polarisation. Their methodology opens up the possibility of performing spectroscopy experiments by varying the RF field frequency and looking for resonances in the difference between the μ^+SR spectra recorded with and without the applied RF field. They also plan to perform pump-probe-style experiments by using the RF field to change the state population and subsequently measuring the resulting μ^+ relaxation. Additionally, extending the RF coil design to allow microwave frequencies (0.3–30 GHz) will permit measurements of electronic (as opposed to nuclear) spin phenomena. This study paves the way for manipulating and understanding a wide variety of complex spin systems with continuous RF-μ^+SR.



Experimental μ^+ asymmetry for $LiY_{0.95}Ho_{0.05}F_4$ at T=50 K for both RF-on and RF-off, at excitation frequencies of (a) $\omega_{on}/(2\pi)$=550 kHz and (b) $\omega_{off}/(2\pi)$=825 kHz, together with those calculated for the F—μ—F complex (μF2) and the $\mu F_2Li_2F_2$ cluster. The improved agreement with experiment from accurately modeling the decoherence effect (by including the local environment of the F—μ—F complex to form the $\mu F_2Li_2F_2$ cluster) is evident. Importantly, the on-resonance asymmetry difference cannot be caused by a simple change in relaxation rate.

Instrument: Emu

Related publication: Radio-frequency manipulation of state populations in an entangled fluorine-muon-fluorine system, *Physical Review Letters*, 129, (2022), 077201

DOI: 10.1103/PhysRevLett.129.077201

Funding: EPSRC and the European Regional Development Fund.

Authors: D Billington, E Riordan, M Salman, D Margineda, GJW Gill, SR Giblin (Cardiff University), SP Cottrell (ISIS), I McKenzie (TRIUMF), T Lancaster (Durham University) and MJ Graf (Boston College)

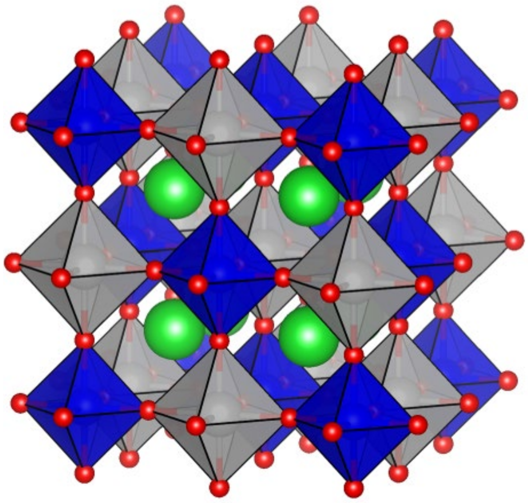
Using neutrons and muons to investigate exotic quantum states

Compounds made of 4d and 5d transition metal compounds are being investigated as potential hosts for exotic quantum states of matter, such as spin liquid states, multipolar order and valence bond glass states. Inelastic neutron scattering and muon spectroscopy have provided valuable and unique insights in this study of complex magnetic behaviour.

Ba_2YMoO_6 and Ba_2LuMoO_6 are both double perovskites, with a single $4d^1$ magnetic cation. Ba_2YMoO_6 has previously been studied, with the experimental results showing that the ground state is a valence bond glass, where nonmagnetic spin singlets gradually form in a disordered fashion as the temperature is decreased, while some orphan spins remain paramagnetic. But it has also been proposed as a spin liquid.

A UK research team, led by Dr Otto Mustonen and Professor Eddie Cussen, studied Ba_2LuMoO_6, whose ground state is not known. Their initial magnetic susceptibility measurements were supplemented by muon spin rotation and relaxation (μSR) experiments and inelastic neutron scatting (INS). Muons were used as a highly sensitive local probe of both static and dynamic magnetism, while INS was used to probe the magnetic excitations, looking for the nonmagnetic spin singlets expected in a valence bond glass state.

While μSR revealed a lack of magnetic order or spin freezing in Ba_2LuMoO_6 down to 60 mK (unlike Ba_2YMoO_6), indicative of a valence bond glass state, INS showed evidence of a singlet-triplet excitation. Therefore the researchers determined that the ground state could best be described as a valence bond glass state, similar to Ba_2YMoO_6, but without freezing of orphan spins. The absence of this spin freezing makes Ba_2LuMoO_6 a more promising valence bond glass candidate.



The double perovskite structure of Ba_2LuMoO_6. Ba, Lu, Mo, and O are represented by the green, grey, blue, and red spheres, respectively.

> **This work highlights the exotic and varied quantum magnetism observed in perovskite oxides and reveals differences between 4d and 5d compounds. Neutrons and muons are essential tools for investigating quantum magnetism. Only by combining both techniques, it became possible to understand the unusual quantum ground state of this material.**
>
> Dr Otto Mustonen, University of Birmingham

Instruments: MuSR, Merlin

Related publication: Valence bond glass state in the $4d^1$ fcc antiferromagnet Ba_2LuMoO_6, *npj Quantum Materials*, 7, (2022), 74.

DOI: 10.1038/s41535-022-00480-4

Funding: The Leverhelme Trust, Winton Programme for the Physics of Sustainability - University of Cambridge

Authors: OHJ Mustonen (University of Sheffield, University of Birmingham), HM Mutch, C Pughe, EJ Cussen (University of Sheffield), HC Walker, PJ Baker, GBG Stenning (ISIS), FC Coomer (Afton Chemical Ltd.), RS Perry (University College London, ISIS), C Liu and SE Dutton (University of Cambridge)

Dr Otto Mustonen wins the 2023 BTM Willis Prize

Recognising outstanding contributions by early-career scientists in the field of neutron scattering.

The 2023 BTM Willis Prize was awarded to Otto Mustonen from the University of Birmingham for his work on the design, synthesis, and investigation of unique realisations of long-sought models of quantum magnetism using neutron diffraction and spectroscopy and muon spin relaxation techniques.

“Multiple neutron scattering techniques underpin all of these studies and it was Otto's contribution of planning, performing and understanding the inelastic and polarised neutron scattering experiments that led to the key insights. It is a measure of both Otto's drive and the esteem in which he is held that the collaborations that underpin these experiments were put in place by him. His elegant application of this range of neutron techniques and the quality of his scientific discoveries makes him a highly meritorious recipient of the Willis Prize."

Professor Eddie Cussen, University of Sheffield

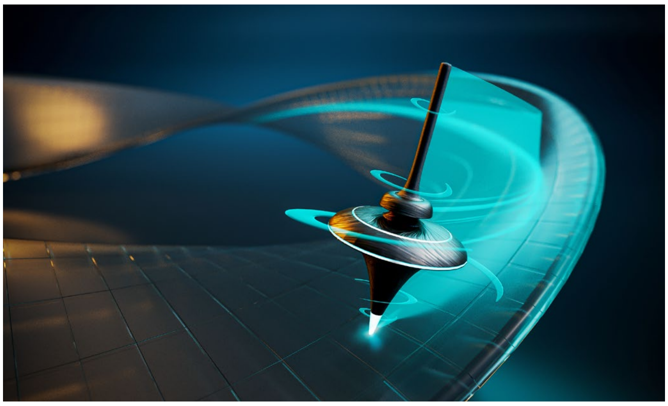
Magnetic excitations for information transfer without heat loss

Since neutrons are sensitive to magnetic fields, they are well suited for the study of magnetic materials. For this international research collaboration, neutron scattering proved to be the only technique capable of detecting spin waves on circular orbits with sufficient resolution over very large length and time scales.

Just as electrons flow through an electrical conductor, magnetic excitations (known as magnons) can travel through certain materials. Currently, the transport and control of electrical charges serve as the foundation for most electronic components. A major disadvantage is that the flow of electric currents generates heat due to the electrical resistance. Magnons could potentially facilitate the transportation of information more efficiently than electrical conductors, offering high energy efficiency.

When throwing a stone into water, you bring the water molecules out of their equilibrium position. They start to oscillate, and a circular wave spreads out. In a very similar way, the magnetic moments in some materials can be made to oscillate. In this process, the magnetic moment performs a gyroscopic motion with respect to its rest position. The precession of one moment affects the vibration of its neighbour, and so the wave propagates.

For applications hoping to use these magnetic waves, controlling properties such as wavelength or direction is important. Skyrmions are tiny whirlpools of magnetic spin with potential to act as carriers of information in future devices. An international collaboration employing polarised inelastic neutron scattering has now proven that the propagation of magnetic waves perpendicular to skyrmions does not occur in a straight line as it does in conventional magnets, but rather on a circular path.



Twisted Spin Wave, Credit: Christoph Hohmann / MCQST.

> **The spontaneous motion of spin waves on circular orbits, whose radius and direction arise from the vortex-like structure of skyrmions, opens up a new perspective for realising functional devices for information processing in quantum technologies, such as simple couplers between qbits in quantum computers.**
>
> Christian Pfleiderer, Technische Universität München

Instrument: LET

Related publication: Topological magnon band structure of emergent Landau levels in a skyrmion lattice, *Science*, 375, (2022), 1025-1030

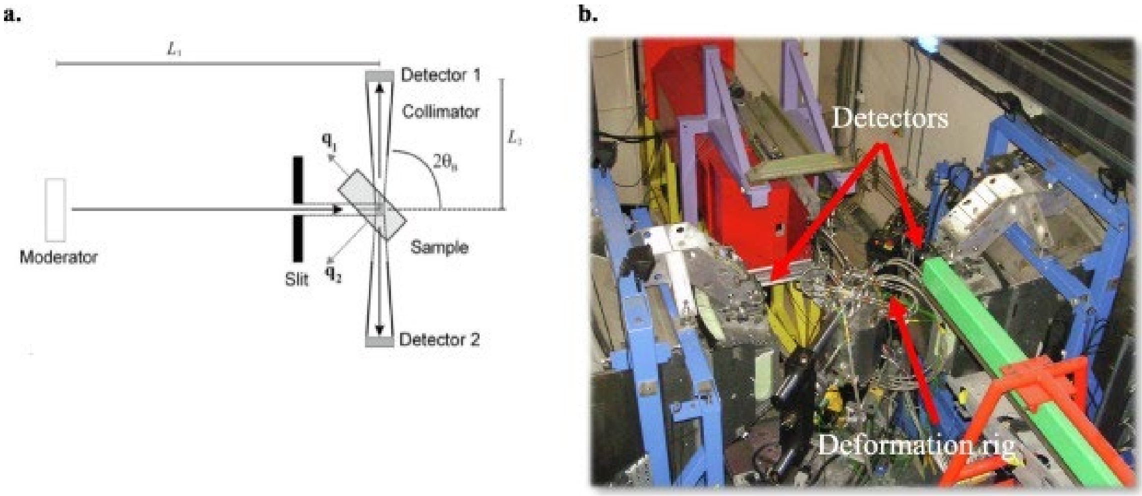
DOI: 10.1126/science.abe4441

Funding: European Research Council, German Research Foundation, Los Alamos National Laboratory, and the Institute for Materials Science at Los Alamos

Authors: T Weber, P Steffens, M Böhm (Institut Laue-Langevin), D M Fobes (Los Alamos University), J Waizner (Universität zu Köln), GS Tucker (Paul Scherrer Institute, École Polytechnique Fédérale de Lausanne), L Beddrich, C Franz, H Gabold, M Skoulatos, R Georgii (Technische Universität München, MLZ), R Bewley (ISIS), D Voneshen (ISIS, Royal Holloway University of London), G Ehlers (Universität Zürich), A Bauer, C Pfleiderer, P Böni (Technische Universität München), M Janoschek (Los Alamos University, Paul Scherrer Institute and Universität Zürich) and M Garst (Universität zu Köln, Technische Universität Dresden and Karlsruhe Institute of Technology)

Siemens Energy test a new gas turbine production method

Additive manufacturing is a production technique that builds a component layer by layer, to the specification of a 3D model. However, using this manufacturing process affects the texture of metal alloys in a different way to conventional techniques. A specialised setup on the Engin-x beamline meant that the researchers were able to study the internal structure at the same time as compressing the materials, to test how they would behave in a real-world scenario.



(a) The schematic of Engin-x neutron diffractometer and (b) the experimental setup at Engin-x.

Additive manufacturing enables intricate parts to be made at a small scale without the need for large investment in rarely-used manufacturing equipment. However, as the mechanical properties of a material are very dependent on this internal texture, it is important to understand how the production process influences what is happening inside the alloy.

One type of additive manufacturing is laser powder bed fusion, where a powder is applied to a substrate and then a laser melts this powder into a given shape. There are many parameters that can be controlled, each influencing the microstructure and texture of the end component.

In this study, a Canadian research collaboration, including Siemens Energy, used neutron diffraction to understand the microstructural changes caused by altering different parameters during this type of additive manufacturing. They focussed on components made from a nickel-based superalloy known as Hastelloy-X, which is used to make gas turbines.

As neutrons can penetrate up to several centimetres into the superalloy, they are an ideal tool to probe internal structures. By studying samples made using a variety of laser powers and scanning speeds, the team were able to determine that both parameters influence the microstructure, with increasing laser power inducing a preferred orientation of the grains in the alloy. This confirmed the importance of controlling each parameter of this production method, as this will determine the structure, and therefore properties, of the end component.

> **The laser powder bed fusion additive manufacturing process produces an intense temperature gradient within the fabricated components as a result of the fast thermal and cooling cycles that occur during the process. Therefore, residual stresses and deformations are inevitable in the manufactured parts. In order to minimise deformation, residual stresses must be measured and analysed to optimise the laser powder bed fusion process parameters. Due to the capabilities available at Engin-x, we were able to measure residual stresses precisely.**
>
> Ali Bonakdar, Siemens Energy

Instrument: Engin-x

Related publication: Deformation mechanisms of additively manufactured Hastelloy-X: A neutron diffraction experiment and crystal plasticity finite element modelling, *Materials & Design*, 222, (2022), 111030.

DOI: 10.1016/j.matdes.2022.111030

Funding: Natural Sciences and Engineering Research Council of Canada

Authors: A Aburakhia (Western University), A Bonakdar (Siemens Energy Canada Ltd.), M Molavi-Zarandi (National Research Council Canada), J Kelleher (ISIS) and H Abdolvand (Western University)

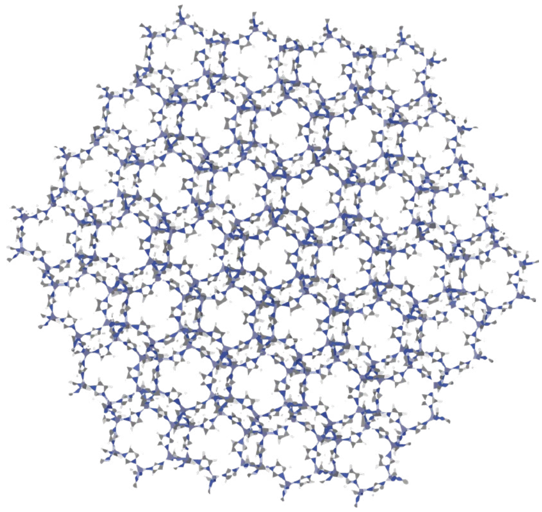
Demonstrating the viability of a scalable route to synthesise a gas storage material

Sustainable technologies company, Johnson Matthey, used neutron scattering to track the synthesis of a commercially relevant porous material, suitable for gas storage and catalysis. The results provided insights to develop a more economic, sustainable and scalable production pathway.

Zeolitic imidazolate frameworks (ZIFs) are porous materials with many potential applications, including gas separation, catalysis, electronic devices and drug delivery. For ZIFs to be used industrially, large-scale production routes are needed. However, conventional, small-scale syntheses often use large quantities of expensive and toxic solvents, so more economic and environmentally friendly production routes are sought.

Researchers from Johnson Matthey wanted to investigate the feasibility of preparing ZIF-8 by first synthesising a different material, ZIF-L, and then transforming this into ZIF-8 in a novel route using much less water and organic solvent. By using neutron spectroscopy, the Johnson Matthey team gained better understanding of the chemistry of their production process and showed that the synthesis of ZIF-8 was successful. The study also demonstrated that neutron spectroscopy could be used to track the reaction in real time, which would be beneficial in material scale-up to determine when the transformation of ZIF-L to ZIF-8 is complete.

On scaling production, Johnson Matthey successfully synthesised one kilogram of ZIF-8, with the potential to increase industrial production to 15 tonnes per year. The pilot formed the basis of an economic analysis that showed this synthesis route could produce over six times more ZIF-8 than direct methods.

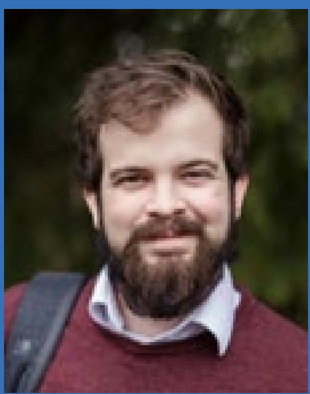


A stylised version of the ZIF-8 framework.

ISIS Impact Awards 2023

2023 Economic Impact Award Winner: Timothy Johnson, Johnson Matthey, UK

Awarded for his work demonstrating the viability of a scalable route to synthesise a gas storage material.



> **Inelastic neutron scattering spectroscopy conducted on the Tosca beamline at ISIS allowed scientists at Johnson Matthey to probe the structure of ZIF-8 and its polymorph ZIF-L. Data collected on Tosca gave our scientists high confidence when working towards an accurate and predictive cost model with the ultimate aim of Metal-organic Framework commercialisation.**
>
> Timothy Johnson, Senior Scientist, Johnson Matthey Challenge

Instrument: Tosca

Related publication: Understanding the ZIF-L to ZIF-8 transformation from fundamentals to fully costed kilogram-scale production, *Communications Chemistry*, 5, 2022, 18

DOI: 10.1038/s42004-021-00613-z

Funding: European Union MEMBER project

Authors: A Deacon, L Briquet, F Massingberd-Mundy, TL Hyde, S Poulston, T Johnson (Johnson Matthey), M Malankowska, J Coronas (Universidad de Zaragoza), S Rudić and H Cavaye (ISIS)

Investigating materials to create novel superconductors

Superconductors are materials that can conduct electrons without resistance when cooled below a critical temperature (T_c). This property could find applications across a vast range of industries, but superconducting materials tend to only show these exotic properties at extremely low T_c. New research aims to not only discover superconducting materials with a higher T_c, but also to uncover the mechanisms behind these unusual properties.

The material $Ba_{0.6}K_{0.4}BiO_3$ exhibits superconductivity up to a relatively high temperature. One prevailing model involves the electron orbitals from the oxygen ions in the structure interacting with those from the bismuth (Bi) ions, causing charge density transfer and creating new energy levels and accessible oxygen ligand holes for resistance-free electron transfer. To investigate this model further, Minu and his team decided to make the same material but with antimony (Sb) rather than bismuth.

In their quest to create this material, the team took their inspiration from geoscience. Recreating conditions deep within the Earth's mantle by using pressures of over 20 GPa and temperatures of 1900°C, they were able to synthesise a series of compounds with the formula $Ba_{1-x}K_xSbO_3$.

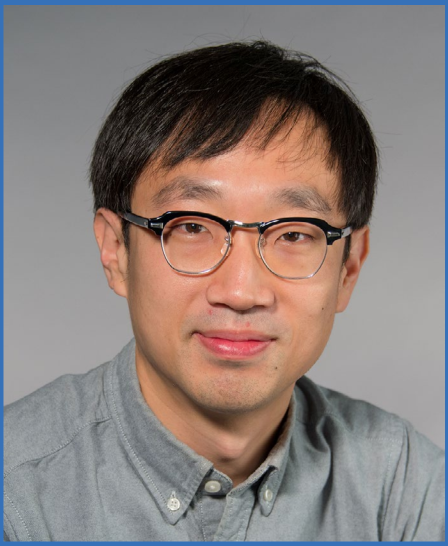
By measuring the Sb-O bond lengths in $BaSbO_{3-\delta}$ using neutron diffraction on WISH, they could see that there was strong covalency between the antimony and oxygen ions, leading to a stronger interaction than in the bismuth equivalent. Further neutron diffraction experiments enabled them to create a phase diagram for the $Ba_{1-x}K_xSbO_3$ series, from which they identified a particular phase that may exhibit superconductivity.

The highest T_c, of 15 K, was observed for $Ba_{0.35}K_{0.65}SbO_3$. Although lower than the T_c of $Ba_{0.6}K_{0.4}BiO_3$, it is higher than the bismuth-equivalent at a similar potassium doping level. This suggests that, if it could be possible to stabilise the structure of an antimony equivalent at the same potassium level, the T_c could be even higher. Crucially for the field of superconductivity, this research indicates that the direction of charge transfer may not be critical for the mechanism, as the opposite correlation is observed for these two series of materials. These findings sparked renewed interest in exploring similar high T_c materials, which could potentially lead to the development of novel superconductors.

ISIS Impact Awards 2023

2023 Science Impact Award Winner:
Dr Minu Kim, Max Planck Institute for Solid State Research, Germany

Awarded for his work investigating a new class of superconductor.



Instrument: WISH

Related publication: Superconductivity in $(Ba,K)SbO_3$, *Nature Materials*, 21, (2022), 627–633

DOI: 10.1038/s41563-022-01203-7

Funding: Max Planck-UBC-UTokyo Centre for Quantum Materials

Authors: M Kim, GM McNally, H-H Kim, T Takayama, A Yaresko, U Wedig, M Isobe, RK Kremer, B Keimer (Max Planck Institute for Solid State Research), M Oudah, DA Bonn (University of British Columbia), AS Gibbs, P Manuel (ISIS), RJ Green (University of British Columbia, University of Saskatchewan), R Sutarto (Canadian Light Source, University of Saskatchewan) and H Takagi (Max Planck Institute for Solid State Research, University of Tokyo)

One of the toughest known materials on Earth, which gets tougher in the cold

Most metals are more likely to crack as you lower the temperature, yet a global research collaboration has been studying alloys that do the exact opposite. Their research has resulted in the characterisation of a new class of alloy that is amongst the toughest ever recorded, even at very low temperatures.

Unlike traditional metal alloys such as steels, which are mainly made up of one element with others added in small amounts, high and medium entropy alloys have multiple principal elements in almost the same amount. There are almost opens endless possibilities to combine elements in this way, so finding a good alloy is like finding a needle in a haystack.

A unique property of one such family of alloys is the ability for the materials to get stronger and less likely to crack at lower temperatures. This is the opposite of the behaviour of most metals, which normally get stronger but more brittle at low temperatures. Alloys derived from the combination of chromium (Cr), cobalt (Co) and nickel (Ni) demonstrate this unusual property, maintaining their resistance to fracture even down to -253°C.

An international collaboration studied the mechanical properties of Cr-Co-Ni medium entropy alloys at temperatures as low as -253°C. The research revealed that the Cr-Co-Ni-based alloys were extremely tough, with their resistance to both crack-initiation and growth at the lowest temperatures being amongst the highest ever recorded. By using neutrons and electron microscopy to study the microstructure around a deliberately initiated crack, they were able to determine what was happening at the atomic and grain scale that caused this impressive toughness.

Being able to create materials that remain strong at these very low temperatures is extremely useful for applications such as transporting liquid hydrogen as a method of energy transport in a hydrogen-based economy, or in creating materials that can be used in space or on other planets.

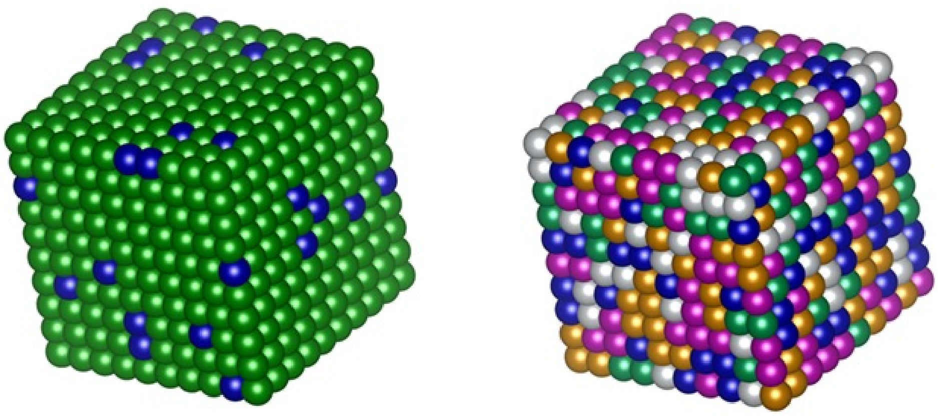


Figure showing conventional alloys (left) and high entropy alloys (right). The different colored spheres represent different elements.

Instrument: Engin-x

Related publication: Exceptional fracture toughness of CrCoNi-based medium- and high-entropy alloys at 20 Kelvin, *Science*, 378, (2022), 978-983

DOI: 10.1126/science.abp8070

Funding: US Department of Energy, Engineering and Physical Sciences Research Council, Australian Research Council, and the UNSW Scientia Fellowship.

Authors: D Liu, M Jiang, P Forna-Kreutzer (University of Bristol), Q Yu (Lawrence Berkeley National Laboratory), S Kabra (ISIS), R Zhang, M Payne, F Walsh, M Asta, AM Minor, RO Ritchie (Lawrence Berkeley National Laboratory, University of California - Berkeley), B Gludovatz (University of New South Wales) and EP George (Oak Ridge National Laboratory, University of Tennessee, Ruhr University Bochum)

Using SANS to study super duplex stainless steel

Duplex stainless steels (DSSs) are multicomponent Fe-Cr-Ni-based alloys with high strength, corrosion resistance and weldability. The name, duplex, refers to the two-phase microstructure of these materials, which comprise roughly equal proportions of two different crystal forms of iron. A study of phase separation in super duplex stainless steel could help to develop future alloys that are less susceptible to long-term thermal degradation.

DSSs are widely used as engineering materials, particularly for corrosive environments, such as gas pipelines and chemical reaction vessels. High-alloy DSSs, known as super duplex stainless steels (SDSSs), are more expensive but their higher chromium, nickel and molybdenum content offers even greater resistance to stress corrosion cracking.

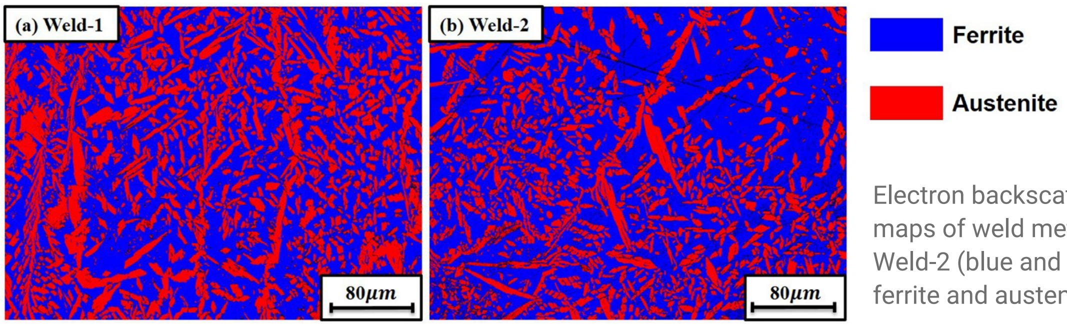
Despite their useful properties, the application of SDSSs is limited to temperatures around 250°C due to changes in mechanical properties caused by decomposition of the ferrite phase. This poses an even greater issue when welding SDSS, as welds are more susceptible to thermal embrittlement.

Tungsten inert gas (TIG) welding is commonly used to create SDSS weldments, but the products are extra sensitive to thermal embrittlement. To understand how TIG welding affects the microstructure of SDSS in the longer term, a team from Sweden studied phase separation in an SDSS base metal and two weldments by small-angle neutron scattering (SANS).

SANS data revealed that aging the base metal (300°C, 48,000 hours) and weldments (300°C, 35,000 hours) increased their hardness due to Cr clustering in the ferrite phase. The effect was more pronounced in the weldments than in the base metal, showing that TIG welding accelerated phase separation, especially during prolonged aging. The pronounced phase separation in the weldments was attributed to two factors: the accelerating effects of their higher Cr and Ni content, and residual strains caused by the welding process. It was found that internal residual strain was exacerbated when using a higher heat input in each welding pass.

Already, the information from neutron scattering is enabling the design of SDSSs that are less prone to thermal embrittlement. The development of new alloys could help to expand the engineering applications of SDSSs, enabling their use under even more demanding conditions.

> **The application of SANS to study phase separation in Fe-Cr based alloys has provided significant new fundamental knowledge and we are currently exploiting this know-how for innovations in the field. So far, we have submitted one patent application for a new duplex alloy and one patent for a new process route, both aiming at mitigating the thermal embrittlement.**
>
> Peter Hedström, KTH Royal Institute of Technology.



Electron backscatter diffraction phase maps of weld metal for (a) Weld-1 and (b) Weld-2 (blue and red colours represent ferrite and austenite, respectively).

Instrument: LoQ

Related publication: Small-angle neutron scattering study on phase separation in a super duplex stainless steel at 300 °C – comparing hot-rolled and TIG welded material, *Materials Characterisation*, 190, (2022), 112044.

DOI: 10.1016/j.matchar.2022.112044

Funding: Vinnova, EIT RawMaterials EndureIT project, China Scholarship Council, Jernkontoret Forskningsstipendium.

Authors: J Liu, Y Das, RP Babu, J Odqvist, P Hedström (KTH Royal Institute of Technology), S Wessman (Swerim AB), JY Jonsson (Outokumpu Stainless AB) and SM King (ISIS)

A research adventure that led to a 'technically perfect' study

Multiferroic materials can exhibit both magnetic and ferroelectric properties at the same time. This unusual behaviour makes them subject to some remarkable physics, as well as candidates for future data storage materials.

Type-II multiferroicity, where there is strong coupling between the magnetic and ferroelectric properties, is of particular interest for data storage applications. However, most multiferroic materials only exhibit these properties simultaneously at very low temperatures. Now, a UK-Japanese collaboration has demonstrated that a simple material can become multiferroic at room temperature.

For the first time experimentally, single crystal neutron diffraction revealed that, by using high pressures, the two properties can be present at once at room temperature in the material CuO. Although it was predicted that the transition temperature above which the multiferroic phase of CuO exists could increase under pressure, the community was divided as to whether this was the case. As well as their experimental studies, the group developed a new model to describe the system that maps onto its real-life behaviour.

By being able to prove that multiferroic behaviour can be present at room temperature, this study opens a route to developing materials that could be used under the normal operating conditions of electronic devices.

Pascal Manuel, Noriki Terada and Dmitry Khalyavin on the WISH beamline.

> **"The paper was described as 'technically perfect' by the editor, which is a nice reward. It is a great example of how tenacity and believing in your ideas pays off in the long run. The study was a human adventure as well as an interesting piece of science."**
>
> Pascal Manuel, co-author and beamline scientist on WISH

Instrument: WISH

Related publication: Room-temperature type-II multiferroic phase induced by pressure in cupric oxide, *Physical Review Letters*, 129, (2022), 217601

DOI: 10.1103/PhysRevLett.129.217601

Funding: Japan Society for the Promotion of Science, Japan Science and Technology Agency, European Union Horizon 2020, Engineering and Physical Sciences Research Council, and University of Oxford-ShanghaiTech University collaboration project

Authors: N Terada, T Naka (National Institute for Materials Science, Japan), DD Khalyavin, P Manuel, F Orlandi, CJ Ridley (ISIS), CL Bull (ISIS, University of Edinburgh), R Ono (Italian Institute of Technology), I Solovyev (National Institute for Materials Science, Japan, Institute of Metal Physics, Russia, Ural Federal University), D Prabhakaran and AT Boothroyd (University of Oxford)

Using diffraction to understand the differences between healthy and diseased skin

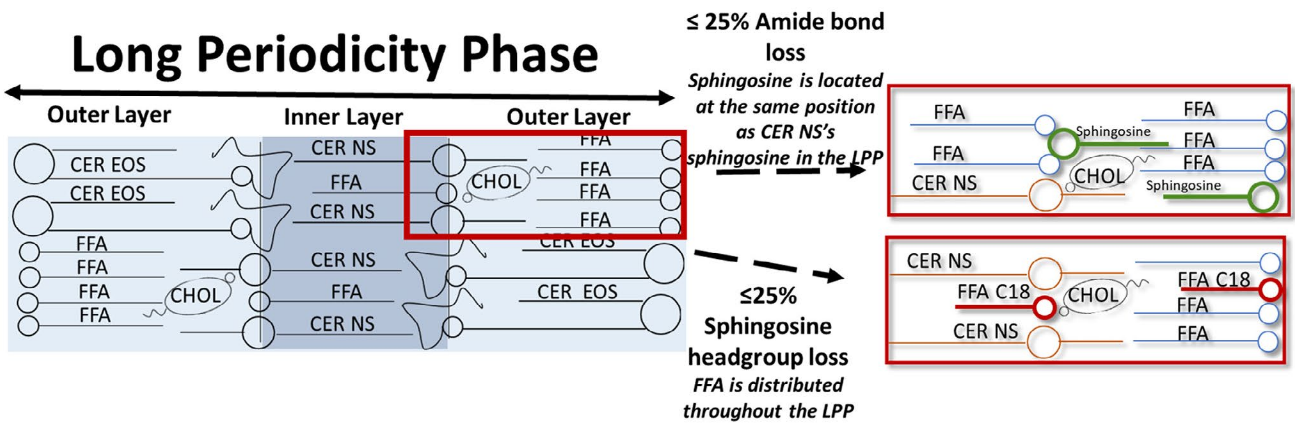
Our skin acts as a barrier between the inside of our body and the external environment. The outer later, the stratum corneum, is crucial to this function. It is made up of lipid bilayers arranged in an ordered matrix. Disruption to this matrix is a key contributor to skin diseases, and so understanding how this happens is key to learning how to treat them.

At ISIS, membranes are usually studied using reflectometry, where you can measure a single film in contact with water. However, in these recent studies, researchers from the Universities of Leiden and Manchester used neutron diffraction to study a model skin membrane with almost atomic resolution.

In the first experiment, the sample was supported on a silicon substrate and measured in a saturated water atmosphere. The sample itself was a spray coated film, hundreds of bilayers thick. These conditions allowed a precise measurement of the arrangement of the molecules in the system without the need for complex modelling.

By analysing the data from a series of samples with different levels of hydrogen and deuterium, the researchers could probe the structure of the membrane.

By measuring multiple samples in this way, the researchers found that the composition of the lipid played a significant part in the structure and therefore behaviour of the lipid matrix. By changing the lipid headgroup, they saw changes to the dispersion of particular lipids within the membrane, which disrupted the structure. This disruption could be a factor in certain types of skin diseases.



Schematic diagram of the lipid arrangement of the LPP both unmodified (left) and when under ≤25% amide bond loss, with the substitution of sphingosine (green) and FFA C24 (blue) with CER NS (top right). Or ≤25% sphingosine headgroup loss, with the substitution of FFA C18 (red) and FFA C24 (blue) with CER NS (bottom right).

Instrument: Larmor

Related publication 1: The importance of ceramide headgroup for lipid localisation in skin lipid models, *Biochimica et Biophysica Acta (BBA) – Biomembranes*, 1864, (2022), 183886

DOI: 10.1016/j.bbamem.2022.183886

Authors: CM Beddoes, GS Gooris, JA Bouwstra (University of Leiden), DJ Barlow, MJ Lawrence (University of Manchester), RM Dagliesh (ISIS), M Malfois (ALBA Synchrotron) and B Demé (Institut Laue-Langevin)

Related publication 2: Phytosphingosine ceramide mainly localizes in the central layer of the unique lamellar phase of skin lipid model systems, *Journal of Lipid Research*, 63, (2022), 100258

DOI: 10.1016/j.jlr.2022.100258

Authors: CM Beddoes, GS Gooris, JA Bouwstra (University of Leiden) DJ Barlow, MJ Lawrence (University of Manchester), RM Dalgliesh (ISIS), M Malfois (ALBA Synchrotron) and B Demé (Institut Laue-Langevin)

Funding: National Institutes of Health

Life under pressure

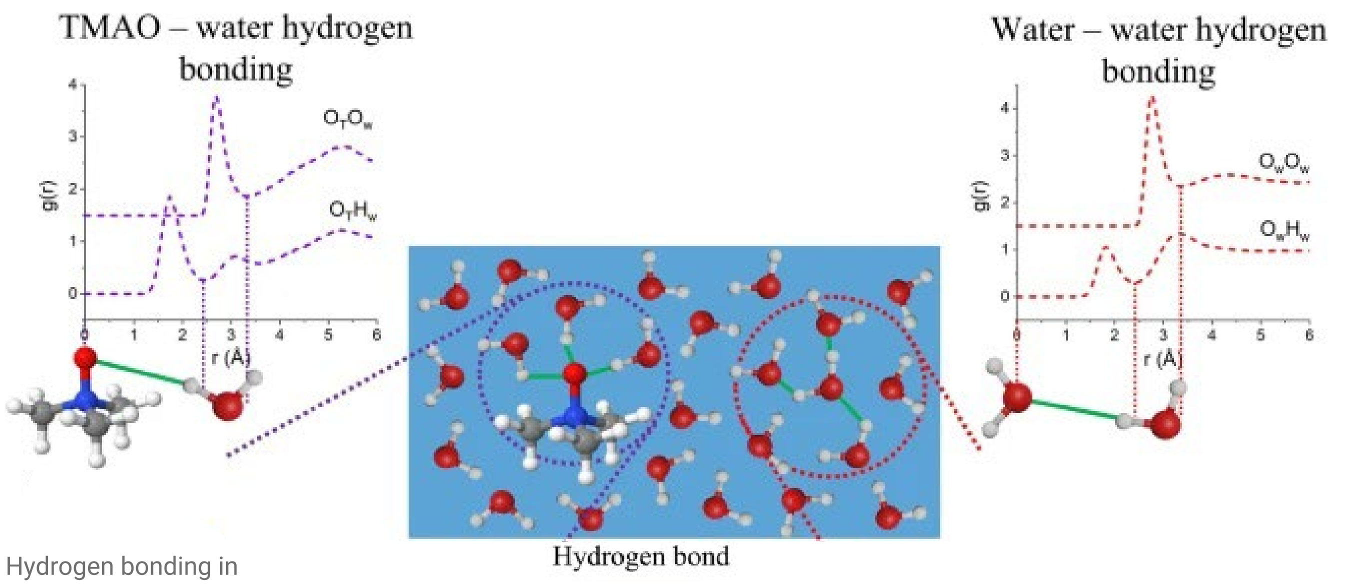
Extremophiles are organisms that can survive and thrive in extreme environments, enduring conditions such as high salinity, temperature and pressure. These organisms are found in habitats inhospitable for humans all over Earth, from boiling and acidic volcanic areas to the deep depths of the Mariana Trench. Biophysicists from the University of Leeds have been using neutrons to unravel the mechanisms behind survival under extreme pressures.

Extremophiles that have adapted to high pressures are known as piezophiles. An example of their adaptation is the ability to accumulate organic molecules that ensure stability within the cells by maintaining the fine balance of interactions between biomolecules, such as proteins and DNA, and water. If we know how these organisms survive at extreme pressure, we can apply these findings to our understanding of biomolecular stability in extreme conditions.

Previous studies show that organisms living under comparable pressures have similar levels of trimethylamine N-oxide (TMAO) within their cells.

Research has so far suggested that the TMAO molecule acts indirectly, meaning that it does not act on the biomolecule itself, but instead influences the water molecules surrounding the biomolecule. While scientists have previously explored how TMAO perturbs water structure and have studied the impact of high pressure on water structure, the potential competition between TMAO and pressure is not clear. If this combination of conditions is understood, scientists can develop their understanding of how life survives at extreme pressures, and particularly the role of TMAO on water and biomolecules.

A team from the University of Leeds investigated samples of pure water, and water with TMAO, at ambient pressure and at a pressure equivalent to 4000 times atmospheric pressure at sea level. Using neutron diffraction, computational modelling and a custom analysis developed by ISIS Facility Development student Dr Harrison Laurent, the researchers were able to build a 3D picture of the positions of the atoms within the sample, revealing the interactions between TMAO and water under pressure.



Hydrogen bonding in aqueous TMAO.

Instrument: NIMROD

Related publication: The ability of trimethylamine N-oxide to resist pressure induced perturbations to water structure, *Communications Chemistry*, 5, (2022), 116.

DOI: 10.1038/s42004-022-00726-z

Funding: EPSRC

Authors: H Laurent, L Dougan (University of Leeds), TGA Youngs, TF Headen and AK Soper (ISIS)

2023 Don McKenzie Paul Thesis: Dr Harrison Laurent, University of Leeds

Awarded by the Neutron Scattering Group, a joint Interest Group of the Institute of Physics and the Royal Society of Chemistry, in recognition of a successfully examined PhD thesis in which the use of neutrons plays a significant role in addressing a scientific challenge or describes notable development of neutron instrumentation or techniques.

“Harry is an exceptional scientist and on an upwards trajectory as a leader in neutron science."

Dr Laurent’s PhD supervisor, Professor Lorna Dougan, University of Leeds

Ionic liquids offer a new way of controlling protein aggregation

An international collaboration, led by Professor Antonio Benedetto from University College Dublin and University Roma Tre, studied the effect of ionic liquids on amyloid fibrils, finding that they can be used to tune their morphological and electrical properties.

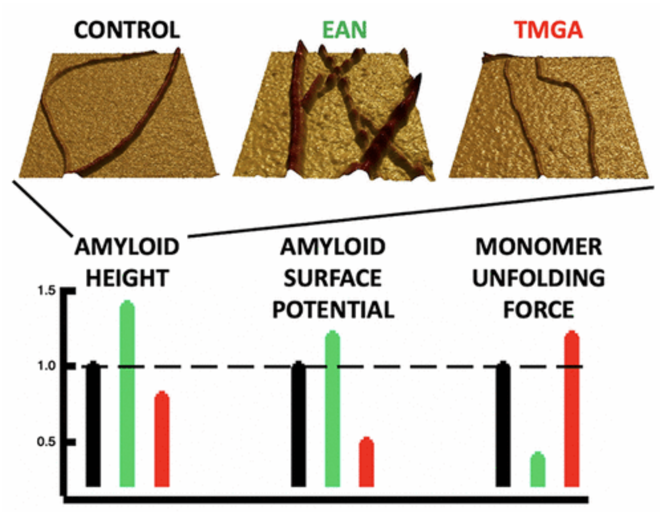
Amyloid fibrils are aggregated protein structures that are involved in many biological processes, but also observed in diseases such as Alzheimer's and Parkinson's. They can also be used in other applications, such as biomedicine and materials science. Controlling their formation could lead to new strategies against amyloid-based diseases, as well as new opportunities in material sciences and nanotechnology.

Previous studies have demonstrated that the ionic liquid ethylammonium nitrate (EAN) enhances the formation of amyloid fibrils by the protein lysozyme, while tetramethyl guanidinium acetate (TMGA) inhibits it. However, why this is the case was not known until now. By using a combination of atomic force microscopy (AFM), optical tweezers and neutron scattering, the group were able to conduct a comprehensive investigation into the effect of EAN and TMGA on the aggregation of lysozyme.

The unique ability of neutron scattering experiments to focus on selected hydrogen atoms by exchanging the other hydrogen atoms with deuterium atoms was exploited during their experiments. They discovered that the EAN interacts with the protein directly, whereas TMGA reacts with its solvation shell. They also observed that the presence of EAN leads to thicker amyloid fibrils, whereas the presence of TMGA leads to thinner ones. As well as this structural control, the presence of the different ionic liquids influences the surface electrical potential of the fibrils, which could result in differing interactions between the fibrils and surrounding biosystems or cells.

This ability for ionic liquids to control not only the morphology of the amyloid fibrils formed, but the way they interact, combined with the variety of ionic liquids available, offers up a whole new landscape of novel ways to use ionic liquids to influence fibril formation for advanced biomaterials. For example, by inhibiting the formation of pathological protein aggregates, they could lead to the formulation of novel effective therapeutics or, by controlling the mechanical properties of amyloid fibrils, they could be exploited in advanced biomaterials.

More information on the "Biophysics of Ionic Liquids" research carried out by the NanoBioPhysics Lab led by Prof Antonio Benedetto can be found at www.antoniobenedetto.eu



Atomic force microscopy has shown that the addition of EAN and TMGA leads to thicker and thinner amyloid fibrils of greater and lower electric potential, respectively, with diameters finely tunable by ionic liquid concentration.

Instruments: Tosca, Iris

Related publication: Controlling amyloid fibril properties via ionic liquids: the representative case of ethylammonium nitrate and tetramethylguanidinium acetate on the amyloidogenesis of lysozyme, *Journal of Physical Chemistry Letters*, 13, (2022), 7058–7064

DOI: 10.1021/acs.jpclett.2c01505

Funding: Science Foundation Ireland, Italian Ministry of University & Research, UCD School of Physics

Authors: VVS Pillai, P Kumari, S Kolagatla, BJ Rodriguez, M Rubini (University College Dublin), V Garcia Sakai, S Rudić (ISIS), KM Tych (University of Groningen) and A Benedetto (University College Dublin, University of Roma Tre, Paul Scherrer Institute)

Understanding how plant diseases cause damage

Plant diseases are common and can cause widespread damage to crops, making them a serious threat to global food supply. These diseases are spread by pathogens such as bacteria and fungi, which then secrete proteins that cause the damage to the host plants. Understanding the way that these proteins interact with the plant cells is key to developing ways to protect the plants from disease.

An international group of researchers focused on proteins known as NLPs (Necrosis and ethylene-inducing peptide 1 (Nep1)–like proteins), which affect a wide range of widely used crops such as potato, soybean, and tobacco. They used a range of biophysical approaches to study how these NLPs interact with the plant plasma membrane, the part of a plant cell that forms a selective barrier between the inside of the cell and the external environment. They looked at how NLP_{Pya}, from a common water mould, interacted with a model membrane made from tobacco leaf glycosylinositol phosphorylceramides (GIPCs). GIPCs have been identified through other studies as the part of the membrane that the NLPs bind to.

Using computational techniques, the researchers modelled how the NLP and GIPCs interact with one another, and then used neutron reflectometry to see if their simulations were correct. They also used a deuterated NLP version, so they could see it clearly within the hydrogen-rich membrane.

Their results showed that the NLP molecules form a layer on the outside of the membrane, rather than moving inside it. The GIPC-attached protein molecules may then interact with the surrounding GIPCs in the membrane, causing them to reorganise and cluster. This causes pores to form within the membrane, from which small molecules in the plant plasma leak out, harming the plant.

Membrane damage by formation of pores is a common way for bacteria to breach the integrity of animal cells but has rarely been seen in plants. The pathogens must have adapted in a way that means they can produce proteins with a structure that interacts with the specific components present in the membrane, releasing small molecules from the plant cytoplasm that boosts their nutrition. By understanding the way these pathogens break down the plant membranes, the researchers hope to open new ways to protect plants and maintain the security of global food production for our planet's future.

Instrument: Inter

Related publication: An oomycete NLP cytolysin forms transient small pores in lipid membranes, *Science Advances*, 8, (2022), 10,

DOI: 10.1126/sciadv.abj9406

Funding: Slovenian Research Agency, Japan Science and Technology Agency, Magnus Ehrnrooth foundation grant, Alfred Kordelin foundation grant, University of Helsinki, Faculty of Pharmacy.

Authors: K Pirc, T Snoj, M Srnko, J Borišek, M Podobnik, G Anderluh (National Institute of Chemistry, Slovenia), LA Clifton (ISIS), N Yilmaz, K Numata (RIKEN Center for Sustainable Resource Science), A Saltalamacchia (International School for Advanced Studies, Italy), M Mally, N Žnidaršič, J Derganc (University of Ljubljana), P Parkkila (University of Helsinki, Chalmers University of Technology), I Albert (Eberhard-Karls-University Tübingen, FAU Erlangen-Nuremberg), T Nürnberger (Eberhard-Karls-University Tübingen, University of Johannesburg), T Viitala (University of Helsinki), A Magistrato (International School for Advanced Studies, Italy, National Research Council Institute of Material, Italy) and JH Lakey (University of Newcastle)

Using neutrons to study self-assembling molecular water pipes

Water is one of the most common molecules found upon our planet. Yet, due to hydrogen bonding, it has some unique and complex physical properties, which are embedded into every aspect of life on Earth.

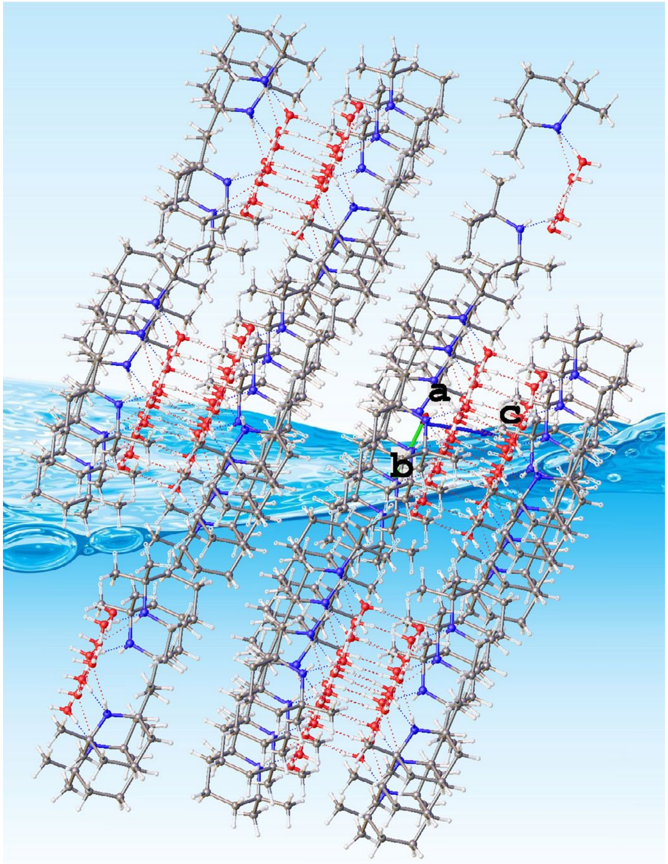
The transport of water through biological membranes has always been a water interaction that has generated a lot of interest. Internal membrane proteins, called aquaporins, transport the water at high speed via single file water wires. The possibility that certain materials can generate self-assembling molecular pipes, like those found in nature, has opened the possibility to engineer water channels for specific applications.

A team from Bangor University were investigating a material that consists of water and 2,2,6,6-tetramethylpiperidine (TMP) in an exact 2:1 ratio, which was found to self-assemble into a 3D structure with molecular water channels. To better understand the role of water and hydrogen bonding in assembling and stabilising the structure, single-crystal neutron diffraction was performed at 100 and 10 K. Data collected from this analysis revealed the positional disorder of the hydrogen atoms in the water molecules. It was observed that the layout of the TMP molecules creating a water channel was similar to other materials with artificial water channels but with a larger diameter.

In addition, inelastic neutron scattering (INS) spectroscopy on the TMP water adduct revealed that the structure consists of quartets of TMP water molecules stacked along the 'a' crystallographic axis, forming channels filled with pseudo-cubic octameric water clusters that are stacked face-on-face. These clusters are quite unusual to find within crystalline structures, especially in this arrangement.

The presence of these clusters in this new structure can help lead to a greater understanding and methods to improve the future design of artificial water pipes.

It is anticipated that this is just the first example of similar adducts that may have played a significant role in the evolution of life.



Structure of the water–TMP complex at 10 K from neutron-diffraction data, viewed down the 'a' crystallographic axis, showing the two water channels.

Instruments: SXD, Tosca

Related publication: The spontaneous self-assembly of a molecular water pipe in 3D space, *IUCrJ*, 9, (2022), 364-369

DOI: 10.1107/S2052252522003396

Funding: EPSRC

Authors: IR Butler, DM Evans (Bangor University), PN Horton, SJ Coles (University of Southampton), SF Parker and SC Capelli (ISIS)

Surprises found in combined diffraction and spectroscopy study

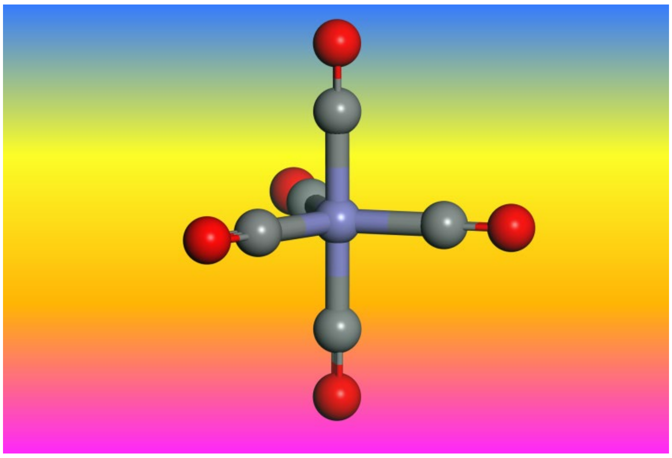
Using high-resolution neutron powder diffraction and neutron spectroscopy, ISIS scientists have been able to re-examine the structure and vibrational spectroscopy of iron pentacarbonyl, $Fe(CO)_5$, a compound which is extensively used in industry and inorganic synthesis. Unexpectedly, their results uncovered a new phase, and show that the true behaviour of the molecule differs from that predicted by computer modelling.

Although $Fe(CO)_5$ was the second metal carbonyl to be discovered, its unusual low symmetry means that aspects of its vibrational structure continues to be under investigation. A comprehensive investigation here examined both the structure and vibrations of the compound across a wide temperature range covering both the solid and liquid forms.

Firstly, by exploiting neutron diffraction on the HRPD instrument, HRPD Instrument Scientist Dominic Fortes and ISIS Catalysis Scientist Stewart Parker discovered a previously un-reported phase transition. This transition proved to be ferroelastic, thought to be the result of Van de Waals strain caused by the bond lengths shrinking on cooling. Then, using inelastic neutron scattering (INS), the team were able to observe all the internal modes of vibration in the molecule for the first time by exploiting the lack of selection rules for INS spectroscopy.

By combining their INS results with additional optical spectroscopy collected at the Research Complex at Harwell, they were able to correctly assign all the vibrational modes, finding that the previous literature was incorrect in multiple areas.

A bigger surprise was in store when the team went to compare their results to those calculated using Density Functional Theory (DFT). Previous studies of other metal hexacarbonyls showed excellent agreement with DFT calculations - this was not the case for $Fe(CO)_5$.



The structure of iron pentacarbonyl.

> **We still don't understand why the results differ from the DFT calculations. The accuracy of the molecular bond distances and angles was similar to that for the hexacarbonyls, but in this instance the calculations do not fit the results.**
>
> Stewart Parker, ISIS Catalysis Scientist and Molecular Spectroscopy Group Leader

Instruments: HRPD, Tosca

Related publication: Structure and spectroscopy of iron pentacarbonyl, $Fe(CO)_5$, *Journal of the American Chemical Society*, 144, (2022), 17376–17386.

DOI: 10.1021/jacs.2c01469

Funding: STFC

Authors: AD Fortes and SF Parker (ISIS)

Using neutron diffraction to investigate how solutes dissolve in solvents

When two or more chemical components are combined to produce a material with a lower melting point than any of the pure constituents, this is known as a eutectic mixture. Although first reported many years ago, their potential use as a more environmentally friendly alternative to volatile organic solvents has only quite recently gained attention.

Eutectic mixtures are now being explored in applications from extraction of active species from plants, through to carbon dioxide capture. However, the fundamental understanding of the physical chemistry of these deep eutectic solvent systems has not kept up with their use, which may be hindering their full potential.

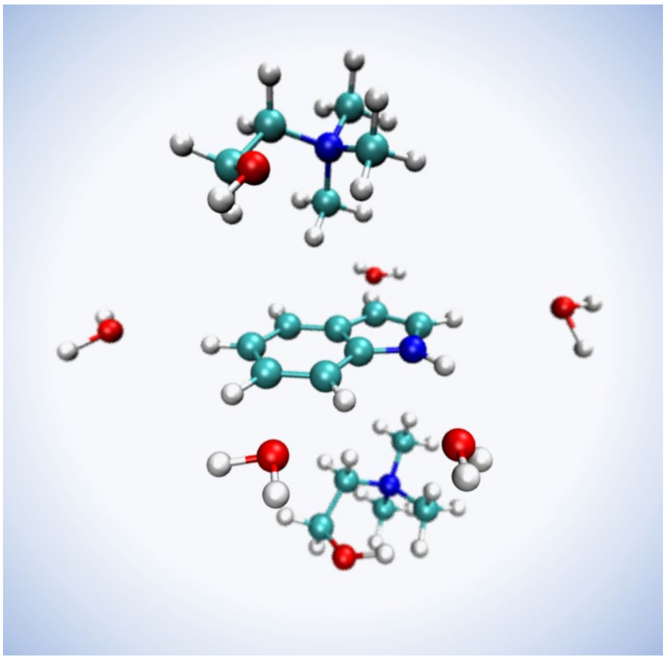
A team of researchers from the University of Bath and ISIS used neutron diffraction to investigate the mixture of the deep eutectic solvent formed by mixing choline chloride and malic acid with indole and water.

They chose this system as both components of the solvent can be naturally sourced and, separately, have been well characterised. Indole was used as a good proxy molecule for testing key aspects of biomolecule solvation and associated chemistry.

The aim was to understand how the indole is accommodated within the solvent environment and whether this was influenced by the presence of water. Through the isotopic labelling of samples (specifically exchanging hydrogen for deuterium), neutrons could be used to study specific interactions between different chemical sites to be resolved, which is a capability currently unique to neutron science.

By fitting empirical potential structure refinement models to their neutron diffraction data, the group were able to understand the interactions between the different components of the system. Multiple structural states were observed for the solvent, likely contributing to its reduced melting point. Interestingly, the interactions between the components of the solvent were not changed significantly when the indole was added.

Water normally prefers to occupy the spaces above and below the aromatic plane of the indole molecule, but in these deep eutectic mixtures, the solvent cation wins the game of musical chairs, and gets there first. Therefore, as more water is introduced, it is forced to take a worse seat, around the hydrophobic parts of the indole molecule, which is typically unfavourable. Their results not only provide an insight into this particular system and how it assembles but are also of interest to those studying the solvation of biological systems such as those present inside our cells.



Indole solvation in choline chloride: malic acid deep eutectic solvent forces water to interact with more hydrophobic parts of the molecule.

Instrument: NIMROD

Related publication: Neutron diffraction study of indole solvation in deep eutectic systems of choline chloride, malic acid, and water, *Chemistry – A European Journal,* 28, (2022), 41.

DOI: 10.1002/chem.202200566

Funding: EPSRC and STFC

Authors: OS Hammond (University of Bath, University of Stockholm), R Atri (University of Bath), DT Bowron (ISIS) and KJ Edler (University of Bath, Lund University).

Transcontinental testing of electronic chips

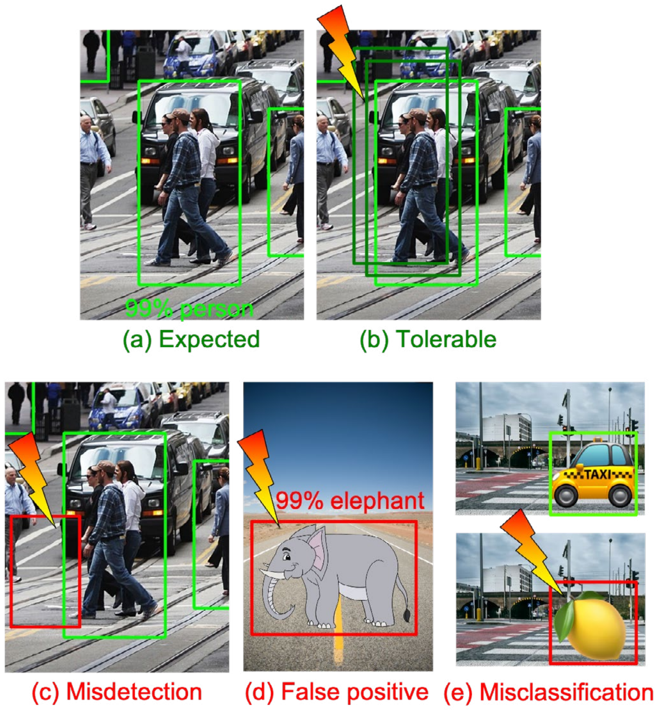
During a period of travel restrictions, researchers from Brazil and Italy were able to test the resilience of Graphics Processing Units (GPUs) and Tensor Processing Units (TPUs) through remote access to ISIS. Their research sought to understand the causes of Silent Data Corruptions (SDCs) and Detected Unrecoverable Errors (DUEs), and how a device could be adapted to mitigate these errors if they do happen.

During the COVID pandemic, travel restrictions meant that most of the experiments that took place at ISIS were led by staff, with the users being remote. For most instruments, the data are collected locally on the instrument's data acquisition system to allow for immediate diagnostics, as well as some initial analysis during the experiment. So, with the hands-on support of on-site staff and existing data connections, users were able to conduct many experiments remotely.

However, for ChipIr, which tests the resilience of electronics chips to atmospheric neutrons, the samples themselves are collecting large amounts of real time data whilst being bombarded by neutrons. Each requires constant monitoring, reprogramming, rebooting, power-cycling, and sometimes replacing if they fail completely. With multiple devices being tested at once, a typical experiment requires someone to be always present. By rethinking physical setup, data connections and methodologies, an international team were able to fully control the electronics remotely and simultaneously from their home institutions in Italy and Brazil, while the task of installing and managing the physical test set-up at ISIS was carried out by the ChipIr Group, which included industrial placement student Sujit Malde.

The group were able to study the sources of SDCs and DUEs in NVIDIA GPUs and Google TPUs executing artificial neural networks for object detection and other critical tasks. Using a virtual private network, the researchers could monitor and adjust the applications of the different GPUs and TPUs remotely, turn on and off the devices and perform power-cycling and reboots when needed. This allowed them to explore how the built-in error correcting code or the software error mitigation solutions they have designed were able to reduce the error rate in some instances, but not all.

Although experiments now see users return to the beamline cabin since restrictions were lifted, this method is likely to be used alongside an in-person presence to make future experiments easier and to widen access beyond those who can travel to ISIS.



Example of (a) expected output of a classification Deep Neural Network, (b) tolerable errors (more than 50% of the original object is still detected in the Bounding Box, (c) a misdetection (the existing object is not detected, thus reducing Recall), (d) a false positive (an un-existing object it identified, thus reducing Precision), and (e) a classification error.

Instrument: ChipIr

Related publication: Experimental findings on the sources of detected unrecoverable errors in GPUs, *IEEE Transactions on Nuclear Science*, 69, (2022), 436-443

DOI: 10.1109/TNS.2022.3141341

Funding: European Union Horizon 2020 and the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brazil

Authors: F Fernandes dos Santos, L Carro (Universidade Federal de Rio Grande do Sul), S Malde, C Cazzaniga, C Frost (ISIS) and P Rech (Politecnico di Torino)

Investigating hydration in ancient Egyptian leathers

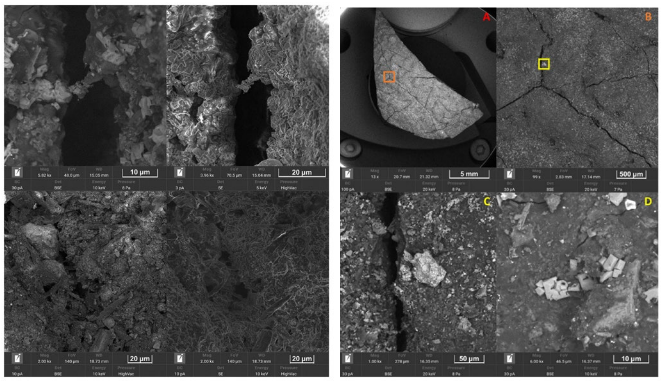
Studying organic ancient artefacts such as leather can tell us much about the history of the age it came from, as well as different conservation techniques through the millennia. The artefact will have been exposed to many outside influences throughout history that can impact on its structure and preservation, from curing processes to pollution. Researchers from the ISIS@MACH ITALIA collaboration used a variety of neutron and laboratory experiments to investigate these effects on a collection of Egyptian leathers dating from 2700 BC – 600 AD and uncovered information on the hydration levels.

A collection of various leather objects, including sandals and parts of stools, were brought over to ISIS from Museo Egizio, Turin. To gain a fingerprint of the molecules contained within each sample, the team used inelastic neutron scattering and built on this by measuring hydrogen levels using deep inelastic neutron scattering.

Using these techniques, they were able to compare the hydration levels of the collection to that of a highly hydrated and highly dehydrated control. Interestingly, each sample gave remarkably similar results, indicating that the whole collection has a shared/similar history, from the age it was created to how it was handled throughout history.

In addition to the neutron studies, the team also used surface techniques such as infrared spectroscopy, scanning electron microscopy and X-ray fluorescence These were available via the ISIS@MACH ITALIA Unit of the Universities of Roma Tor Vergata and Messina.

All these techniques played a role in determining how the surface of the samples may have been treated over time. This includes specific tanning and curing techniques that could have been used on the leather during their creation, or even the effect that pollution may have had on the artefacts. Currently, neutrons are not commonly used in these types of processes, but this fundamental study has shed light on how useful the techniques could be for future investigations.



(a) (b)

(a) SEM images of leather samples S1 (top) and S3 (bottom) obtained from back scattering (left) and secondary electrons (right). For each sample, the left and right panels correspond to the same region. (b) SEM images collected from sample S1 overall (A), magnification of the region delimited by the orange square (B) and two details in the region within the yellow square (C,D).

> **With some artefacts weighing less than eight milligrams, which is very small for neutron experimentation, we were proud to be able to test all of their samples. Combining both the ISIS experiments and the laboratory techniques will lead to improved methodology to learn about historical artifacts like these and how we treat them.**
>
> Giovanni Romanelli, Università degli Studi di Roma Tor Vergata

Instruments: Tosca, Vesuvio

Related publication: Neutron-enhanced information on the laboratory characterization of ancient Egyptian leathers: hydration and preservation status, *Information*, 13, (2022), 467

DOI: 10.3390/info13100467

Funding: Regione Lazio, Ministero dell'Università e della Ricerca and Consiglio Nazionale delle Ricerche.

Authors: G Romanelli, C Andreani, S Licoccia, E Preziosi, R Senesi (Università degli Studi di Roma "Tor Vergata"), E Ferraris, C Greco, V Turina (Museo Egizio di Torino), S Ikram, AJ Veldmeijer (The American University in Cairo), G Paladini, V Venuti (University of Messina), SF Parker (ISIS) and L Skinner (University of Southampton, University of Messina)

Meteorite or meteor-wrong?

The physical, chemical and mineralogical characterisation of meteorites is of paramount importance in the study of the formation of the solar system. An Italian research collaboration aimed to develop a new analytical protocol to investigate the elemental and mineralogical composition of meteorites and hence the formation of the solar system.

Research conducted by the team enabled them to establish a methodology to identify a meteorite and then classify and characterise it non-destructively. The first stage for the team to classify a sample as a meteorite was the detection of cosmogenic radionuclides, such as ^{26}Al, by means of γ-ray spectroscopy performed at Laboratori Nazionali del Gran Sasso (LNGS, Italy). Once the team had confirmed this, they could use neutron and muon techniques to study the composition of the bulk of the sample. In parallel, lab-based techniques, such as optical microscopy investigation, micro-Raman spectroscopy and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM/EDS), were applied in a complementary way. This innovative combination looked at the elemental and mineralogical phase composition, with particular attention to the crystallinity state of the phases.

The crystalline phases were characterised using neutron diffraction, and the combined results of diffraction on the bulk micro-Raman and SEM-EDS on a thin section provided a full mineralogical description of the meteorite. Using neutron resonance capture analysis (NRCA) and neutron resonance transmission imaging (NRTI), the researchers were able to determine some of the elements present in the meteorite, and its homogeneity on a millimetre scale. Thanks to muonic atom X-ray emission spectroscopy (μXES), they could quantify the weight ratio of the main elements in the sample.

This study proves that it is possible to identify a sample as being a meteorite and characterise the bulk of it non-destructively. The methodology will be used to study other meteorites belonging to museum collections as well as those that will arrive to Earth from space in the future.

The three samples from the same meteorite studied in this work: R001 and R002 are bulk samples, whereas R003 is a standard petrological thin section.

Instruments: Ines, RIKEN facility, MuX

Related publication: A new multidisciplinary non-destructive protocol for the analysis of stony meteorites: gamma spectroscopy, neutron and muon techniques supported by Raman spectroscopy and SEM-EDS, *Journal of Analytical Atomic Spectroscopy*, 38 (2023), 293-302

DOI: 10.1039/D2JA00263A

Funding: Consiglio Nazionale delle Ricerche, STFC, Laboratory STELLA (SubTErranean Low Level Assay) of the Laboratori Nazionali del Gran Sasso (LNGS) and the Cultural Heritage NET (CHNET) of the INFN

Authors: R Rossini (University of Milano-Bicocca, Milano-Bicocca Division - INFN, University of Pavia, ISIS), D Di Martino, G Gorini, M Clemenza (University of Milano-Bicocca, Milano-Bicocca Division - INFN), T Agoro, AD Hillier, A Scherillo (ISIS), M Cataldo, G Marcucci (University of Milano-Bicocca, Milano-Bicocca Division - INFN, ISIS), M Laubenstein (Laboratori Nazionali del Gran Sasso (LNGS) - INFN), M Musa (University of Milano-Bicocca) and MP Riccardi (University of Pavia)

World-class technology and infrastructure

With the UKRI's goal to be net zero by 2040, we have made significant strides at ISIS over the past 12 months in our efforts to minimise our own environmental impact. In this section, learn about our helium recovery system, Sustainability Network and other ways the facility is aiming to reduce its carbon footprint.

The Endeavour Programme – to deliver new instruments and significant instrument upgrades – was approved this year, and we continue to take forward plans for a next-generation facility, ISIS-II. Developments of the ISIS accelerator, target station and instrument suite, along with detector, sample environment and computing progress, all help to keep the facility at the forefront of accelerator-based neutron and muon sources.

Image left: Raheema Hafeji, former industrial placement student, working on a μRWELL detector.

Helium recovery at ISIS

Helium is critical for ISIS, as it enables the cooling of experimental samples to very low temperatures in our specialist sample environment (SE) equipment.

However, helium is a finite resource in need of preservation. In order to reduce our helium consumption, ISIS uses a helium recovery (HR) system. This allows us to recover helium used in experiments, store it and reuse it later on, thus reducing our dependence on external sources. This system has been in place for almost six years now. It began with a recovery rate of 50% but has become more efficient year on year and currently recovers over 90% of the helium used at ISIS. This is fantastic news as it means we do not need to obtain as much helium from diminishing natural sources. However, for a sustainably goaled process, helium recovery requires a lot of energy.

In a new study, members of the ISIS SE Cryogenics Group have calculated the carbon footprint of both our helium recovery process and the production process from the supplier. Considering the transportation and energy used in each process, it was calculated that 500 g of CO_2 is produced per liquid litre of helium (so the carbon footprint is 500g CO_2/l He). In comparison, the carbon footprint of the gas suppliers process is 712g CO_2/l He, making the output from our system 30% smaller. However, once the separation process from the supplier is taken into account, their carbon footprint dramatically increases to the point where our HR system footprint seems negligible at 99.02% smaller than that of the supplier.

Regardless of the comparison, the team are always looking for ways to improve this carbon footprint. Later this year the addition of a liquid nitrogen pre-cooler system will mean that the temperature of the incoming helium gas can be lowered to approximately -190 ℃ before liquification, resulting in a quicker liquefaction rate from 20 liquid litres per hour to 40 liquid litres per hour. Consequently, the energy required to power the process is halved to 1.036LHe/kWh with a subsequent reduction of 7.3 Tonnes CO_2e annually.

Helium recovery facility welcomes helium from Diamond Light Source. Left to right: Ken Jones, Adam Rankin (Diamond Light Source), Chris Lawson, Matt Baston, Dale Keeping and Richard Down (ISIS).

Related publication: Carbon footprint of helium recovery systems, *Low Temperature Physics*, 49, (2023), 967-970

DOI: 10.1063/10.0020164

Authors: AT Jones, RBE Down, CR Lawson, D Keeping and O Kirichek (ISIS)

Meet Skip Doran, Cryogenics Technician

Skip is a Cryogenic Technician, specialising In helium recovery. She works to recover, recycle and reuse all helium used on the ISIS site, implementing and managing the logistics and data of ISIS helium recovery.

How did your career as a technician kickstart?

I completed an Advanced Engineer Technician Apprenticeship at UK Atomic Energy Authority at the Culham Science Centre. This involved gaining practical experience and theoretical knowledge, working towards qualifications through academics, including an HND.

How did you first learn about ISIS?

I first learned about ISIS when I was in college. STFC did a presentation about the work at this site when advertising the apprenticeship. But I did not realise the true scale of all the work at ISIS until I started to work here.

What is a typical day like for you?

A typical day for me includes taking stock of all liquid cryogens, placing orders to replenish stock, monitoring information and data to manage stock, leaks, servicing, logistics, organising and doing movements of liquid helium orders. I manage the helium recovery system and complete dewar fills when required. I also work on projects, including ideas to help helium recovery and the Cryogenics Group, as well as outreach projects to inspire the younger generation about the amazing things science and engineering has taught us.

What do you enjoy the most?

Personally, I really enjoy managing the logistics and data about helium recovery. From collecting the data, I can show what an impact recovering helium makes to ISIS but also the environment. I can monitor where we have losses and ensure historical data is available to show how helium recovery has improved over the years.

What have been the main benefits so far of working at ISIS?

For me, it's having a supportive and caring team. Everyone in the Cryogenics Group has been lovely and it is a pleasure to work alongside them. I have been able to work on projects that were much needed in my team to improve efficiency and data recording. I have implemented new systems and documents so that we now have clear records of how much helium we are recovering, as well as being able to look at where losses have occurred.

Alongside data recording, I also produced an ordering system to not only aid in record keeping, but in easing and improving communication. This has been something that was much needed and has already made great improvements in its first month of use so far.

How would you encourage young people to get into the discipline you have chosen? What words of advice would you give someone hoping to make it into a career?

For me, going down the route of an apprenticeship allowed me to gain knowledge in both theory and practical skills. This was key in developing my career and finding the path I wanted to follow. I would advise young people to take every chance to learn something new as possible. You may find out something amazing and new, that you never even knew existed.

New cooling system for Target Station 2

The towers provide cooling for the accelerator, target and instrument systems associated with Target Station 2. They are five closed towers, providing a total cooling capacity in the region of 3.2 MW. They will be replaced with newer technology adiabatic coolers, which will maintain the operational requirements whilst significantly reducing the water consumed and the electricity required to operate the cooling system, by using modern energy efficient technology. The new cooling system will reduce water consumption by 6,000 m^3 per year and save 2,000 m^3 entering the RAL site wastewater system.

RIKEN solenoid to be replaced

ISIS is currently working to replace the existing RIKEN muon beamline superconducting solenoid magnet. The current solenoid relies on liquid helium at cryogenic temperatures to operate and this involves a helium compressor. Replacing the solenoid with a cryogen free system will reduce helium consumption and significantly reduce the electrical power consumption. In operation, each year the RIKEN solenoid creates 379 tonnes CO_2. It is calculated that this figure will reduce to 47 tonnes CO_2 per year.

Lowering our carbon footprint via our Waste Electrical and Electronic Equipment management

During 2021 and 2022 the combination of increased demand for new devices for working from home and a constant flow of staff with different user requirements called for the IT teams around site to think of new ways to manage the approximately 20 tonnes of Waste Electrical and Electronic Equipment (WEEE) that requires processing annually. The Facilities IT Team have been taking part in the new computer recycling scheme to try and work towards a greener future and disposing of the increased amount WEEE waste in a responsible manner.

Green machine has helped us dispose of over 10 tonnes of IT hardware, which is estimated to have lowered our carbon footprint by approximately 54,277 kilograms through the responsible reuse and recycling of WEEE waste generated by STFC.

This outcome will mean that we will be one step closer to meeting our sustainability goals and it will hopefully set a precedent to be more careful when disposing of WEEE waste.

Delivering sustainable software

The vision of the Research Software Engineering Group is to champion the adherence to modern software engineering standards while designing, developing and maintaining the cutting-edge scientific software tools at ISIS. Our mission is to deliver useful and maintainable software that enables and advances the world-class science research performed by ISIS staff and users. Below are some highlights of the currently on-going projects within the team.

Reflectometry: RAT/RasCAL

- Refactor existing RasCAL suite into computational backend and user-facing frontend
- Add comprehensive suite of automated tests
- Complete user and developer documentation

Molecular Spectroscopy: MDANSE

- Replace third-party code that is no longer supported with modern equivalents
- Cross-intergration with other scientific software

Disordered Materials: Dissolve

- Spiritual successor to EPSR software of the same name but written form scratch for larger and more complex systems
- Use modern development methods

ISIS Sustainability Network

The ISIS Sustainability Network (ISN) is set up and meeting on a regular basis with a remit to support, influence and challenge ISIS to embed sustainability in all our activities. Initial working groups are focussed on biodiversity, transport, energy, waste and LEAF (Laboratory Efficiency Assessment Framework). The ISIS Green Computing group will also report via the ISN. The ISN will be responsible for annual reporting on ISIS sustainability activities and developing the next generation of ISIS environmental sustainability strategy. The ISN will be focussing on our own operations but will also be looking to develop links and collaborations with other STFC sustainability network groups.

AAAS 2023

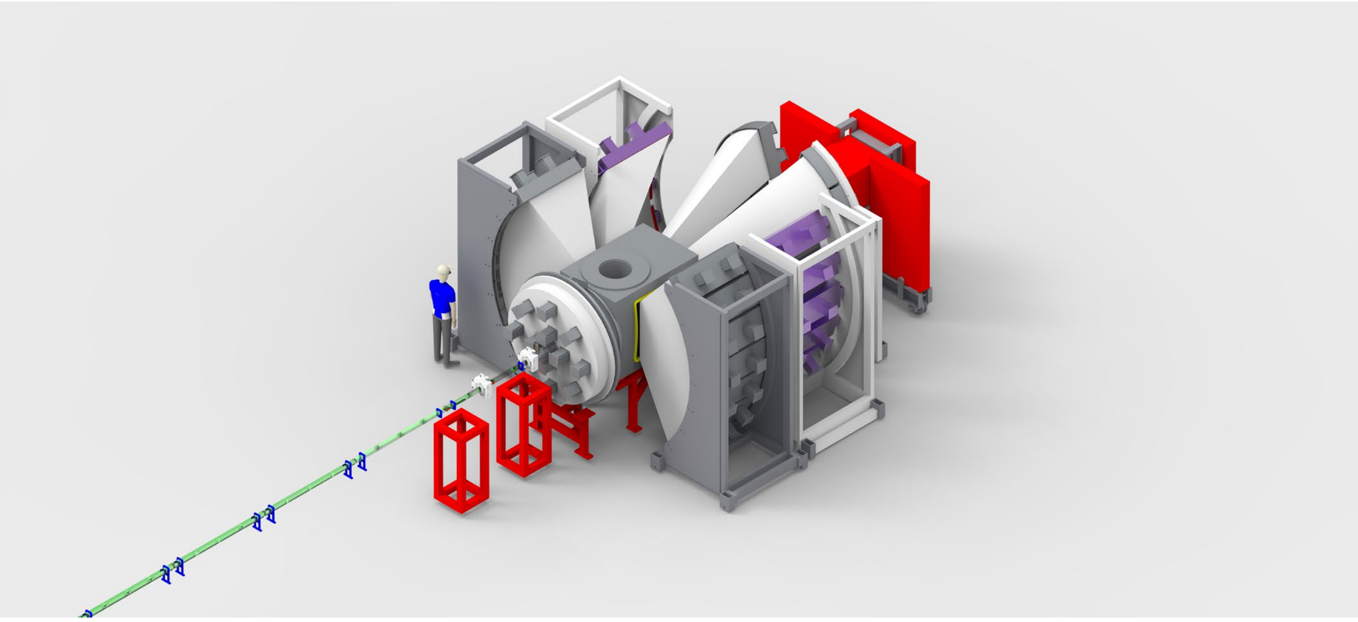
Representatives from ISIS attended the American Association of the Advancement of Science (AAAS) Annual Meeting on 3rd March in Washington, DC. This is a unique, interdisciplinary blend of more than 120 scientific sessions, attended by hundreds of people worldwide, so being allocated a session is highly competitive!

The theme of the meeting was 'Science for Humanity' and the ISIS science session focused on Clean Energy Storage. Our first speaker was ISIS scientist Professor Bill David, who explained the need for clean energy storage. Monash University's Dr Alexandr Simonov then highlighted the work of his group on an alternative, less energy intensive ammonia production to the Haber Bosh process. Our final speaker was Professor Serena Cussen from University of Sheffield who discussed developing sustainable battery technologies. Overall, the ISIS trip to AAAS was highly successful, and sets a high bar for future proposals.

Left image: ISIS experimental halls have now been covered with photovoltaics to help offset facility energy usage.

Endeavour: a £93M programme to supercharge the ISIS Neutron and Muon Source

Our Endeavour programme was officially launched in June 2023. It will enable the delivery of new instruments and significant instrument upgrades that ISIS will carry out over the next ten years. Nine projects are included – new instruments Mushroom, Wish-II, eMAP, LMX and upgrades to HRPD-X, SuperMuSR, Tosca+ and Sandals-II with a total programme cost of £93M.



HRPD-X is a significant upgrade to the existing high-resolution powder diffractometer, setting the benchmark for similar instruments worldwide.

The process to secure funding for Endeavour had taken around three years, but in May 2023 we heard that final approval was given by the UK Treasury, following business case reviews by UKRI and the government department, BEIS. Endeavour will increase ISIS capacity and capability, enabling our user base to explore new areas of science, including research in priority areas such as net zero, circular economy, hydrogen and healthcare. Through work such as this, Endeavour will expand the scope of our facility to attract global talent and further investment.

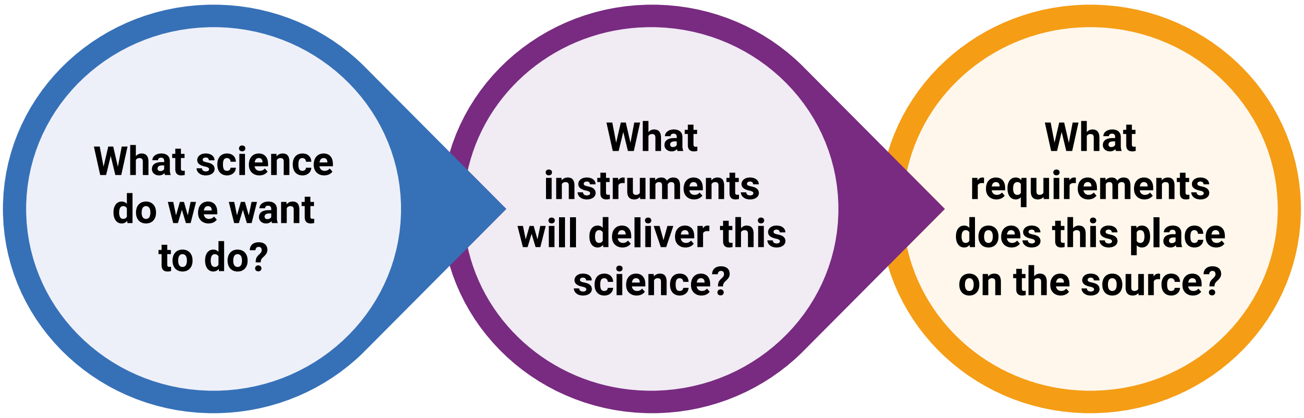
Two of the instrument projects have now been moved into full implementation: HRPD-X, a rebuild of the high-resolution powder diffractometer, and SuperMuSR, a development of the MuSR muon spectrometer. As these projects move to procurement and build, other instruments will be moved to implementation in a phased way over coming years.

Endeavour is mainly funded by the UKRI Infrastructure Fund and represents a major investment in ISIS and its science. It will also attract international collaboration and funding and will enable the training of next generation STEM workers (apprentices, graduates, year-in-industry students and PhD students).

> **Investment in critical research infrastructure such as this is essential to equip UK scientists to remain at the cutting edge of scientific progress and innovation, to address the ever-changing needs of society. Through Endeavour, STFC will facilitate new research that will play a key role in helping us to protect against threats from global health crises to climate change. It will provide UK researchers with world-leading tools to transform our understanding of new materials and chemical processes that will support the UK's ambitious science and technology strategy.**
>
> Professor Mark Thomson, STFC Executive Chair

ISIS-II: Designing the UK's next-generation neutron and muon source

ISIS-II is a project to explore and develop the design of a short-pulse neutron and muon source that is a suitable successor to ISIS. As Europe enters a neutron drought in the coming decade due to decommissioning of reactor-based sources, ISIS-II is expected to be a key player in neutron-based science and complement other European neutron facilities in the second half of the 21st century. Work on feasibility, design studies and R&D is currently underway.



The requirements for the facility are being driven by the scientific interests and needs of the ISIS user community. Some key parameters include smaller samples, enhanced complexity of materials and faster measurement capability. The instruments required for this science drive the parameters for the source. To deliver these requires not only a reliable, sustainable facility but also the supporting instrumentation and infrastructure.

The current phase of ISIS-II is supported by the UKRI Infrastructure Fund and is focused on the creation of high-level requirements, resource planning and environmental sustainability estimates as well as how these impact the design of the accelerators. Key design considerations include the match of the accelerator, target and moderator technologies.

With the front end based on the Front End Test Stand (FETS) project, accelerator options being considered for ISIS-II include:

- A low energy linac injecting into a Rapid Cycling Synchrotron (RCS) or Fixed-Field Alternating-gradient Accelerator to bunch compress and accelerate up to 1.2 GeV.
- A full energy linac (1.2 GeV) injecting into an accumulator ring (AR).
- A 180 MeV linac upgrade for injection into the present ISIS synchrotron.

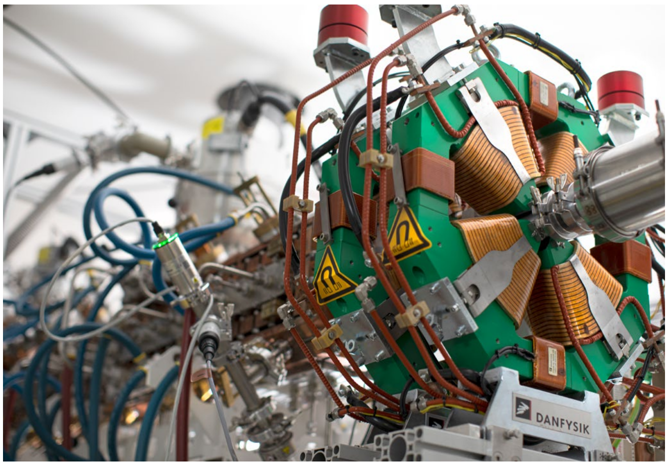
Examining siting and planning for the accelerator options is underway alongside identification of where long-term R&D and prototyping is required to establish feasibility. The proposal for ISIS-II will be developed over the next decade and the facility is expected to go into operation in the 2040s.

Front End Test Stand gets its first beam

Neutron sources of the future will need to be equipped with more powerful accelerators - a critical component of which is the 'front end', responsible for the first part of the acceleration process.

The Front End Test Stand (FETS) is a research and development project to build the front end of a linear accelerator to test new techniques, physics and other components. This could eventually feed into larger experiments and contribute to the development of future high-power accelerators, such as ISIS-II. The main component of FETS is the Radio Frequency Quadrupole (RFQ), a low energy accelerator designed to accelerate an H^- ion beam to 3 MeV with high efficiency and beam quality.

The first beam was successfully accelerated through the FETS RFQ on 26 March 2022. This was primarily an opportunity to perform surveys to assess the radiation levels produced as well as to check the safety systems and procedures;, a respectable 27 mA of H^- ion current was accelerated. Now operational, FETS is a valuable resource for ISIS staff to perform beam experiments and test new equipment, or possibly exploit the beam in other ways.



Part of the Front End Test Stand.

Medium Energy Beam Transport (MEBT) to improve efficiency of ISIS linac

Controlling beam loss is critical in high power accelerators as it reduces efficiency and causes activation of components, making maintenance harder. The addition of a Medium Energy Beam Transport (MEBT) will improve the efficiency of the ISIS linac by up to 30% by properly matching the beam from the Radio Frequency Quadrupole (RFQ) accelerator into the first tank of the drift-tube linac. The new MEBT will also provide a beam chopper that can allow the creation of pulsed beams with arbitrary time structures. The MEBT is currently being assembled on the pre-injector test stand where it will be soak-tested with the new Radio Frequency (RF) Volume Ion Source for a year before installation on ISIS in 2025.

For the last 40 years, the H^- beam for ISIS has been produced by a Penning surface plasma source. The lifetime of this type of ion source is fundamentally limited by sputtering and deposition - flaking processes that cause blockages and shorts. The source currently has an average lifetime of two weeks. The ion source relies on hot (500°C) caesiated surfaces that require daily tuning. Furthermore, ion source variability is a major source of machine instability and lost time during the user cycle.

The efficiency improvements provided by the MEBT reduces the beam current requirement on the ion source and opens the door to using a different type of ion source: an RF Volume Source. Employing permanent magnets to control the H^- volume production process and an RF drive coil positioned outside the ceramic plasma chamber makes this source effectively 'maintenance free'. It runs at room temperature, and therefore has no stability or start-up problems.

First beam was extracted from the RF Volume Source on the pre-injector test stand. Work is currently underway to integrate the spare ISIS RFQ on the test stand so that beam can be delivered to the MEBT for soak testing before installation on ISIS in 2025.

Image right: FETS team celebrating first beam being successfully accelerated through the FETS RFQ.

Muon accelerator opportunities

ISIS's accelerator scientists are coordinating the UK collaboration in a major new Horizon Europe project, led by CERN, to develop high-brightness muon beams. The four-year project, which started in March 2023, aims to design a radically different collider, based on muons, to follow on from the Large Hadron Collider when it finishes running around 2040. Muon beams can have a much greater science impact than electron or proton beams, but colliding muons is no mean feat. To study matter at the edge of our understanding, the accelerator team will need to produce an intense muon beam, accelerate it, and then compress it to a collision point just 1 micron across. This is hard enough, but it must all be done on the time scale of the muon lifetime, just 2 μs.

The UK team will look at challenges across the design of the facility but in particular, muon beam compression, which is needed to obtain the high brightness required of particle colliders. Novel target solutions will be designed to withstand the powerful proton beams required to produce a high muon current. This UK collaboration is also examining potential applications of these new technologies to the production of muons in ISIS and ISIS-II as well as other muon facilities worldwide.

New target manufacturing capabilities at ISIS

The target manufacture section within the Operations Group is responsible for manufacturing the targets used on Target Station 1 and Target Station 2 in-house. A variety of machines and equipment are used, from electron beam welders and ultrasonic polishers, to wire cutting and die sink electrical discharge machining.

By having in-house manufacturing capability, the ISIS Design Division can adjust target designs for each target we manufacture. It also means that the team are also able to feedback information from the manufacturing process to the design team which assists in future design decisions.

The hot isostatic pressing (HIP) is used in target manufacturing to obtain a diffusion bond between the tungsten core of the target and the tantalum cladding fitted around it.

As well as bonding dissimilar materials, HIP machines can also be used to increase the density of materials, remove porosity in 3D printed parts and increase the service life of components by removing material imperfections.

Installation of new muon collimator

The muon collimator is a critical component in the extracted proton beam just behind the muon target. It protects the quadrupoles from damage from the scattered proton beam. The collimator developed a major leak just before the last cycle before the long shutdown and without significant work to minimise the water losses, the muon target would not have been able to be inserted. However, a rapidly developed project was instigated, and the collimator has now been replaced.

Target Manufacturing Group, (left to right) Grace Fenemore, Micheal Hellier, Daniel Cross, Alan Prothero.

Full-time called on part-time DPhil for ISIS Group Leader Rob Williamson

Rob Williamson is Accelerator Physics Group leader at ISIS and has been researching for a DPhil with the John Adams Institute at the University of Oxford part-time. In June 2023, he successfully defended his thesis on beam instabilities encountered in high-intensity hadron accelerators and their impact on facility operations. Rob joined the ISIS Neutron and Muon Source as a graduate trainee in 2006, following an undergraduate MPhys degree at Trinity College, Oxford. He began research for a part-time DPhil in October 2014 whilst working full-time in a dual role: helping set up and operate the ISIS accelerators, alongside researching developments to improve operations and push the intensity frontier for new facilities such as ISIS-II.

Beam instabilities are a common and significant challenge to the operation of high-intensity hadron accelerators, particularly as they can drive beam-loss. To allow for regular hands-on maintenance of the machine, the beam loss and related radiation dose levels are carefully controlled and minimised. A key feature of beam instabilities is that their strength increases with beam intensity, thereby leading to an associated limit in the beam intensity achievable.

On the ISIS synchrotron, a head-tail type instability was identified soon after commissioning and was mitigated to a reasonable degree. However, as the accelerator was developed, the beam intensity achievable increased to such an extent that the instability became a hard limit due to the associated beam losses. Rob's research has measured and characterised the instability as a function of key beam and accelerator parameters in both normal operations and in a new operating mode: bunched beams stored at injection energy. Comparison of this extensive campaign of measurements with instability simulations and theoretical predictions provides essential tests of state-of-the-art models.

The thesis highlighted limitations in present theories and models, the development of which are important for the better performance of both current and future high-intensity hadron machines, not least ISIS and ISIS-II. The next steps following the thesis include pursuing studies to identify components that are driving the instability in the ISIS synchrotron, which is the focus of another DPhil being undertaken by another ISIS employee, David Posthuma de Boer. This naturally leads to possible cures, or at the very least focused mitigation for this particular instability. A prototype instability damping system has also been developed which successfully minimises unstable motion and associated beam-losses. Further work is planned to make this system dependable for consistent use throughout the user cycles.

> **I'd always wanted to pursue a PhD but thought that ship had already sailed when I started the graduate training scheme at RAL. However, when my colleague began his, I kept a close eye on what was involved and when the opportunity arose for me to start, I jumped at the chance.**

Rob Williamson (centre) with Prof Phil Burrows (left), internal examiner and Dr Elias Métral (right) from CERN, external examiner.

Reflectometer developments for Inter and Surf

Inter on Target Station 2 is currently being rebuilt with a new detector tank, detector and motion control system. The upgraded instrument is scheduled to take beam in late 2023, during which extensive commissioning will be undertaken.

Surf on Target Station 1 is also being rebuilt, with a new mirror guide tank installed before the sample position. The instrument will be ready to take beam in late 2023 but full commissioning will only be possible when we have a working hydrogen moderator on Target Station 1 in early 2024.

Osiris silicon analyser upgrade

Osiris is currently being upgraded with the addition of a silicon analyser. The current pyrolitic graphite analysers (PGA) provide a maximum spectral resolution of about 25 μeV at the elastic line, enabling access to relaxation times up to 140 ps. Using the (111) reflection plane of a silicon analyser, Osiris will extend these timescales to ca. 400 ps as a result of an improvement in spectral resolution by a factor of 2.5 (resolution of 11 μeV). The solid angle of the silicon analyser is about 2 sr and hence will be almost twice the present one. An inherent advantage of the silicon analyser is that the increase in spectral resolution does not affect the wide momentum-transfer range currently available on the instrument. Moreover, the use of position-sensitive detector technology will also enable access to four-dimensional data sets, of particular relevance to single-crystal studies of quantum materials, a new feature of the instrument.

Degrading Emu!

A small project with a big impact! A simulation of the Emu spectrometer revealed that the inclusion of degraders could improve the data quality, and so new degraders were procured and installed. We have seen a significant improvement in the muons signal – the initial asymmetry of the muon polarisation – without affecting the muon spot size.

RIKEN-RAL Muon Facility refurbishment

The RIKEN-RAL refurbishment, a £3.5M project, was completed during the ISIS long shutdown. The RIKEN-RAL beamlines are about 35 years old, and this was the major intervention that will ensure the future of these beamlines. The work consisted of replacing the magnet cooling water circuits, magnet power supplies, vacuum pumps, shielding (to allow for better access during a breakdown or service) and refurbishment of the sample environment (flow cryostats and He-4 systems). A new cryostat has been purchased (the same as the south side muon cryostats that will have two sample sticks, He-3 insert and a dilution insert). The instruments detector systems have been refurbished as well. The initial retuning of the RIKEN beamlines has shown a substantial increase in flux.

New windows for SANS2D

Work has continued to re-engineer the windows at the front of the SANS2D guide. The changes require the installation of a new, clamped sapphire window to replace the existing glued silicon window. This will improve the reliability of the guide system and ensure that the likelihood of window failure is radically reduced. The new windows and mountings are currently undergoing stress testing to ensure that they meet the predicted performance.

Sandals upgrade

Sandals underwent a major upgrade during the long shutdown of ISIS in 2021-2022, with a full rebuild of its front end. Incident flux has been doubled by increasing the instrument's view of the moderator, with count rates on standard flat-plate samples now 2.5 times higher. Backgrounds have been lowered and signal-to-noise improved by the addition of a 50 Hz frame-overlap chopper and a new fully-evacuated primary shutter. Beamline logistics and flexibility have also been enhanced through the addition of three sets of collimating and beam-defining motorised jaws, including an additional pair of incident beam monitors.

Image right: Matthew Krzystyniak (ISIS) working at Vesuvio.

Vesuvio - planning for the future

The programme of work to prepare the ground for an entirely new epithermal neutron spectrometer, Etna, is underway, using Vesuvio as a test bed. Novel data acquisition electronics (DAE) for the yttrium-aluminium-perovskite (YAP) gamma detectors, which are used to detect neutrons in forward scattering on Vesuvio, will be installed. The count rate of the YAP detectors will be increased by detecting gamma emission of the gold resonant analyser foils installed on Vesuvio to select the energy of scattered neutrons within the range of 100-300 keV. Simultaneously, by vetoing gamma emission in the energy window outside the 100–300 keV range, a great deal of suppression of unwanted background signals from the instrument blockhouse can be achieved. Moreover, the novel DAE will enable recording two-dimensional spectra (as a function of both neutron time-of-flight and gamma energy) for concurrent high-sensitivity neutron and gamma spectroscopic measurements in the future.

Larmor spin-echo improvements

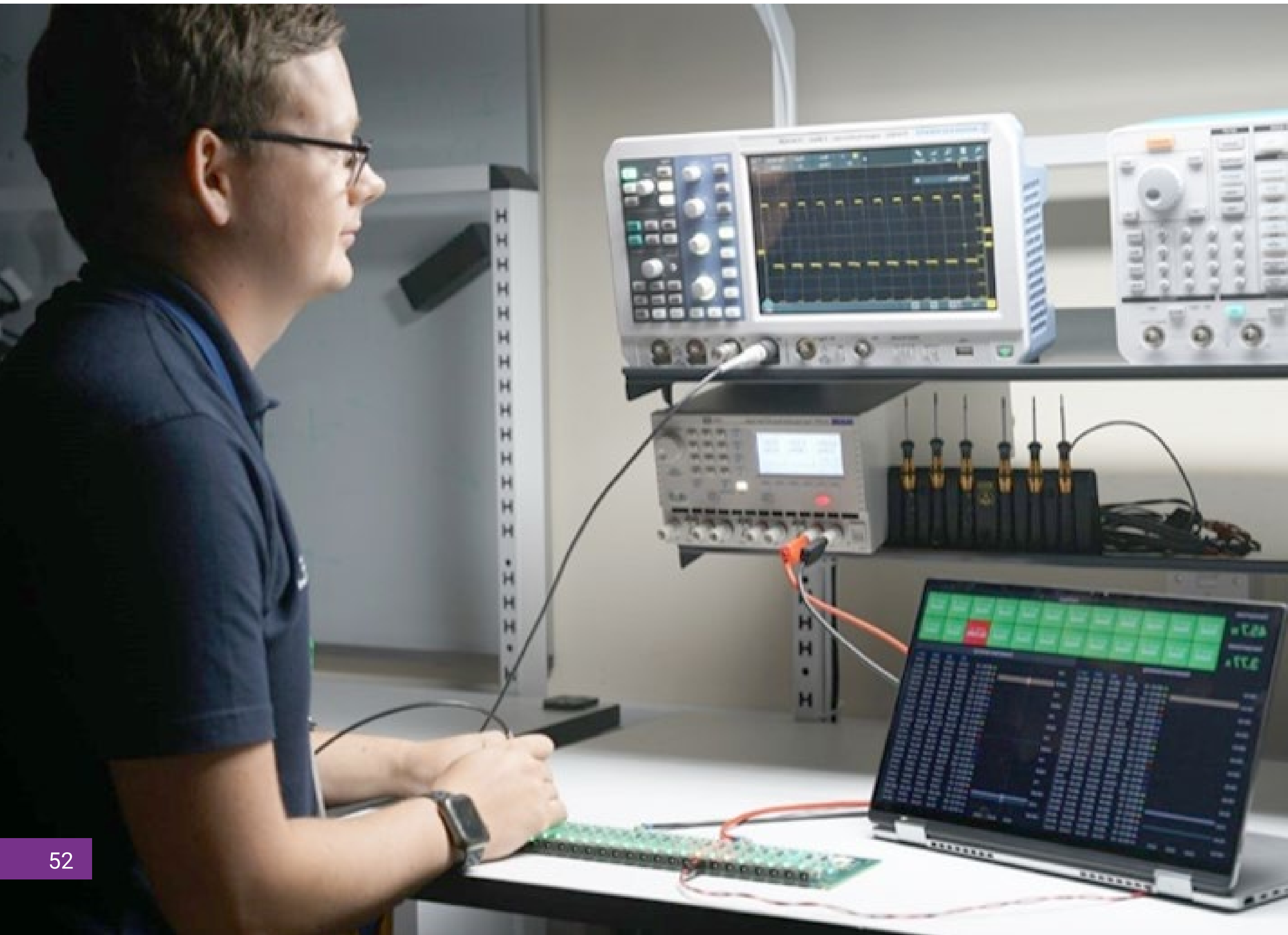
The Larmor neutron spin-echo system was recommissioned throughout 2022-2023 with re-engineered components to aid performance and reproducibility. The system is now significantly more stable and available for routine use. The highest length scale setting of the instrument has also been successfully tested and is now achieving the spin-echo SANS (SESANS) record of 35 microns. The instrument team are now working to improve usability and data analysis software, in addition to continuing to develop new sample environment equipment that is compatible with the precessing neutron beam.

Detectors for SuperMuSR

A prototype 'detector stave' for the SuperMuSR instrument, part of the Endeavour Programme, has been successfully tested using muons. Developed with industrial partners and RAL Technology, the detector system will be the first major deployment at ISIS of photon sensors know as silicon photomultipliers. A novel control mechanism has been developed, a 'serpentine heater', which keeps the sensor's temperature stable to a fraction of a percent. The full detector will have almost one thousand scintillator elements in a compact cylindrical geometry and is one of the first detector systems to be developed for Endeavour.

A new type of ^{3}He gas detector

A significant amount of development has been carried out on a new ^{3}He-containing micro-pattern gas detector called the μRWELL. The Detector Systems Group has built on the success of the high-energy physics community to produce the first neutron-sensitive μRWELL detectors using a mixture of ^{3}He and CF_4 (a gas used to increase the position resolution of the detector). So far, high neutron detection efficiency, the possibility of obtaining 0.5 mm position resolution and count rates better than 100,000 neutrons per second per cm^2, have been demonstrated. These new detectors could have many applications, including SANS, reflectometry and imaging.

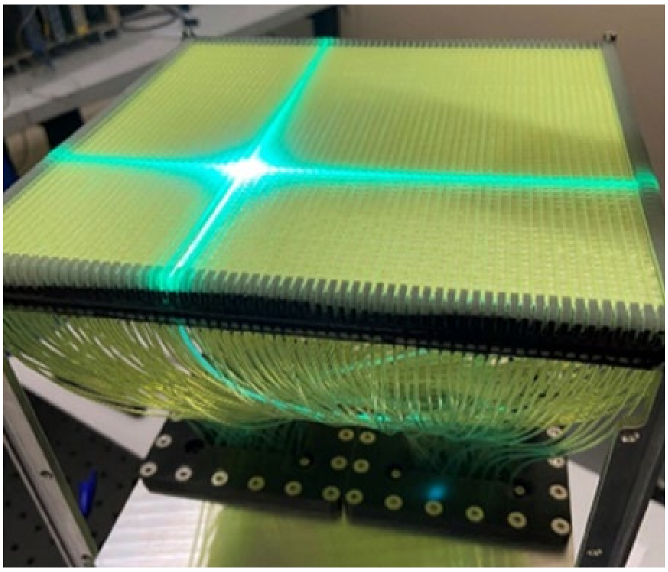


New neutron detector systems for SXD and Inter

Major detector systems were delivered to both SXD and Inter this year following extensive development programmes based on ZnS:Ag/^{6}LiF scintillators and wavelength shifting fibre (WLSF) light collection. The new SXD system has a detection efficiency of over 75% for thermal neutrons, more than a factor of 3.5 improvement on the current detectors with even larger gains for shorter wavelengths. As a result, the entire detector suite will be replaced on SXD, serving as a blueprint for future 2D detector needs such as LMX and WISH-2.

The new detector for Inter uses the same detector technology but adapted to meet the different requirements for neutron reflectometry. This detector can achieve neutron count rates 16 times higher than Inter's previous detector due to its unique geometry, optimised light collection and signal processing. In addition, the detector is the first WLSF detector to operate in vacuum, reducing the neutron background. These performance improvements should give an order of magnitude enhancement of Inter's signal to noise ratio.

The team are continuing to investigate data streaming directly to a PC as a successor to currently used DAE-II and DAE-3 systems, eliminating the need for additional detector cards. Maps and PolRef have been configured to run data streaming in parallel with their existing DAE electronics. Once operational, data streaming will enable sample environment information to be seamlessly integrated into the detector data, enabling new types of experiments.



2D WLSF based neutron detector for single crystal diffraction with a blue laser shining on one pixel.

Image left: Jack Day testing a new 12V distribution board and its web interface for use on future WLSF detectors including IMAT, Inter, SXD and Endeavour Programme Instruments.

Additive manufacture for soft matter

Soft matter encompasses a wide range of substances such as polymers, surfactants (including detergents), liquid crystals, micelles (clumps of polar molecules), and microemulsions. All of these share the same basic properties – weak interactions between structural units and large numbers of ways to arrange themselves internally. Characterisation requires information over a wide range of microscopic distances and timescales to control practical effects such as rubber elasticity, detergency, stickiness, and lubrication.

The Soft Matter Group within our Sample Environment Group regularly design and build specialist experimental setups which allow users precise control of a variety of parameters. Additive manufacture for engineering components has enabled them to create devices which would be extremely challenging to make using traditional machining methods.

Devices produced by this method include a humidity cell designed by Xiao Wang (Mechanical Development Engineer), and the Delft Furnace modifications, worked on by Harry Oliver (Soft Matter Sample Environment Technician). The existing furnace was originally developed and manufactured by TU Delft. The desire was to further develop this design to allow more, different samples to be used in this tightly made assembly. Harry from the Soft Matter Group collaborated with the Delft Group to produce a sample holder which can hold a sample of 12.5mm diameter and 300 microns thick, 3D printed from boron nitride which is an excellent thermal insulator and can withstand temperatures in excess of 2000℃.

The ISIS Soft Matter Group consists of four technical experts who continuously develop our offering to the science community, whilst simultaneously providing frontline support to the experimental programme. The team have benefited from the ISIS apprentice programme: two technicians in the team are a result of this scheme.

Development of an automatic cryostat controller

A considerable proportion of experiments at ISIS require some sort of cryogenic sample environment. A popular option is the legendary 'Orange Cryostat,' originally designed by the Institut Laue-Langevin in Grenoble. Temperature is controlled through balance between heating and cooling. Heating is provided by an electrical heater; cooling is provided via a cryogenic needle valve which directly controls the flow of helium being evaporated in the cryostat's heat exchanger.

Historically at ISIS, users have enjoyed automated control of the heating; however, the cooling circuit has always been controlled manually. There are many situations where automatic control of heating and cooling, in combination, would be advantageous. This is not as simple as it may seem as it requires a correct balance between the heating and cooling control loops. To achieve this full cryostat control, a controllable cryogenic needle valve was designed and installed on all 15 Orange Cryostats. A controller was then developed to both drive the cryogenic needle valve and measure all relevant control variables. Lastly, an algorithm to interpret all these parameters was created and refined, allowing a user to simply enter a required temperature and have the Orange Cryostat go there directly without further interaction.

This is a new capability for the Orange Cryostats at ISIS. It offers easier access to cryogenics for users with less experience in that area, as well as improving cryostat operational efficiency.

Image right: Jonathan Timms of the ISIS Cryogenics Group guiding the lowering of 3D magnet from an overhead crane into the supports in order to diagnose a fault and conduct the repair.

Humidity cell assembled for leak checking and wiring

A humidity cell has been developed using advanced additive manufacturing techniques. The bulk of work in SANS involves a humidity range of 20 to ~90%, which may be provided by saturated salt solutions and simple humid air pumping systems. There are, however, some systems, such as fuel cell membranes, which require a range of 0-100%. Changing the deuteration level of the humid atmosphere is also required. Current cells can take several hours to equilibrate following a change of humidity or deuteration level; cells able to accommodate much faster changes are needed for SANS measurements, with automatic control of humidity, deuteration level and temperature.

The newly-developed humidity chamber is currently on track for leak testing and wiring. It will then undergo testing in a live instrument to confirm its behaviour with neutrons. The Soft Matter Group are also actively sharing their experience in this development with other facilities, such as the ESS.

Repair of the 3D magnet

The 3D magnet is a critical piece of sample environment, which sees heavy use on the SANS beamlines in particular. The magnet features a nested set of three superconducting coils which provide a 2T magnetic field in any direction. The coils are cooled by a recondensing helium cryostat, which also provides a sample space with temperatures from 1.8K to 300K. The control of this variable temperature sample space is given by an electrical heater, buried right at the centre of the cryostat.

This heater suffered a complete failure and needed to be replaced. This alone is a challenging operation (requiring the total disassembly of an almost 1-ton magnet) but additional steps were taken to provide resilience to the magnet by installing a spare heater, along with new capillary-unblocking heaters which have the potential to quickly resolve blockages in the cryogenic system and thus save experiments.

The Cryogenic and Electrical experts at ISIS were critical in the delivery of this project. The next upgrade of this magnet will be the installation of superconducting wiring for the cryostat's temperature control. Superconducting wires conduct heat poorly (which is advantageous in this situation), whilst simultaneously allowing for much higher currents than resistive wires.

Raman scattering for diffraction

HRPD's combined Raman scattering and neutron powder diffraction system has entered the user programme. The system focuses a laser onto a sample directly adjacent to the sample in the neutron beam (and therefore under the same environmental conditions) and then collects the scattered light. The system has undergone extensive commissioning on HRPD as part of a Facility Development Studentship held jointly between Diamond Light Source and the University of Exeter. Student Johannes Meusburger used the system to characterise the phase transitions in calcium nitrate. More recently, the system has been adapted for use with single crystals and been commissioned on the instrument SXD as part of another Facility Development studentship; Sarah Dugdale (Keele University) has employed the technique to study photochromic and thermochromic crystals as a function of temperature.

Deuteration for Neutron Scattering Meeting

The fourth Deuteration for Neutron Scattering Meeting was a huge success, attracting over 60 participants from the UK, US, Sweden and France. The meeting took place at Milton Hill House and ran from 26-27 September 2022.

Birthday celebrations were also in order for Professor Bob Thomas, who celebrated his "80th-plus-one" birthday at the meeting. Professor Thomas is a pioneer in the development of neutron scattering and reflectivity techniques and instrumental in the Oxford Isotopic facility establishment, which is now the ISIS Deuteration Facility.

The Deuteration for Neutron Scattering Meeting is held every 18-24 months and will next be held in 2024.

Sample environment for Small-Angle Neutron Scattering (SANS)

Size-exclusion chromatography is a size-based separation technique that, when used in-line on SANS instruments (SEC-SANS), ensures samples flow directly from a SEC column into a SANS measuring cell, allowing the separation of polydisperse mixtures and determination of the solution structure of monodisperse samples. SEC-SANS, in conjunction with contrast matching and deuteration, allows the investigation of protein complexes, multiprotein assemblies, or protein-DNA/RNA complexes. Other SANS developments this year include *in situ* LED-illumination and temperature-controlled cells for the study of the structure of thylakoids in cyanobacteria and photoactivable soft matter; and levitation-SANS.

High temperature, high pressure gas handling for QENS

A remarkably high temperature and high pressure *in situ* gas handling cell has been developed for Osiris. The stainless steel *in situ* cell has works within the furnace, with temperatures up to 800ºC and 10 bar. The design allows gas flow from the bottom of the cell to maintain the sample in a gaseous environment under fixed conditions of temperature and constant pressure. This cell has been used to investigate, in *operando*, the dynamics of hydrogen (H_2) on Ru-doped polar MgO surface using quasi-elastic neutron spectroscopy (QENS). As H_2 diffusion in extreme *operando* condition is important in other similar catalytic surfaces, as well as H_2 storage materials and fuel cells, this sample container can be used in future studies.

Cool science

Our Ultra Low Temperature (ULT) science program is returning to the pre-COVID level. Over the five 2022 cycles, 38 ULT experiments were delivered. In only the first two cycles of 2023, 23 ULT experiments were delivered, putting us on track to deliver around 60 ULT this year.

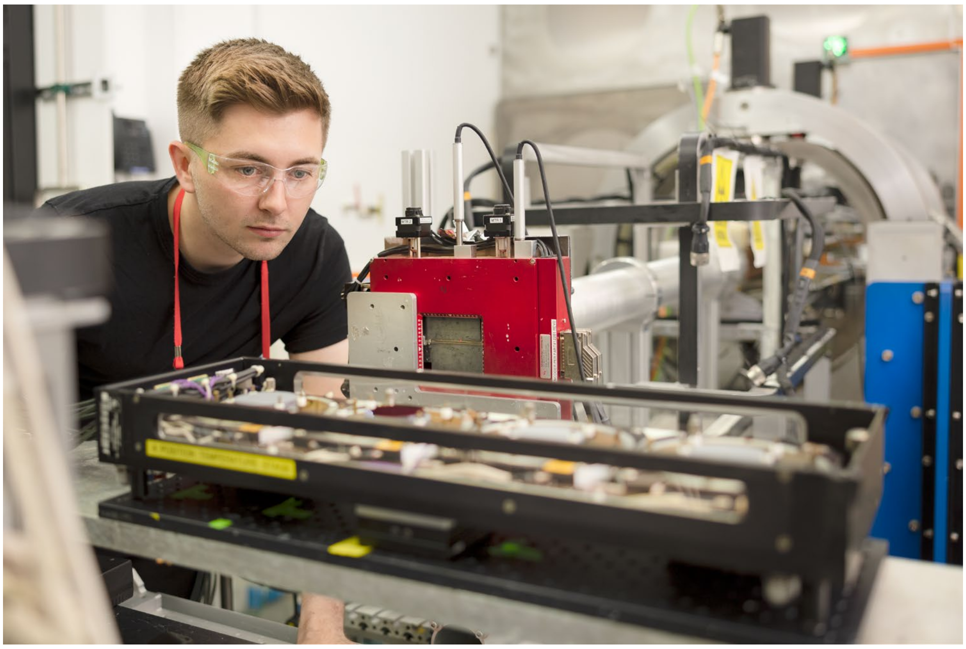


Image left: Najet Mahmoudi (ISIS) using new sample environment equipment on SANS2D. Image above: Callum Bannister (University of Durham) studying the influence of cure conditions on barrier properties and interface of epoxy coatings.

Cybersecurity

A new cybersecurity officer joined ISIS in late 2022 to help establish a robust cybersecurity culture within the department. A comprehensive gap analysis has identified the strengths, weaknesses, and areas for improvement within ISIS. Based on these findings, a cybersecurity strategy and roadmap has been developed to shape the role of cybersecurity in the department over the next few years.

Looking ahead, the department has set ambitious goals for the future. One of these goals is to achieve the Cyber Assessment Framework, aligned with the requirements set by the UK Government. This framework will serve as a benchmark for measuring and improving the department and organisation cybersecurity posture.

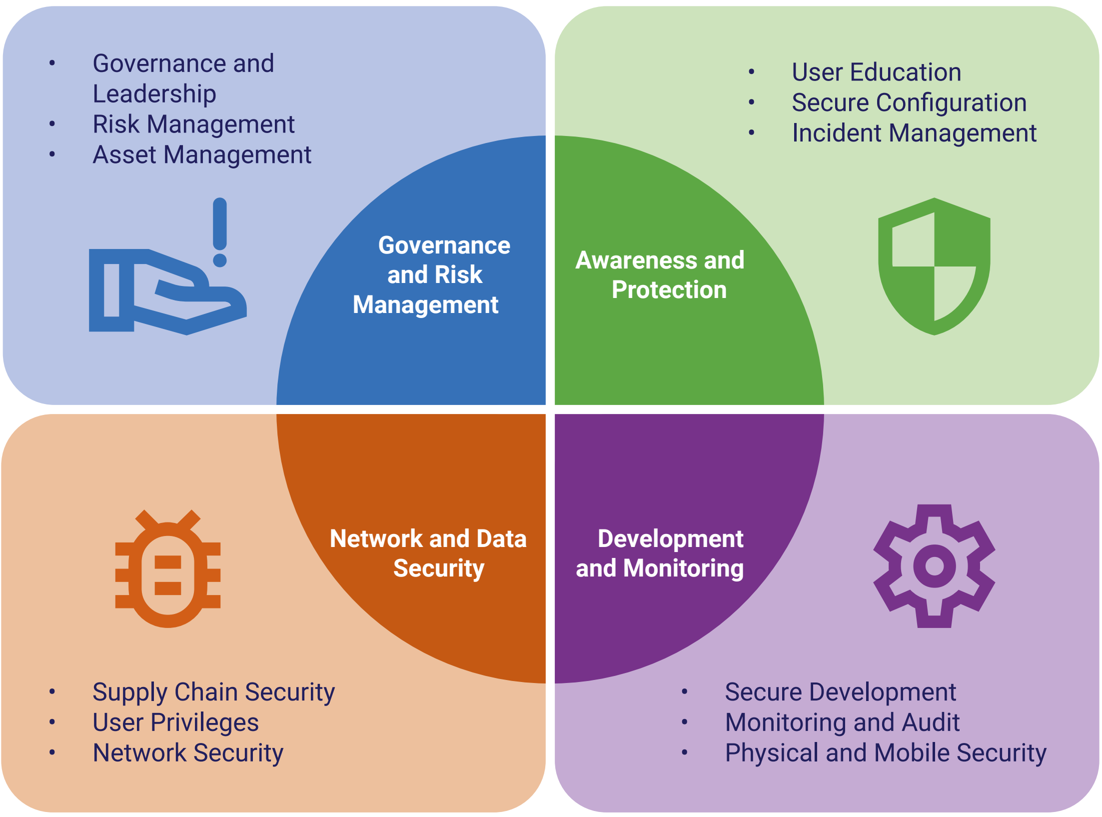
New virtualisation infrastructure

Our existing virtualisation cluster and underlying storage infrastructure was approaching end of life, having been in service since 2016, and needed to be replaced.

Two new virtualisation clusters, together with associated storage and networking upgrades, were successfully delivered, providing the significant increase in both compute and storage capacity, with all existing virtual systems migrated across without downtime or service interruption. This was especially important given that numerous services critical to delivering the ISIS user program, such as the ISIS User Office and Proposal systems, are hosted on this platform.

These new virtualisation clusters will support business and scientific workloads for ISIS and the wider National Labs until the end of the decade.

NCSC Cyber Assessment Framework



The Cyber Assessment Framework offers a structured approach to evaluating an organization's cybersecurity practices, controls and identifying areas for improvement.

Streamlining Mantid with Conda-based packaging

Members of the Data Reduction team, part of the Scientific Software Group (Left to right: Gemma Guest, Tom Hampson, Jonathan Haigh) ensemble programming on Mantid.

Mantid, the core software framework for data reduction, analysis, and visualisation of ISIS data, has recently undergone a significant transformation. The Mantid Group at ISIS recognised the need for a more maintainable approach to managing third-party libraries across different operating systems. To address this, they migrated the framework to a Conda-based package management system.

Previously, the management of third-party libraries in Mantid varied significantly on each operating system. This disjointed approach significantly increased the maintenance overhead and prevented us from defining a single version of a given package across the entire project.

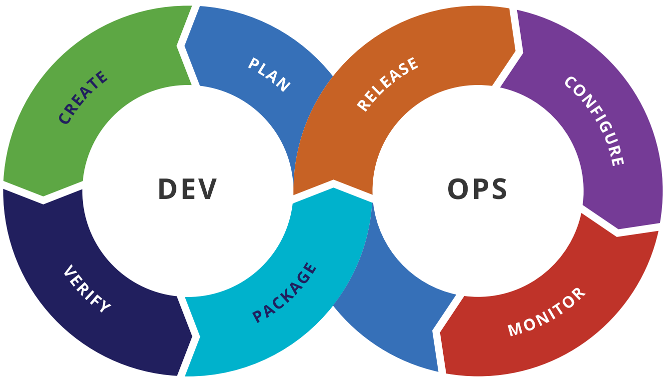
To address these challenges, the Mantid Group made the decision to adopt Conda - a cross-platform package manager that supports various languages, including Python and C++. The result is a streamlined process for users and developers across all operating systems. Mantid can now be installed into a Conda environment on all target OS, while Windows and macOS users retain the option to install using standalone package installers.

Integration of Development and Operations

The integration and automation processes between software development and IT operations (DevOps) has allowed us to improve the process of delivering services quickly for our users.

In Mantid, a virtual team has been created out of volunteers from other teams. They collaborate to enable developers to produce high quality, tested, software releases.

In User Programme Software (UPS) and System Operations, the DevOps responsibilities include creating pipelines that allow automation of system testing and releases, version control of code to allow multiple people to work on the same code base and managing infrastructure such as Kubernetes clusters and servers hosted on the STFC cloud using a shared responsibility approach with SCD.



An illustration of the standard DevOps feedback cycle.


ISIS Neutro
and Muon
Industrial use of I

Partnerships and collaborations

Our external relationships continue to grow: from constructing state-of-the-art instrumentation for the ESS, extending our agreement with the Jawaharlal Nehru Centre for Advanced Scientific Research in India, or signing a new agreement with Neutrons Canada to support the Canadian user community – amongst many other partnership developments over the past year. Collaboration is key as we share our scientific and technical knowledge, pushing the boundaries of neutron and muon science to enable new discoveries that benefit society.

Image left: ISIS Director, Roger Eccleston (right) explains facility operations to Indian Science and Technology Minister, Dr Jitendra Singh (centre), and Professor Ajay Kumar Sood, Principal Scientific Advisor to the Government of India (left), as part of a visit celebrating the longstanding collaboration between India and ISIS Neutron and Muon Source.

Grants help to boost industry engagement

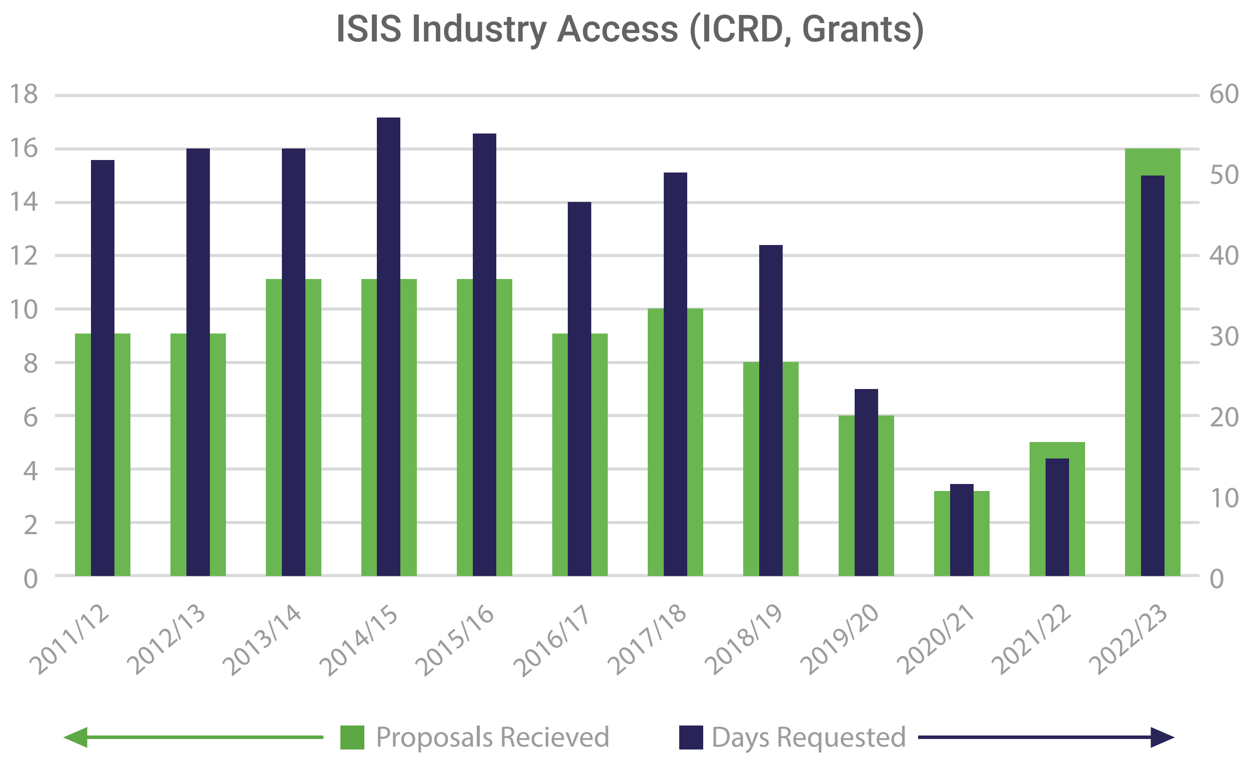
During the last year, ISIS has seen a resurgence in direct industrial users. After a period of limited beamtime due to the COVID pandemic and planned facility shutdown, the full operation of Target Station 2 and anticipated restart of Target Station 1 led to a record number of proposals from established and new industrial users. This uplift has been enhanced by the availability of several grant programs, which support private companies' access to UK national labs run by Innovate UK, BBSRC, and STFC's Business and Innovation Directorate, in addition to the established ISIS Industrial Collaborative R&D ICRD route.

These grants can cover the commercial costs of ISIS beamtime for private companies, as well as staff costs for the ISIS scientists and technicians who contribute to the projects. In total this year, ISIS was awarded more than £420,000 of grants supporting industrial access, resulting in 23 days of grant-funded beamtime. Examples of these include:

- Neutron diffraction on fast-charging lithium-ion battery materials to understand aging mechanisms to improve the cycle life at high temperature (Polaris)
- SANS on lipid nanoparticle (LNP)-mRNA based therapies for reversal of liver fibrosis to understand the structural similarities / differences of highest performing LNPs and low performing LNPs in LNP delivery systems (SANS2D, Zoom)
- Combined X-ray and neutron diffraction for simultaneous stress mapping of surfaces and bulk of engineering components (Engin-x).

Exploitation of these funding opportunities and grants for industrial use of ISIS is an element of the Industry Engagement Strategy. The Industry Liaison Group will be providing information and assistance to the user community and to ISIS staff in how to access these.

These funding programs complement the additional access routes available to businesses: academic access via the FAP program, the ICRD access route and proprietary access.



The NanoVation Tx UK (NTxUK) team about to run their first SANS experiments in May 2023 on lipid nanoparticle-mRNA systems. This was funded through a successful A4I grant (NTxUK, ISIS and the National Measurement Laboratory) which set out to better understand LNP-mRNA technologies and investigate the use of AF4 (Asymmetrical flow field-flow fractionation). (Left to right) Graham Hayes (Senior Scientist), Martin Atwood (Senior Scientist), Georgie Girt (Senior Scientist), Julia Fernando (Scientist), Hanna Barriga (Head of Biophysics), Fred Campbell (Scientific Director).

ISIS delivers for ESS

ISIS continues to develop state of the art instrumentations for the ESS. Two instruments, LoKI and FREIA are currently under development. LoKI is a small-angle instrument with a large simultaneous dynamic range to study complex hierarchical and multi-scale systems. FREIA is a reflectometer with an advanced optical guide system, opening up new frontiers in the structural and kinetic study of soft condensed matter and the life sciences.

This year has seen considerable progress on LoKI, with large quantities of equipment being delivered to and installed at the ESS. A major deliverable has been the completion of the extensive detector modules and support frames.

FREIA has undergone extensive progress in a range of areas including the completion and integration of the bunker wall insert and testing of new technologies for the large chopper disks required for the FREIA design.

New proposals submission system

It is coming up to two years since the replacement proposal submission system was first used at STFC, replacing the old system and streamlining the submission process for beamtime application proposals across CLF (Central Laser Facility) and ISIS. The collaborative effort between the Submissions Group with the ISIS Computing Division and the European Spallation Source (ESS) has resulted in a flexible and configurable system that can adapt to changing facility requirements and support multiple facilities. Initially launched for CLF, the system has expanded its capabilities to encompass various ISIS access routes, including ISIS Direct Access, where it has successfully processed over 1000 proposals across two rounds so far, with very positive feedback from system users.

Once proposals have been submitted, they go through the peer review (FAP) process. To support this, a standardised and easy-to-use tool for panel secretaries to collate their panel scores has been introduced. The FAP scoring site holds all the proposal information reviewers need to give their feedback and uses an automated permissions system to ensure that proposals and feedback are only seen by the right panels.

Members of the Submissions Group (Simon Fernandes, Chi Kai Lam, Farai Mutambara, George Flecknell) discussing requirements with the User Office Group leader (Emma Gozzard).

Meet Rasmia Kulan, Graduate Software Engineer

Rasmia joined ISIS's Computing Division as a placement student, then returned to work for ISIS full time after concluding her degree.

Whilst studying Computer Science at the University of Hertfordshire, Rasmia joined the User Program Software Group of the ISIS Computing Division (ICD) as an industrial placement student. During her placement year she gained experience in the professional field of the software development lifecycle, from capturing requirements and designing a solution, through modelling, coding, testing and development.

She began her placement working with the Reporting Tool, which allows specific members of staff to run a variety of queries on their database, allowing information about experiments, proposals, users, their website and more to be extracted. Rasmia then moved on to contributing to the new proposal system project; a collaboration with the European Spallation Source (ESS).

The motive behind the new proposal system project was to provide all users with an updated interface with a better user experience, and the work was divided into four phases of development. Most of Rasmia's work placement revolved around contributing to the first phase called "Base Integration" which involved setting up the development environment to enable UAT (User Acceptance Testing), friendly user access (BETA testing) from internal staff and external users.

The highlight of her contribution was pairing up with a colleague to design and implement the authentication feature. This would allow STFC users access to the new proposal system using existing login facilities and avoid the need for new accounts when sending proposals thereby lowering the barrier to entry.

To simplify deployment and enable integration with other software, Rasmia set up the database for the new proposal system to be compatible with the STFC Data Integration (DI) Database Services infrastructure. This involved liaising with the stakeholders to obtain their requirements, leading presentations to demonstrate how the data recovery procedure worked, researching disaster recovery and working with the database services team to explore the best options available to set up the database in the development and production environment. After completing her degree, Rasmia re-joined STFC in 2022 as a graduate software engineer. She mainly works on the user office project with the ESS to build a flexible web software that effectively runs and organises user programmes at a variety of science facilities. The software has features that include allowing scientists to submit proposals based on questionnaires and calls defined by user officers.

"I chose to work for ISIS because during my work placement I realised that they really prioritise individuals' mental health and it is made sure that you are feeling fit enough to work. That is one the things that really mattered to me and it felt like it would be a good place for me to get more opportunities to learn and grow in a safe environment.

When I did my placement with STFC that is when I started working from home. It is nice in a way that you can work from the comfort of your own home which does affect your creativity and productivity."

ISIS international partnerships continue to grow and develop. Highlights from the past year include:

India

In December 2022, ISIS signed an extension to our existing agreement with the Jawaharlal Nehru Centre for Advanced Scientific Research, supported by Department of Science and Technology funding, enabling further use of ISIS by Indian researchers and providing additional support for our instrumentation projects.

Italy

In July 2023, ISIS signed a new MoU for partnership working with the University of Rome Tor Vergata, together with an agreement for ISIS to employ a Communications Officer for the ISIS@MACH Italia programme.

Canada

ISIS is working with Neutrons Canada, a group of 14 Canadian universities, which aims to govern, manage and represent Canada's infrastructure program for research with neutron beams. ISIS has recently been awarded funds from the UK's International Science Partnership Fund (ISPF) to develop our partnership with Canadian researchers and further enable use of ISIS by Canada, and has recently signed an agreement with Neutrons Canada for the oversight of this programme.

Switzerland

ISIS continually works with the Paul Scherrer Institut (PSI), as PSI hosts Switzerland's neutron and muon sources, as well as the Swiss Light Source. ISIS, together with Diamond Light Source, has recently received an ISPF award to develop our long-term partnership with PSI – this will include a variety of science and technology projects.

Brazil

ISIS has recently organised a number of webinars for Brazilian scientists interested in using neutrons across a range of science areas. ISPF funding has also been awarded for the next three years to support Brazilian use of ISIS and to enable us to develop partnership working with Brazil.

The Netherlands

ISIS has a long-term partnership with the Technical University of Delft and signed a new MoU for continued partnership working this year.

RIKEN-ISIS Partnership

March 2023 saw the ending of the current partnership arrangements between ISIS and RIKEN. ISIS and RIKEN have had continuous agreements since 1990 for the construction and operation of the RIKEN-RAL Muon Facility at ISIS – a very long-standing and productive science partnership between the UK and Japan. March saw the completion of a large refurbishment project of the facility, ensuring its ongoing use for many years to come. An event at RAL attended by senior RIKEN and embassy staff was held to mark the achievements of the facility and the collaboration. As part of this event, ISIS and RIKEN signed a new MoU for continued partnership working.

Hiroyoshi Sakurai (Director, RIKEN NIshina Centre) and Roger Eccelston (ISIS Director) signing an MoU for continued collaboration.

30 years of RIKEN-RAL Muon Facility operations

Over 800 submitted proposals (580 from Japanese researchers)

2500 days of experiments

More than 500 publications

Collaborations with >90 institutes across Japan

Collaborations with >50 institutes worldwide

Agreements with Malaysian, Indonesian and Korean institutes

Image left: In May, the Swiss Secretary of State for Education, Research and Innovation, Martina Hirayama (bottom row, second from right), and colleagues visited RAL to discuss enhanced UK-Swiss research partnerships.

People and teams

The research conducted at ISIS is supported by about 600 staff - from beamline scientists that run our instruments to engineers that keep the accelerator running to User Office that supports our visiting researchers - everyone at ISIS plays a vital role in its everyday running.

Image left: Ella Ward, one of our apprentices in training.

First Industrial Placement Celebration Event reveals fantastic career paths and inspiring stories from former students

In June, ISIS hosted its first Industrial Placement Celebration Event, where past students returned to Harwell Campus for a day of talks and to share their experiences of working at our national facility.

There were stories of moving onto postgraduate studies, starting careers in various industries and, indeed, returning to ISIS itself! Past students commented on the adaptability and flexibility that the industrial placement offers - from the transferable skills gained, to career progression and offered advice to our current students on how to make the most of their remaining time.

The event was so warmly received by staff and students alike that we now plan to hold this event as a yearly highlight, providing an opportunity for past alumni to reflect, lend their expertise and offer valuable advice, and for current students to learn and be inspired before returning to their studies, secure in the knowledge of all the possibilities their placement at ISIS has opened up for them.

> **My research has taken me on aircraft-based fieldwork campaigns over the remote North Atlantic Ocean and on a ship-based campaign to the Arctic. Although magnetism and atmospheric chemistry sound vastly different, many of the skills that I developed at ISIS have been applicable to my PhD, from leading my own research project to communicating to different audiences.**
>
> Loren Baker, University of York

NMSUM 2023

The UK Neutron and Muon Science and User Meeting took place at Warwick University from 19 - 21 April 2023. Jointly organised by the Institute of Physics and the Royal Society of Chemistry's Neutron Scattering Group, ISIS and Institut Laue-Langevin, the meeting brought together researchers from across the UK, sharing news and updates on the latest Neutron and Muon science.

With key speakers such as Anthony Phillips (Queen Mary University of London), Karen Edler (Universities of Lund and Bath) and George Green (Ashmolean Museum, Oxford), along with breakout sessions for each area of research, the meeting displayed both the full variety of research possible and the capabilities of neutron and muon techniques. The event included a student day where students were able to share presentations on their own research and make new connections within the community.

Participants at the NMSUM 2023 conference at the Warwick University Conference Centre.

Meet our 2022/23 students, reflecting on the value of their placement year

Every year, ISIS hosts a number of industrial placement students in areas ranging from reflectometry to software systems, to communications and public engagement. Industrial placements offer a unique experience for university students to see what life is like at ISIS and how they can contribute to the valuable research being carried out here.

Amongst those who joined us for 2022/23 were Ella, a chemistry student at the University of Bath who was based in Neutron Scattering and Development; Morgan, a physics student at the University of Bath who was based in Neutron Detector Development; Rupo, a chemistry student at the University of Loughborough who completed a Public Engagement placement; and Katie, a biochemistry student at the University of Warwick, who was our Science Communications student.

Rupo

The people I have met have been some of the strangest, funniest and sweetest people out there. They have helped me become the Rupo I am today, and I think the Rupo a year ago would like this one a lot. Following from that, the confidence boost has been wonderful! Public engagement involves a lot of talking to members of the public, which can be very daunting. I was so worried 'what if I mess up and say something wrong?' Been there, done that – I told some students that Buzz Lightyear went to space and life went on. Do not get me wrong, it still is scary, but a lot less so!

Morgan

I have been responsible for the development of the beam monitors for this year, working with not only my manager but also the wider LoKI instrument Group. The trust placed in me to find solutions and work things out has been a fantastic change of pace from university. The impact you can have on a project as a placement student is larger than I expected it to be.

Ella

I am still not sure what I would like to do with my career, but the neutron scattering community is definitely one that I could see myself working within in the future. This year has even made me consider the possibility of doing a PhD, which was a thought that had not crossed my mind previously!

Katie

Releasing my own work into the public domain has given me many proud moments this year, especially my illustrations and videos. Developing creative skills within a STEM setting was something I did not know was possible before this year. I am also proud of how my confidence has soared over this year. Interviewing the numerous world-class researchers just wandering around this site was incredible and terrifying to start with! But I have learnt that my curiosity is more important than insecurity.

Ludmila Mee

Technicians play a vital role in our society and work in virtually every sector and industry. Within ISIS, our highly skilled technicians are critical for installing, maintaining and developing our unique facility. They provide essential service to ensure we can operate our world leading capabilities, which supports our national and international scientific community.

In June 2023, Ludmila Mee, who joined ISIS as Biolabs Manager last year, was appointed as a founding member of the Institute for Technical Skills and Strategy Technical Council, a body of technical staff across the nation who will advise on the aims and initiatives of the UK's ITSS, which launches this year. This new entity will build on the legacy of the MI TALENT programme as well as being underpinned by the advances of the Technician Commitment movement. Officially opening on 1 August, the Institute will be the first of its kind in the UK, funded by £5.5 M investment from UKRI.

The main purpose of the Institute is to invest into academic research of the UK technical force, to find better approaches to culture change and pilot them, to produce a UK-wide policy on the technical force and to engage industry, public and government organisations with the UK technical community.

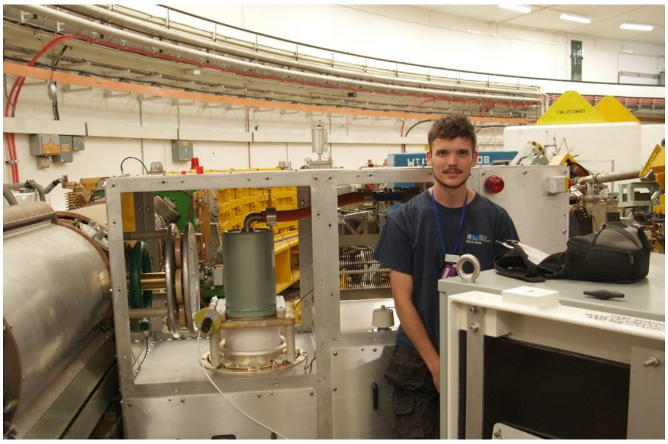
> **I am humbled and truly honoured to become one of the founder members of the Council. I see this as a great opportunity to govern and lead an important initiative on the national scale. They had over 150 applications to choose from, but only 12 places which they negotiated up to 14, which reflects the quality of applications! I am really looking forward to the great and rewarding experience of shaping up the future of the UK Technical workforce.**

Image left: Ludmila Mee at the CL2 BioLab, Target Station 2.

Meet Ryan Allinson, Electronics Technician

Ryan is an Electronics Technician within the Synchrotron Section of the Radio Frequency (RF) Group. He began his career within STFC straight out of GCSEs through the Advanced Engineering Apprenticeship in Electronics. Ryan has recently been awarded a first for his degree and in January 2023, started a new role within the ISIS Diagnostics Group as a Diagnostics Electronics Engineer.

> **"I find ISIS a rewarding place to work as there is flexibility to take a project from concept to commissioning. I find the entire process hugely motivating seeing how I can change an idea to an operational piece of equipment supporting world leading science!"**



Ryan Allinson at the ISIS synchrotron.

How did your apprenticeship begin?

The Advanced Engineering Apprenticeship in Electronics started with a year's full-time study at college, balanced between academic and practical learning across classrooms and workshops. From the second through to the third year, most of my time was spent conducting on-site placements. Placements allowed for developing competence over a range of electronics and with most taking part within ISIS, it naturally led onto securing a full-time position in the ISIS RF Group.

Tell us more about your current role at ISIS?

Throughout this role, I have gained expertise in a range of areas including the operation, maintenance and repair of complex integrated systems encompassing electrical, electronic, high voltage (HV), radio frequency (RF), control loops and cooling components. I have been involved in manufacturing prototype and operationally ready hardware, contributing to documentation, record-keeping and engineering drawings, as well as maintaining spares inventories, handling small order procurement and establishing effective communication with suppliers.

As my role has progressed in conjunction with my degree course, I have taken on additional responsibilities and acquired project management skills, successfully planning and coordinating my own design projects. As the RF Group provides apprentice placements, I have been involved in supervising apprentices within our section. This has been a rewarding experience to give back to the scheme, as well as supporting the progress of developing apprentices. I was very proud and privileged to be the recipient of a Whitworth Scholarship Award, which enables engineers, who have excellent academic and practical skills and the qualities needed to succeed in industry, to take an engineering degree-level programme in any engineering discipline.

How would you encourage young people considering an apprenticeship in engineering?

I would strongly recommend engineering and apprenticeships to any young person considering it. As a practical person, I have found the balance of practical and academic work well balanced. In addition, the first-hand experience provided application in context for classroom learning.

I also feel that starting a career through an apprenticeship provided an ideal pathway into a technical career. Collaborating with experienced colleagues quickly built strong fundamentals, boosting my own competence and confidence both professionally and personally.

Meet Christopher Robinson, Electronics Technician

Christopher is an Electronics Technician with the Radio Frequency (RF) Group's Linac section. After taking his GCSEs, he completed the RAL Apprenticeship Scheme and joined ISIS.

What first piqued your interest in engineering?

I have had an interest in engineering from a young age, particularly in electronics. I would always question how things worked, and why things broke, and would frequently take things apart to find out! I knew that I'd rather learn hands on by doing an apprenticeship than learning from a textbook in a classroom, so I left school after GCSEs and joined the RAL Apprenticeship Scheme. I had one day release learning in the classroom and physical hands-on learning for the remainder of the week. I really enjoyed this balance, and the physical work was always engaging. After completing the first year, I continued to day release to BMW for classroom learning but came on to site to learn on the job. Following the completion of my four-year apprenticeship, I then advanced to a HNC at JTL and OAS where I learned more advanced electronic theory.

Tell us about your current role.

Following my apprenticeship, I moved into the ISIS RF Group linac section. We are tasked with maintaining and developing the 70MeV drift tube linear accelerator, constructed of four tanks, a Radio Frequency Quadrupole (RFQ) and a debuncher, driven by five 200KW amplifiers and four 2MW amplifiers. Parts of the system are over 65 years old - tank 3 for instance was constructed in 1956, so it is particularly important to keep on top of maintenance, and to design new pieces of equipment to aid in the running and protection of the machine, and the equipment that operates it.

What is a typical day like for you?

On a typical day, I'm developing and assembling projects. Most recently, I've been working on a new design for a 130A pulsed power supply for our drift tube magnets to replace our current aging power supplies built in the 1990s. This involves electronic design, printed circuit board design and eventually manufacture and assembly. I also check the linac, inspecting for any early signs of component failure that might need attention in a shutdown.

What do you enjoy the most?

Development is my favourite part of the job. Mainly because I can see it through from start to finish, from a scribble on a whiteboard, to a finished device in service.

Did you ever doubt your abilities? If so, how did you handle these feelings?

When I first started working on the linac, I would worry about potentially worsening a situation or not being able to diagnose a fault. I found that taking time and care and splitting the system down into its separate components makes the task much more manageable. Talking a problem through with other members of staff helps too. Everybody is trying to achieve a common goal and I've found they are generally happy to help!

> **For me, the experiences I've had and the variety of jobs I've completed at ISIS have given me a vast spectrum of knowledge which I can use to perform more complicated repairs and develop more complicated equipment.**

Christopher Robinson at the Linac Modulator 2 in the injector hall.

International Women's Day

This year, International Women's Day happened to occur during one of the biggest events in our public engagement calendar – the RAL Particle Physics Masterclass. During the Masterclass, we typically welcome 100 A-level students visiting every day over four days and many of our staff volunteer to be tour guides. In the past, the Masterclass has been an event dominated by male participation but the coincidence of this event with International Women's Day offered an opportunity to make an impact on young women aspiring to work in STEM. So on this day, all our tour guides and speakers were female, also allowing the opportunity to encourage more women to become tour guides at ISIS. By increasing the diversity of our guides, we, in turn, provide diverse models for our young visitors and the next generation of scientists and engineers.

From left to right – Rupo Mapanga, Preeti Kaur, Ella Chandler, Terri-Louise Hughes, Rhea Stewart, Steph Richardson, Rosie de Laune, Anna Herlihy.

Inspiring the next generation

It has been an exciting and dynamic year for public engagement as we have transitioned back to in-person events after two and a half years of virtual engagement. The continuous evaluation and refinement of our activities has allowed ISIS to develop a successful hybrid public engagement programme that combines the impact of in-person and on-site activities with the benefits of our wider-reaching and more accessible virtual ones.

Over the past year, we have delivered over 50 events – virtual, in-person, on-site and off-site – reaching over 5200 school students, teachers and members of the public across the UK. Alongside our active programme of events, we have continued to develop new online material and innovative content for the ISIS schools webpage, reaching thousands more.

Our activities span a wide range of themes – from particle physics and space science to remote handling and machine learning – reflecting the breadth of work and expertise at ISIS. Engaging diverse and under-represented audiences is also an important part of our Public Engagement programme and we continue to work to increase our engagement with more diverse audiences and those from areas of high deprivation.

We have been actively embedding EDI (Equality, Diversity and Inclusion) into our engagement programme, creating and delivering activities highlighting diversity in STEM, and linking into campaigns including Black History Month and International Women's Day. This year, ISIS also contributed to a hands-on exhibit at the Science Museum in London, inspiring the next generation by showcasing the skills and work of our technicians.

This year, the RAL Engineering Experience Programme (which started as an ISIS initiative in 2021/2022) was expanded across several facilities at RAL, including RAL Space, Central Laser Facility, and the Technology Department. A-level students from five local schools took part in the initiative, working with RAL and ISIS graduates to undertake a real engineering challenge over 6 months.

ISIS also delivered several virtual and in-person activities as part of training days for over 60 educators, offering unique insights into the facility and our science and engineering. In summer 2022, the facility also hosted 35 work experience students from across the UK for week-long placements as part of the online RAL work experience programme, offering opportunities to work alongside ISIS staff across a range of disciplines and areas of work.

The summer also saw two large open days at ISIS for over 650 visitors. The ISIS open days were the first large public events at RAL for two and a half years and were a huge success, allowing us to engage with the local community, under-represented and hard-to-reach audiences, as well as our staff and their families and friends.

From sticky slime and crystal gardens, to artificial intelligence and remote handling challenges, there were interactive activities for all ages and interests. Our staff volunteers engaged with visitors, leading tours, workshops and demonstrations, and sharing their stories with a vibrant excitement and enthusiasm for what we do here at ISIS.

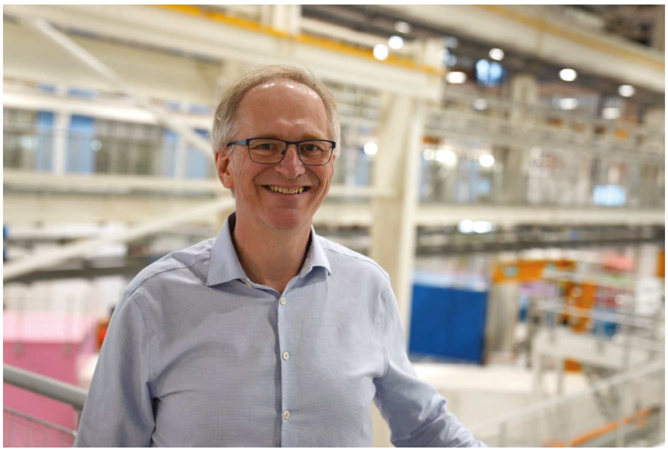
Toby Perring awarded the European Neutron Scattering Association Walter Hälg Prize for 2023

Toby joined ISIS in 1992 and has held various positions as a research and instrument scientist, becoming an STFC Fellow in 2005. In 2007, he became an Honorary Professor in Physics at the London Centre for Nanotechnology, University College London, UK.

> **Toby and I formally started at ISIS on the same day and we worked closely together for several years. I am delighted to see my good friend and colleague recognised in this way for his great contribution to neutron science, instrumentation and software.**
>
> Roger Eccleston, ISIS Director

Through several decades, Toby has been a central leading figure in the evolution of highly pixelated direct time-of-flight spectrometers for the investigation of excitations in strongly correlated electron systems. He has been instrumental in all steps in this revolution, designing, building and commissioning the Maps spectrometer at ISIS, continually monitoring to ensure its scientific success. Maps was the first neutron time-of-flight spectrometer with a large array of position-sensitive detectors, allowing for efficient mapping of large areas in momentum and energy space.

Furthermore, Toby has been instrumental in the evolution of software analysis tools, unlocking the potential of the unprecedented data-volumes achieved with Maps and the latest generation of spectrometers to be fully exploited, leading to hitherto unachievable scientific discoveries. In his own experiments and collaborations, Toby has made seminal contributions to the understanding of the dynamics of strongly correlated electron systems, including giant magnetoresistance manganites, high-temperature superconductors, and quantum magnets. His research has led to a greater understanding of spin waves in layered magnetic systems, spinons in low-dimensional magnets, and complex spin fluctuations in cuprate and pnictide superconductors.



> **The European Neutron Scattering Association and the global international neutron community are grateful to Prof Toby Perring for his paradigm changing contributions to single crystal neutron spectroscopy and enthusiastically congratulate him as the 2023 recipient of the Walter Hälg prize.**
>
> Henrik Rønnow, the current Chair of ENSA

The prize is sponsored by Swiss Neutronics

Regular ISIS user and panel member, Professor Andrew Goodwin, elected as Fellow of the Royal Society

Andrew Goodwin, Professor of Materials Chemistry at the University of Oxford and a regular ISIS user, was elected as a Fellow of the Royal Society this year. He has sat on ISIS Facility Access Panels and represented the user community on the Target Station 1 Refurbishment Project Board.

Andrew's research focuses on understanding and exploiting the dual roles of flexibility and disorder in functional materials. He and his team specialise in the development and application of diffuse scattering methods, which provide an experimental window into the atomic-scale structures of disordered solids. Andrew has used these approaches to resolve the nature of complexity in a range of different systems of both fundamental and technological importance.

Andrew has received several awards for his work in the field of materials chemistry, including the Harrison-Meldola, Marlow, Corday-Morgan, and Peter Day Prizes of the Royal Society of Chemistry. In 2018, he was named the inaugural Chemistry Laureate of the UK Blavatnik Awards for Young Scientists.

Dr Paul Goddard wins Brian Peppard Prize for 2023

ISIS user, Dr Paul Goddard from the University of Warwick, has been awarded the 2023 Brian Pippard Prize for his developmental work on the techniques of angle-dependent magnetoresistance and its application to mapping Fermi surfaces.

The Pippard prize is named in honour of Professor Sir Brian Pippard. It is awarded annually by the Institute of Physics to a scientist working in the UK who has made a significant recent contribution to the field of superconductivity.

Dr Goddard's current research examines materials that combine frustrated magnetism and electrical conduction. He intends to investigate materials that combine the ground states and exotic excitations of frustrated magnets with highly correlated electronic properties and expects the emergence of interesting and potentially useful new physics.

A frequent user at ISIS for his work on molecule-based magnets, Dr Goddard conducts his experiments using WISH and LET.

Dr Goddard hopes his work in organic materials will contribute to important milestones in the creation of more efficient electronic and magnetic devices.

> **"The experiments at WISH and LET have shown us details about the ground states and excitations of these materials that wouldn't otherwise have been uncovered and taught us a great deal about how molecules mediate magnetic exchange interactions. This has fed directly into new publications, new materials and new avenues of research. Just as importantly, the ISIS work has provided important training for several generations of graduate students and been a key ingredient in their PhD theses."**

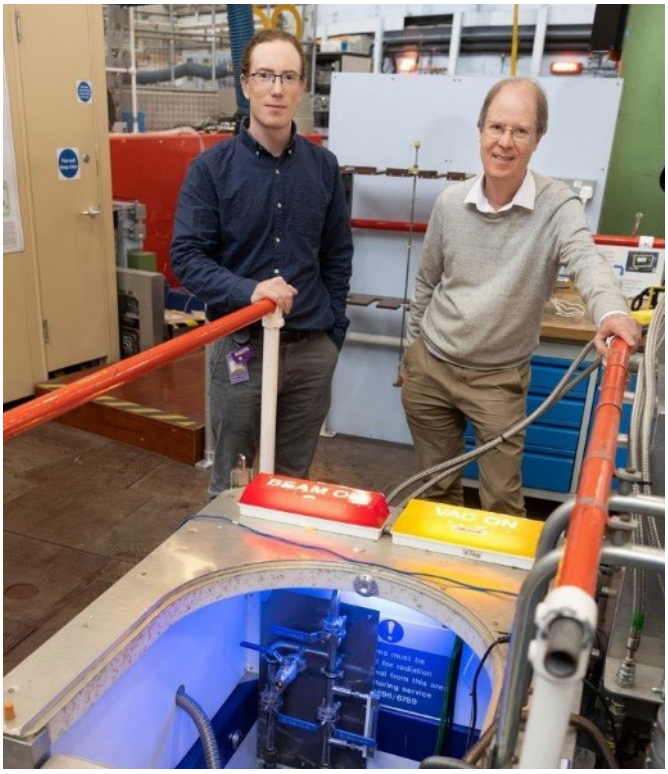
Alex Hannon and Oliver Alderman receive The American Ceramic Society's 2023 Ross Coffin Purdy Award

ISIS scientists, Alex Hannon and Oliver Alderman, alongside Shuchi Vaishnav and Paul Bingham from Sheffield Hallam University, received The American Ceramic Society's 2023 Ross Coffin Purdy Award for their paper "The structure of sodium silicate glass from neutron diffraction and modelling of oxygen-oxygen correlations." The team will receive their award at the American Ceramic Society's Honors and Awards Banquet as part of the Society's 125th Annual Meeting in October 2023 in Columbus, Ohio, USA.

Their paper used neutron diffraction to show that it is possible to calculate the oxygen coordination inside a glassy material, even if the glass has a complex structure or composition. The coordination number can then be used to model the oxygen framework within the glass, enabling the positions of the other elements present to be calculated, and therefore the wider structure.

The researchers used the Gem instrument at ISIS to measure the neutron correlation function of a sodium silicate glass with 42.50 mol% Na_2O. Instead of using the traditional difference method to analyse their results, they developed a more sophisticated interpretation method that can also be applied to other simple glass systems, such as borates and germanates, or to more complex glasses. When studying the sodium silicate glass, contrary to the conclusions of previous glass structure studies, they did not find evidence that the sodium-oxygen bonds are shorter for non–bridging oxygens and longer for bridging oxygens. Instead, the distribution of lengths for the sodium-oxygen bonds for non-bridging oxygens is broad enough to cover both shorter and longer lengths than the bonds with bridging oxygens.

> **I was particularly thrilled to learn about our award for this work, given its basis in methodology I originated during my PhD studies. In the paper that is the subject of the award, Alex has further developed and applied this methodology to gain detailed, unique and somewhat paradigm-shifting insight into a fundamentally important glass system. We expect to continue to exploit and develop this methodology given its excellent applicability to neutron diffraction from amorphous oxides.**
>
> Oliver Alderman, ISIS Scientist



Oliver Alderman (left) and Alex Hannon (right).

Glossary

AFM	Atomic Force Microscopy - a high-resolution imaging technique used to study surfaces.
BBSRC	Biotechnology and Biological Sciences Research Council - part of UKRI.
CERN	Conseil Européen pour la Recherche Nucléaire - a European laboratory for particle physics.
DAE	Data Acquisition Electronics - components responsible for collecting, processing, and recording signals from neutron detectors.
DFT	Density Functional Theory - a quantum mechanical modelling method used to calculate the electronic structure of materials.
DSSs	Duplex Stainless Steels - two-phase alloys with high strength and corrosion resistance.
DUE	Detected Unrecoverable Error - a system fault that has been identified but cannot be corrected, often leading to a disruption or failure in the normal operation of a computer system or application.
EV	Electric Vehicle - a vehicle powered (partially or entirely) by an electric motor.
EDS/SEM	Energy-dispersive spectroscopy / scanning electron microscope - a technique that combines the high-definition surface imaging and elemental analysis.
EPSRC	Engineering and Physical Sciences Research Council - part of UKRI.
ERC	European Research Council - an organisation that funds scientific research in Europe.
ESS	European Spallation Source - a multi-disciplinary research facility under construction in Lund, Sweden, designed to be the world's most powerful neutron source.
FFA	Free Fatty Acid - molecules that consist of a long hydrocarbon chain with a carboxylic acid functional group at one end.
FETS	Front End Test Stand - the front end of a linear accelerator that can be used for testing new techniques, physics and components.
GPU	Graphics Processing Unit - a specialised circuit for parallel processing, originally designed for graphics but now widely used for diverse computational tasks, including scientific simulations.
HIP	Hot Isostatic Press - equipment that simultaneously applies high temperature and pressure to improve material properties.
HR	Helium Recovery - capturing, compressing and storing helium to make it available for re-use.
HND	Higher National Diploma - an academic higher education qualification in the UK.
HV	High Voltage - an electrical potential large enough to cause injury or damage.
ICRD	ISIS Industrial Collaborative Research and Development, a fast-track route for companies with a UK manufacturing or research base to use ISIS.
INS	Inelastic Neutron Scattering - a method for examining the low-temperature atomic vibrations of solids.

ISIS@MACH ITALIA	The hybrid Italian multidisciplinary Research Infrastructure for Complex Materials and Interfaces, a hub of the ISIS Neutron and Muon Source.
LPP	Long Periodicity Phase - a lamellar phase of lipid molecules with repeat distances of approximately 13 nm.
MFM	Magnetic Force Microscopy – a technique used to map the nanoscale magnetic properties of a surface.
MEBT	Medium Energy Beam Transport - a component of a particle accelerator used to transport and condition particle beams in the medium energy range.
MOF	Metal-Organic Framework – a porous and crystalline material that consists of metal nodes connected by organic linkers.
μSR	Muon Spin Rotation/Relaxation/Resonance – a technique that uses muons to study atomic-level structure and dynamics in the bulk of a material.
μXES	Muonic atom X-ray Emission Spectroscopy - a technique to study the electronic and nuclear structure of materials using the X-rays emitted during the decay of muonic atoms.
NERC	Natural Environment Research Council – part of UKRI
NRCA	Neutron Resonance Capture Analysis - a technique to analyse the elemental composition of the bulk of a material.
NRTI	Neutron Resonance Transmission Imaging – an imaging technique that provides information about the elemental composition and distribution of a sample.
OAS	Oxfordshire Advanced Skills, providing high quality training for apprentice engineers and technology business in the Thames Valley.
PGA	Pyrolytic Graphite Analyser - a component used to select neutrons based on their energy.
QAH	Quantum Anomalous Hall effect - a phenomenon where a two-dimensional system exhibits Hall conductivity in the absence of an external magnetic field.
QENS	Quasi-Elastic Neutron Scattering - a technique used to study dynamic processes in a material.
RAL	Rutherford Appleton Laboratory – a national scientific research laboratory in the UK that is operated by STFC.
RF	Radiofrequency - electromagnetic radiation in the range of around 3 kHz - 300 GHz.
RFQ	Radiofrequency Quadrupole - a type of linear particle accelerator.
RCS	Rapid Cycling Synchrotron - a type of particle accelerator that is capable of rapidly accelerating charged particles and transporting them to their destination many times per second.
R&D	Research and Development - any activity that leads to new or improved products, processes, or services.

SANS	Small-Angle Neutron Scattering – a technique to determine micro/nano structure in the range of 1 - 500 nm.
SCARF	Scientific Computing Application Resource for Facilities – a high-performance computing cluster.
SCD	Scientific Computing Department – a department within STFC that provides large-scale high-performance computing facilities, computing data services and infrastructure.
SDCs	Silent Data Corruptions - errors in computer data that do not trigger a notification or warning and may lead to undetected inaccuracies in the stored information.
STEM	Science, Technology, Engineering and Mathematics
STFC	Science and Technology Facilities Council – a UK government agency that conducts and funds research in astronomy, physics and space science, and operates world-class research facilities as part of UKRI.
SdSSs	Super Duplex Stainless Steels - a family alloys known for their high strength, excellent corrosion resistance and enhanced durability.
Tc	Critical Temperature (of a superconductor) - the temperature at which electrical resistivity drops to zero.
TPUs	Tensor Processing Units - specialised accelerators developed by Google specifically for deep learning tasks, particularly those involving neural networks.
TI	Topological Insulator - a class of materials that behaves as an insulator in its interior but conducts electricity on its surface.
UKRI	United Kingdom Research and Innovation - the national funding agency investing in science and research in the UK.
ULT	Ultra Low Temperature - a temperature that approaches absolute zero.
WEEE	Waste Electrical and Electronic Equipment - discarded or obsolete electronic devices and appliances.
WLSF	Wavelength Shifting Fibre - an optical fibre that shifts the wavelength of radiation as it propagates through the fibre.
ZIF	Zeolitic Imidazolate Framework - a class of MOF that comprises metal ions or clusters connected by imidazolate linkers.

Launching our 40th anniversary

As 2023 drew to a close, ISIS kicked off its 40th anniversary celebrations with a staff update and a social gathering featuring photos old and new, including the one shown here, captured at the moment when the first neutrons were detected.

On 16 December 2024, we will mark 40 years since first neutrons and we now look forward to a year of celebration in recognition of this milestone.

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Cover Image: A Combined Inelastic Neutron Scattering and
Simulation Study of the $^3He@C_{60}$ Endofullerene.
Credit: Stephanie Richardson and Mohamed Aouane

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