ISIS Neutron and Muon Source:

Annual Review 2021

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Front cover: Technician Justin Miles working on the new assembly for the TS1 Project.

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Foreword

Foreword

‘Curiouser and curiouser!” cried Alice.

In last year’s foreword I managed to quote from Forrest Gump and Harry Potter. This year I have chosen something written closer to home, actually within a few hundred metres of the source of the ISIS name. The past year has indeed been curious. We do seem to be in a ‘looking glass’ world where some things are the same and some are different, and we don’t quite know how to get back to the other side. However, some things don’t change. Despite all of the constraints and complications ISIS has had another excellent year. To run three operational cycles with about 75% of a normal experimental programme, but 10% of the number of visiting users, is a remarkable achievement. At the same time we have completed the preparatory work so that the long-planned long-shutdown has now started. Users and staff have produced a record number of publications, so somebody has been managing to work from home despite caring or home schooling responsibilities.

> Despite all of the constraints and complications ISIS has had another excellent year. To run three operational cycles with about 75% of a normal experimental programme, but 10% of the number of visiting users, is a remarkable achievement.
> **– Robert McGreevy, ISIS Director**

TS1 will restart operation in 2022 with a new ‘heart’. Preparation for the Endeavour instrument development programme is well underway, and funding has recently been awarded for preparatory work on ISIS-II. We have come a long way since I was employed as a postdoc in 1981 specifically to be one of the first users of ISIS. Possibly there will be a postdoc being employed in 2021 who will be writing the foreword to the ISIS-II Annual Review in 2061? Maybe it’s you? By the time you get there you will fully understand what is meant by ‘teamwork’. Many thousands of people, staff and users, have contributed to the ISIS journey so far. Roger Eccleston will shortly rejoin the journey as ISIS Director – I wish him well. I had no idea where we were going when I joined, but I have been very fortunate to be one of you. Which brings us back to Alice:

‘Would you tell me, please, which way I ought to go from here?’
‘That depends a good deal on where you want to get to.’

Robert McGreevy
ISIS Director

Left: Tatiana Guidi, beamline scientist, on the MARI instrument.

Overview

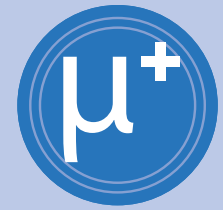
The ISIS Neutron and Muon Source is a world-leading centre for research at the STFC Rutherford Appleton Laboratory near Oxford. Our suite of neutron and muon instruments gives unique insights into the properties of materials on the atomic scale.

We are part of the global research infrastructure, and our science spans a wide range of disciplines, from magnetism to cultural heritage, engineering to food science, chemistry to environmental science.

We contribute to inspiring the next generation of scientists through our public engagement programme as well as supporting training for apprentices, year-in-industry students, work experience students and graduates.

Through spring and early summer 2020, the facility was set up to allow work in a Covid-safe manner, with project work and then operational work restarting with a limited number of people on site.

ISIS operated for two run cycles in the 20/21 year, between September and December 2020.



5 Muon instruments

Neutron instruments

1034 Proposals received from **34 Countries**

Xpress proposals

518 Experiments

Unique principal investigators awarded time

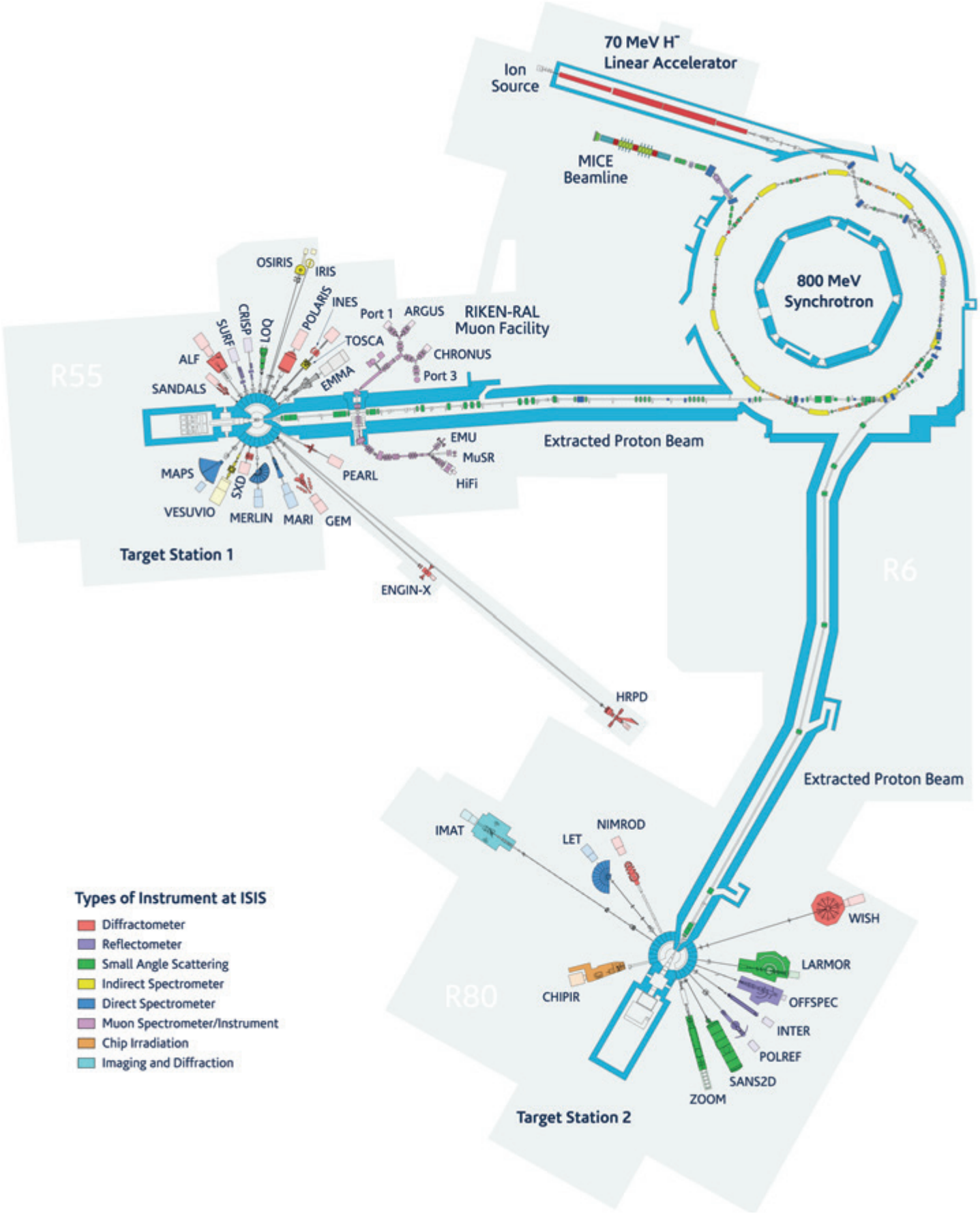
423

New principal investigators

Companies engaging

Journal publications

The ISIS Neutron and Muon Source



The ISIS Endeavour Programme

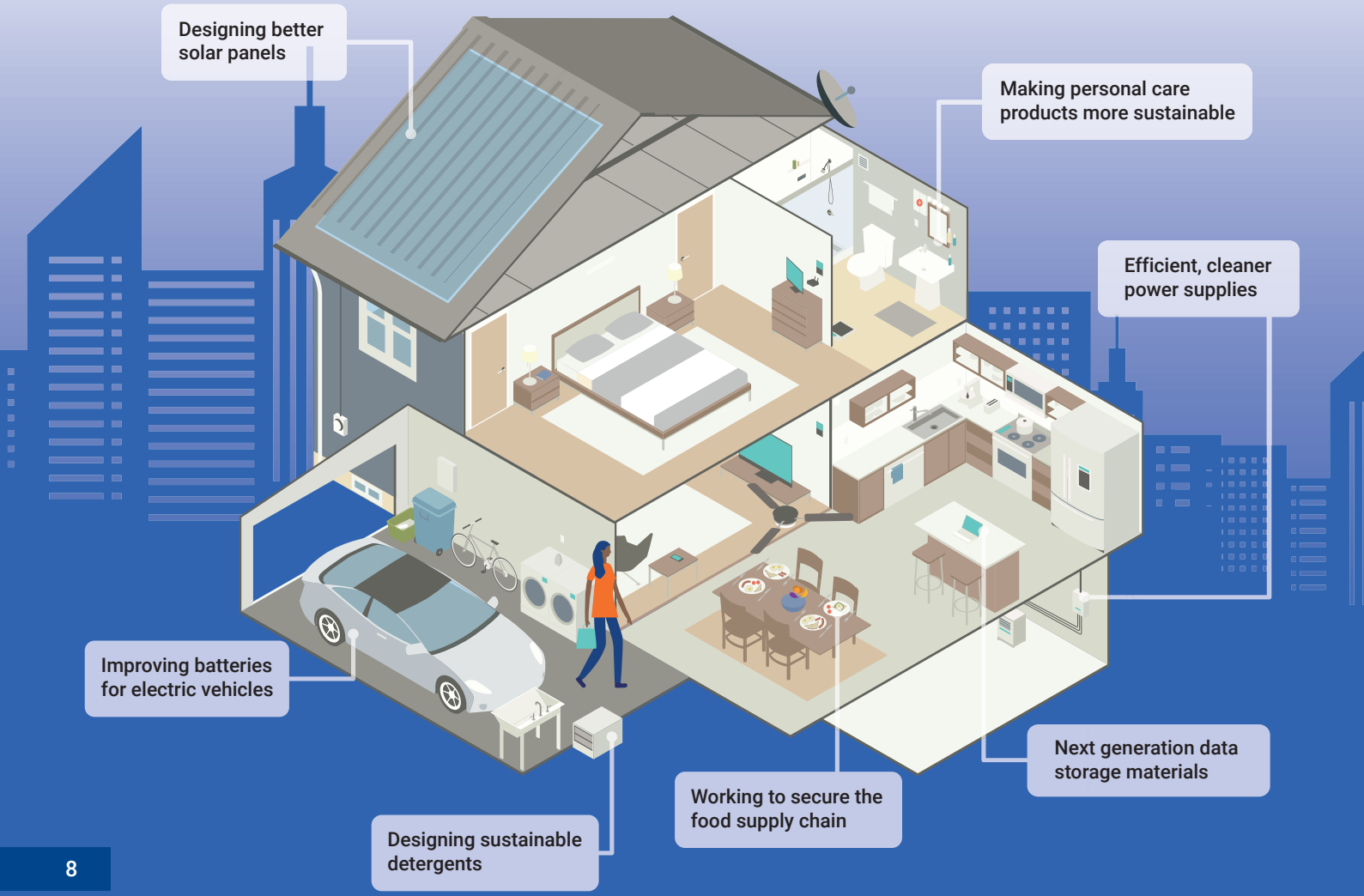
ISIS seeks to continually update and develop its suite of neutron and muon instruments, in order to respond to current research needs and to ensure it remains a world-leading facility and maximises its socio-economic impact. The Endeavour programme will deliver the next generation of instruments and significant instrument developments in support of an extensive range of research across the science disciplines, strongly aligned with the Government's key priority areas.

Advanced Manufacturing – the next industrial revolution

Endeavour will allow the study of real components (often large, thick and complex) with excellent time resolution. A typical example that is not currently feasible is the materials understanding required to realise the potential of small modular reactors (SMRs) in solving the clean energy challenge. SMRs will challenge our current knowledge of processing (e.g. additive manufacturing) and joining technologies. Endeavour will provide the ability to measure strain, plasticity, and crystal structure in real world components, all of which contribute to the performance, safe operation and lifetime of SMRs.

Clean growth and Net Zero – capturing the bad guys

Crucial to reaching Net Zero carbon emissions will be the development of cheap and effective technologies for carbon dioxide capture. Highly porous materials such as zeolites and metal organic framework (MOFs) are likely to be at the forefront in this area. To gain quantitative mechanistic insight into how these disordered systems function requires direct observation of the interactions of CO_2 with these materials. However, CO_2 (and greenhouse gases such as NO_x and SO_x) are on the limit of present capabilities. Endeavour will enable direct observation of the structure and dynamics of CO_2 and other molecules (notably hydrogen where neutron techniques are uniquely placed) in porous systems.



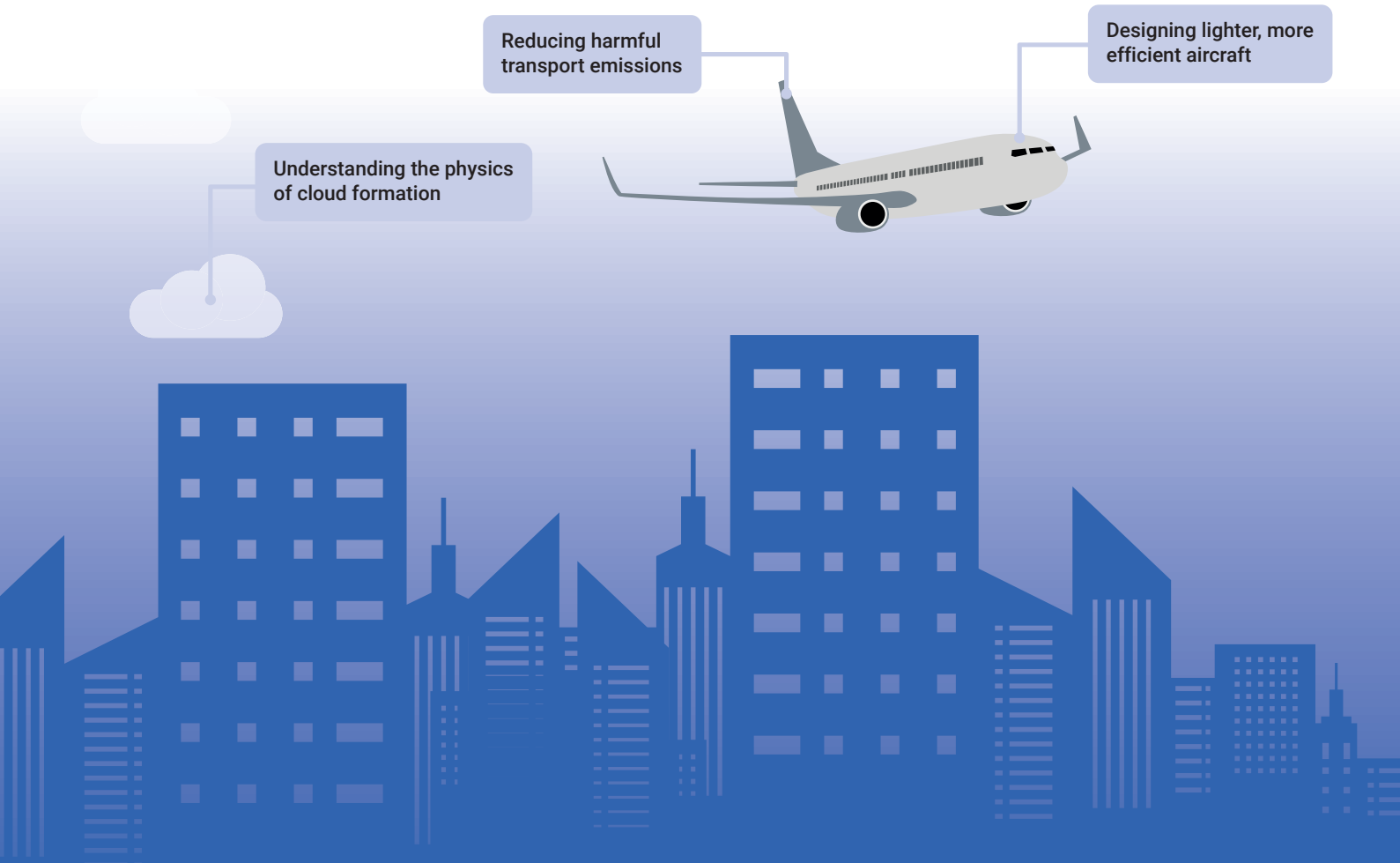
Materials of the future – delivering the promise in transformative technologies

Quantum computing has the potential to be a truly transformative technology. A challenge in achieving quantum computation is maintaining the coherence of quantum states while information is processed. Experiments where the loss of quantum information can be dynamically observed are currently not practical. Endeavour will open a window on the nature of quantum coherence and move us to a quantitative 4D understanding of the dynamics of materials in the nanosecond to sub-picosecond timescale region alongside resolution in momentum space. This complements other techniques that access shorter timescales but which lack spatial information.

Bioscience and Health – a unique contribution

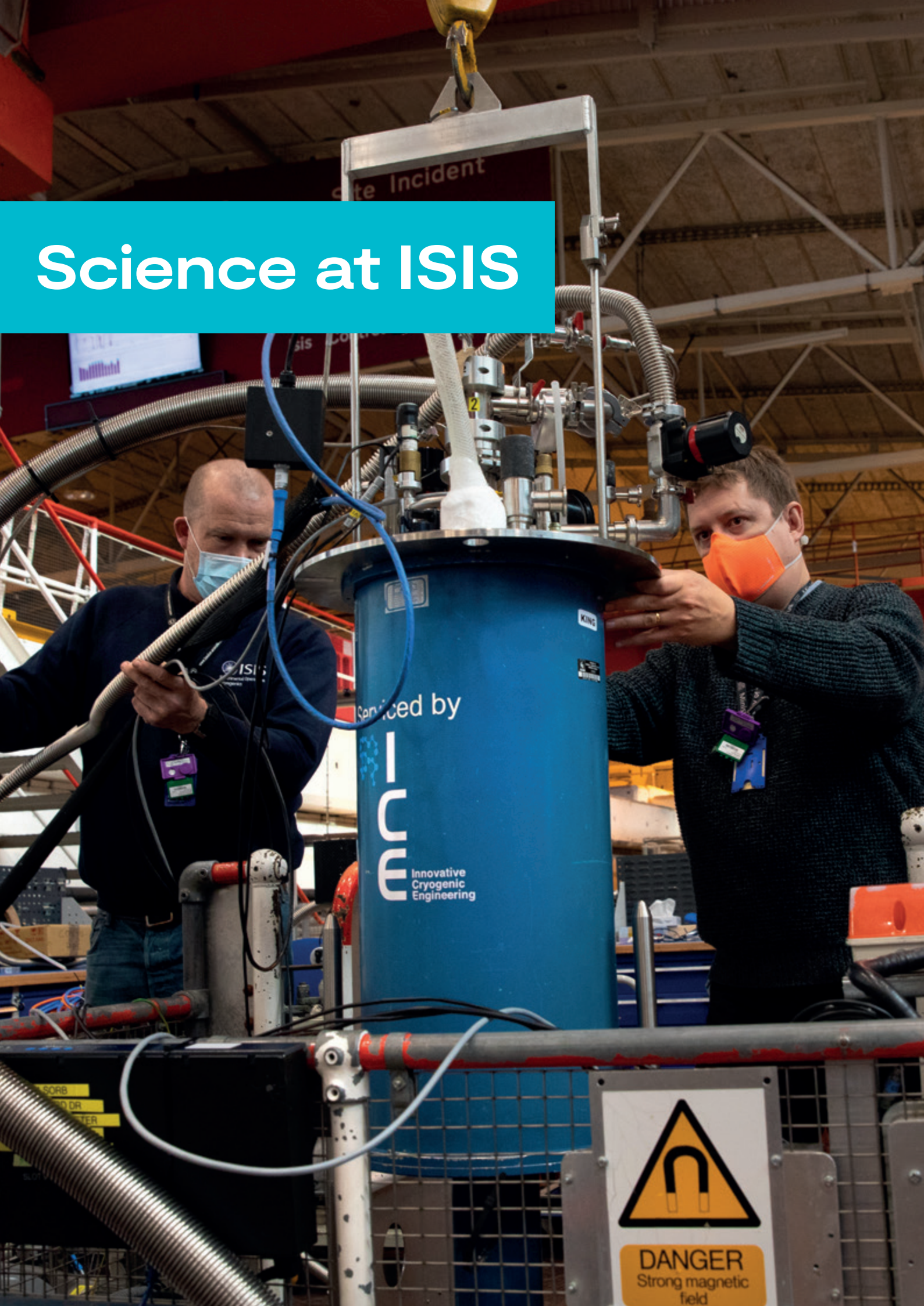
Endeavour will move our structural analysis into significantly larger structures, enabling, for example, the study of the virus reproduction process and the interactions of drug molecules at active sites. Currently this research is not possible at ISIS.

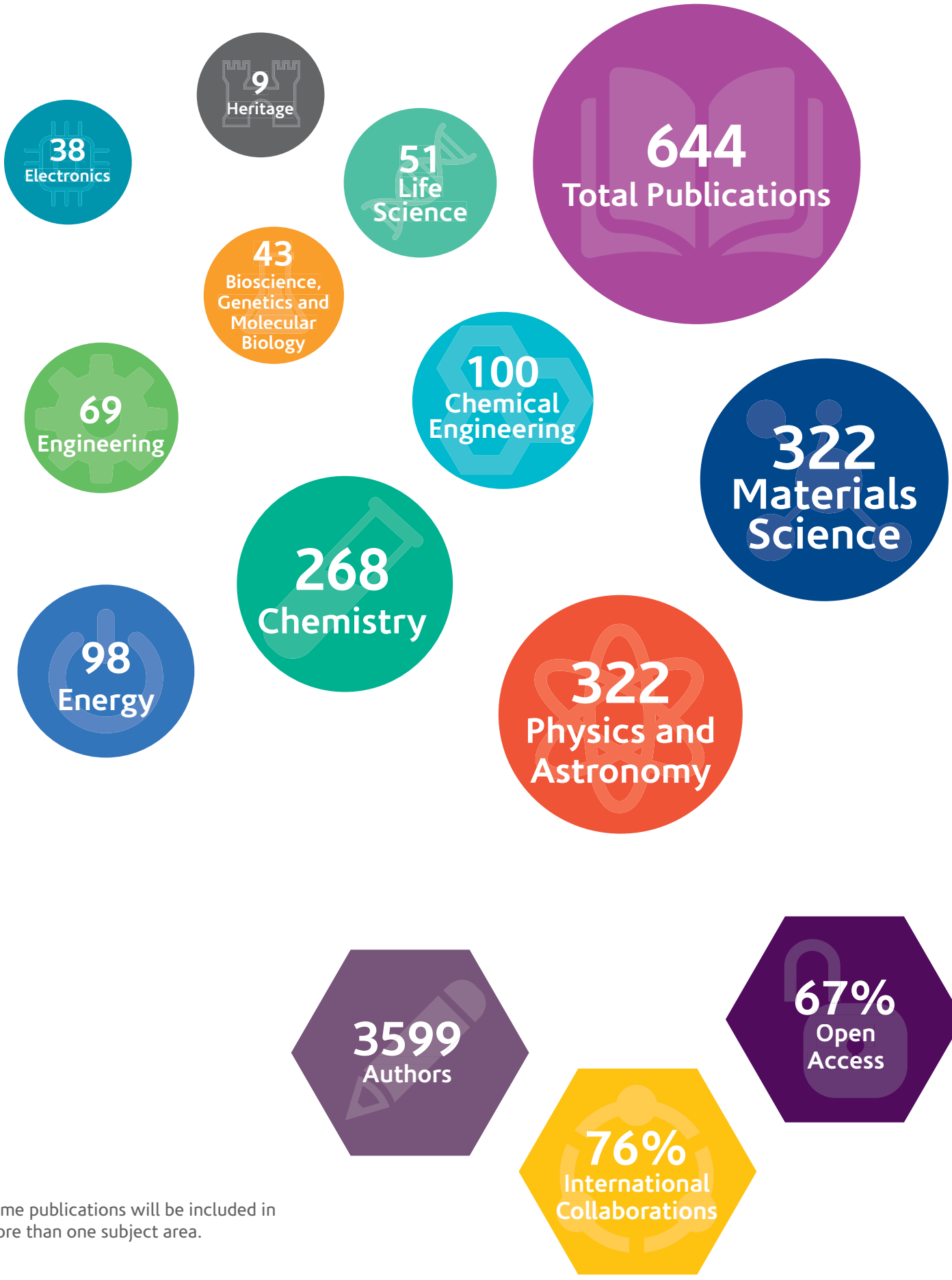
As access to neutrons in Europe is reducing, Endeavour will step up to provide this capability to the research community.



> "The Endeavour programme will make currently challenging measurements routine. The new capabilities will provide access into unknown research frontiers and provide the information for materials databases as part of an integrated cycle of materials discovery."
>
> **Professor Sean Langridge, Head of the ISIS Diffraction and Materials Division**

Science at ISIS





Some publications will be included in more than one subject area.

Left: Paul Frodsham from the Cryogenics team loading a sample into the MuSR instrument with Adrian Hillier.

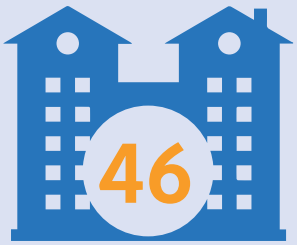
Engaging Industry

In 2020, 85 companies were associated with ISIS proposals across all access routes. Some companies appear in more than one sector.

Review of ISIS ICRD scheme

The ISIS Collaborative R&D programme (ICRD) was established in 2011 as more flexible access route for industry to perform measurements at ISIS than the standard proprietary access and Direct Access (peer–reviewed proposal) routes. Beamtime is free at point of use, and can be obtained very quickly. The proposals are reviewed based on the potential economic benefit to the UK and the results remain confidential during the period of the experiment and subsequent data analysis. The decision to put the results in the public domain or to keep them confidential through purchase is taken by the company after the experiment/measurement has been made and after some analysis undertaken to ascertain the commercial 'value' of the results to the company.

69 Total number of proposals



Companies using the scheme

430 Beam days

30 Publications

3 Patents

Johnson Matthey

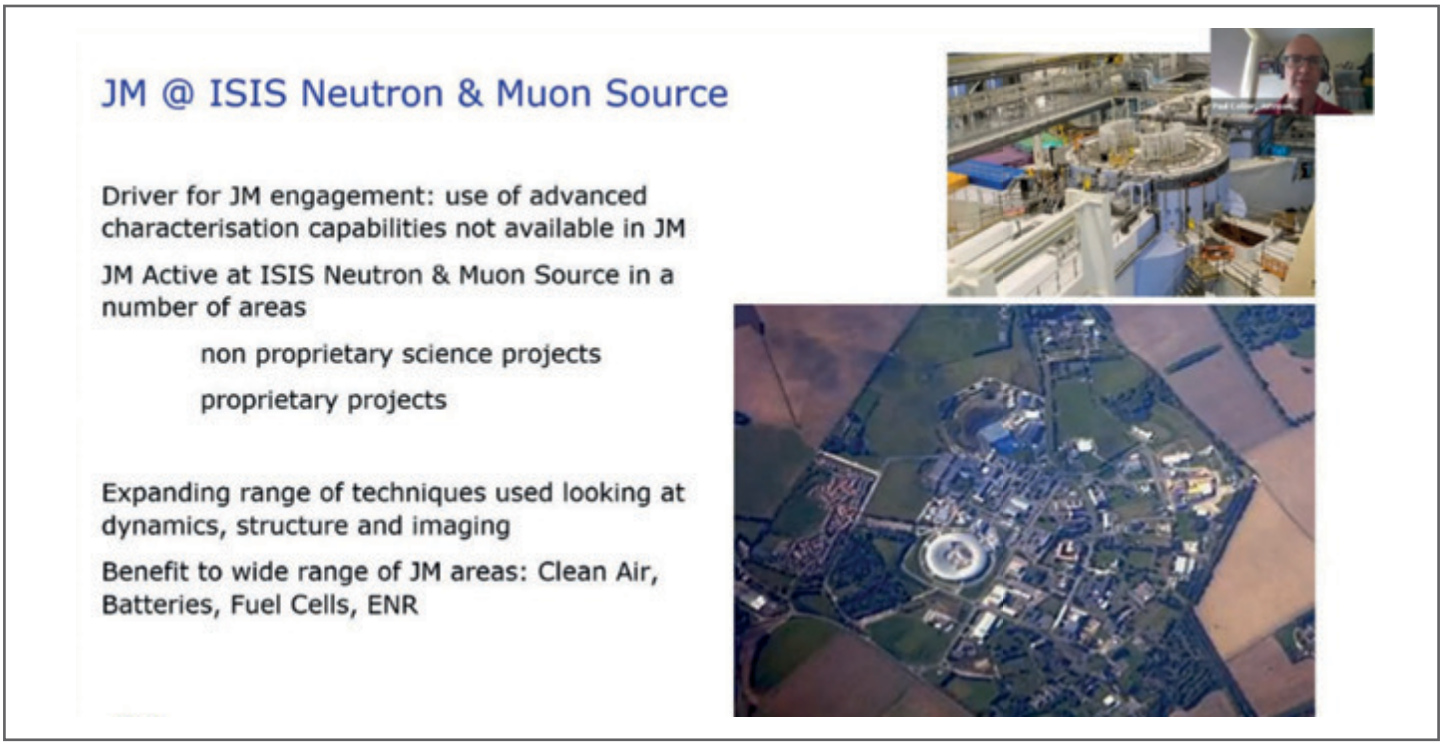
ISIS delivers industry-focussed neutron training to Johnson Matthey staff

On 13 and 21 July 2020, ISIS ran an online ISIS training event for scientific staff from Johnson Matthey to learn about neutron techniques and their applications.

The science and chemicals company Johnson Matthey (JM) has a very unique connection with ISIS: as well as using the facility many times for a variety of experiments, they jointly fund a research fellow, Hamish Cavaye. The aim of Hamish's role is to inform JM staff about neutron techniques, which can involve anything from making introductions to running experiments.

The training day was developed by Hamish, in collaboration with ISIS Business Development Manager, Graham Appleby, and JM Research Manager, Paul Collier. The aim was for JM scientists to gain a better awareness of what problems neutron techniques can solve, and how the techniques should be applied.

Although unable to go ahead with an in-person training day on site, two afternoon training sessions were run remotely on 13 and 21 July covering neutron spectroscopy, diffraction and imaging.



Roughly 30 participants from JM sites across the UK and USA tuned in, and the events were recorded so that other JM staff across the world could watch them later. "The event was very successful," explains Graham, "Surveys taken at the end of each day showed that, beforehand, only 50% of respondents had used neutrons before but, having finished the training, all of them thought that neutron techniques were relevant to their work, with 93% considering using neutrons in the future."

As well as Hamish, JM also jointly fund a research fellow with the Central Laser Facility, Kathryn Welsby, and she is now in the process of setting up a CLF training programme for JM, based on the ISIS one.

> "I think this has had a very positive impact in JM and we will no doubt see further interest in neutron techniques as a result of it."
> **– Paul Collier, JM Research Manager**

Finden and Infineum UK

IMAT helps to understand where and how coking occurs on engine components

A team of scientists from Finden Ltd, in collaboration with Infineum UK Ltd, have used IMAT to help understand where and how coking occurs on engine components. This understanding will help develop more durable, fuel efficient lubricants.

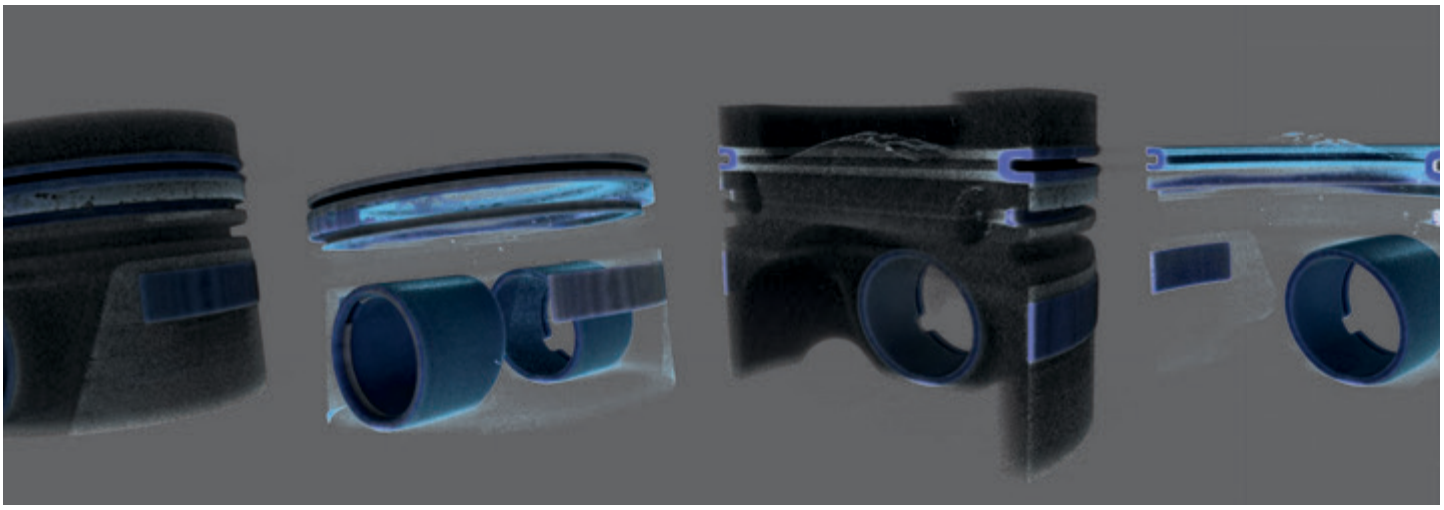
Coking of engine components can reduce efficiency and lifetime of engines (automotive, marine, aviation) through increased wear. Coked components have poorer thermal conductivity and act to insulate the engine components, leading to localised increases in temperature, which in extreme cases can lead to physical failure, e.g. cracking of the component. The coked material can also travel around the engine, blocking filters and narrow regions.

Visual appearance is often used to assess the performance of lubricating oils on components during engine testing; however this doesn't reveal deposit formation within a component. Current methods for assessing internal deposits are destructive, as often the component must be cut open – preventing continued use and damaging brittle coked deposits, potentially distorting the interpretation.

A key challenge in studying carbonaceous deposits on metal components is achieving appropriate contrast of a low-density material (the carbonaceous deposit) on top of a high-density substrate (the metal surface). Whilst X-ray imaging is able to achieve this with small components, the large size of engine components such as pistons or turbochargers strongly attenuates X-rays, meaning that inner surfaces are obscured.

In the proof-of-concept measurements performed at IMAT, the unique properties of neutrons allowed for the lighter carbonaceous deposits to be clearly imaged on both external and internal surfaces of the metal engine components, and quantified e.g. in terms of thickness, volume, area covered. The upcoming diffraction capabilities in IMAT will complement the imaging by revealing if any of the deposits have crystallised, and identifying their chemical composition.

Steve Price, Finden Ltd.
"These results mean that we can now quantify where and when coking occurs within engines – even looking at the same component before, during, and after an engine test, and identify how this is affected by different conditions and lubricants to help build a model of deposit formation and aging."



Neutron tomography performed on a piston at IMAT, allowing carbonaceous deposits on internal and external surfaces to be detected.

Instrument: IMAT

Rolls-Royce

Novel IMAT experiment helps Rolls-Royce Plc with crystal conundrum

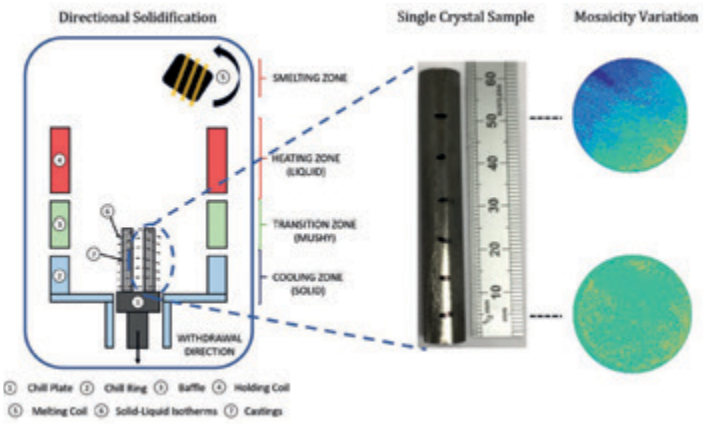
A new characterisation method has been used on the IMAT beamline to determine the 3D structure of materials used in gas turbine engines. For the first time, time-of-flight energy-resolved neutron imaging has been used to understand and visualise the inside of metallic single crystals used in gas turbine engines to improve their mechanical properties at high temperatures.

Trying to make these metallic single crystals is very challenging. The aim is to produce crystals that are large enough to be practical, but where all of the regions in the internal structure are all aligned in the same direction. A common issue with the crystals used in aerospace applications is that some regions are tilted with respect to the others, like in a mosaic, and this can affect the mechanical properties. Thanks to new software developments and the unique set up of the IMAT instrument, researchers have finally been able to investigate the cause of this tilting.

The samples in this study, published in *Scientific Reports*, were brought to ISIS by Rolls-Royce Plc, in collaboration with scientists from the University of Leicester as part of an ICRD measurement.

Joel Strickland, University of Leicester
"This study is of great interest to Rolls-Royce Plc, as mosaicity decreases a turbine blades high temperature performance, which ultimately results in a reduction in jet engine efficiency through lower turbine entry temperatures. Further, any mis-orientation related defects are a major cause of turbine blade non-conformance and scrappage."

This study establishes IMAT as a fundamental characterisation tool for studying the structure and properties of these materials in the future. In fact, the group have already returned to ISIS to continue their experiments on other samples.



Schematic sample preparation geometry and lowest transmission wavelength Bragg-dip distribution maps.

Instrument: IMAT

Related publication: "2D single crystal Bragg-dip mapping by time-of-flight energy-resolved neutron imaging on IMAT@ISIS." Sci Rep, 10, 20751 (2020)

DOI: 10.1038/s41598-020-77572-3

Funding: EPSRC and Rolls-Royce

Authors: J. Strickland, K. Tassenberg, G. Sheppard, B. Nenchev, S Perry, J. Li, H. Dong (University of Leicester), G. Burca (ISIS), J. Kelleher (ISIS), S. Irwin (Rolls-Royce Plc)

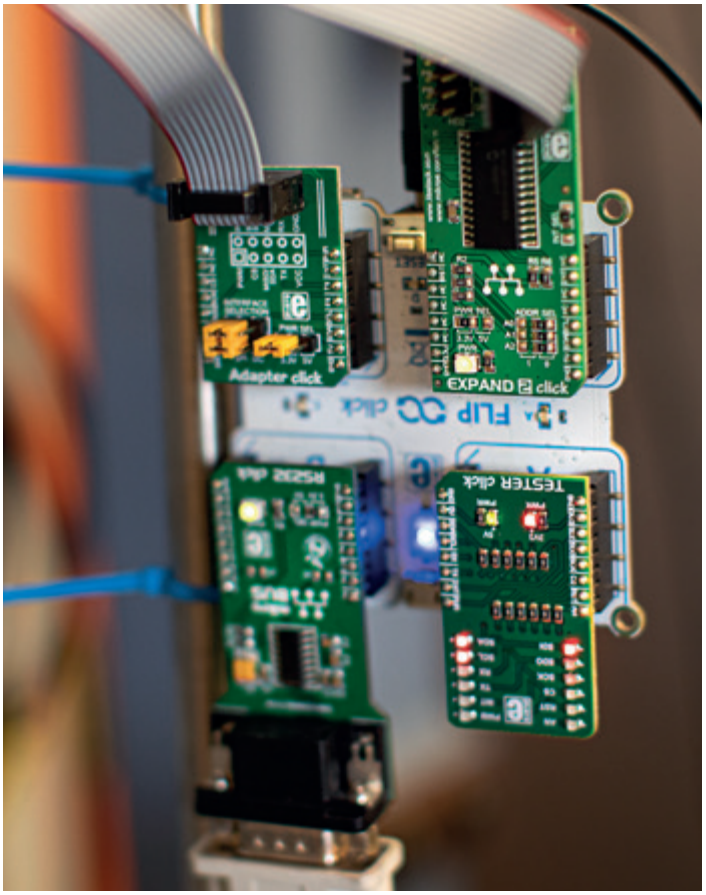
STMicroelectronics

ST tests transistors for aerospace and aviation

STMicroelectronics is a global semiconductor producer, with their products used in systems including the automotive industry, personal electronics and devices that may make up the Internet of Things of the future. Semiconductors are vulnerable to failure due to cosmic radiation, and understanding the potential rate of failure is important for companies like ST and their customers.

Neutron instruments such as ChipIr can replicate many years of neutron irradiation, enabling companies to test their electronics to determine their average failure rate and expected lifetime. In this study, published in *Sensors*, STMicroelectronics tested semiconductors like those used in applications in electrical vehicles, power grids and avionics, to study the effects of neutron damage.

They were able to build a comprehensive picture of how their devices behaved under different conditions by testing almost 2000 devices in a series of experiments at ChipIr and on TRIGA at the Mark II reactor in Italy. Their results enabled them to determine commonalities across different types of device, and the effect of the device technology on failure rate.



Instrument: ChipIr

Related publication: "Accelerated Tests on Si and SiC Power Transistors with Thermal, Fast and Ultra-Fast Neutrons." Sensors, 20, 11, 3021 (2020)

DOI: 10.3390/s20113021

Funding: STMicroelectronics and University of Palermo

Authors: F. Principato (University of Palermo), S. Altieri (University of Pavia and National Institute of Nuclear Physics), L. Abbene (University of Palermo) and F. Pintacuda (STMicroelectronics)

Right: Innes McClelland from the University of Sheffield, supervised by Professor Serena Corr, on the EMU instrument.

Impact Awards

ISIS Impact Awards 2021

2021 Science Impact Award Winner: Serena Corr – Applying muon spin relaxation spectroscopy to investigating ion diffusion in battery materials.

Science

Professor Corr and her team at the University of Sheffield have advanced the application of muon spin relaxation spectroscopy (μSR) to investigating ion diffusion across a range of industrially-relevant battery materials. This included the first in-situ μSR study of a functioning battery cell, permitting the study of diffusion processes occurring within individual battery components at different states of charge and, most recently, in developing a protocol for studying real batteries in operation using μSR.

The team, in collaboration with ISIS Instrument Scientist Dr Peter Baker, began with investigations into olivine cathodes, the positive electrode materials recently introduced in Tesla's Model 3, for which existing lithium diffusion property measurements spanned orders of magnitude. These studies, in good agreement with first principles studies, illustrated the benefit of applying μSR to interrogate ion diffusion across a breadth of these materials.

The team then investigated ceramic candidate solid electrolytes, which are safer alternatives to traditional liquid electrolytes, developing novel microwave chemistry methods to prepare the samples. Again using μSR, the results demonstrated the critical importance of applying multiple techniques to holistically probe diffusion properties. The next step was applying both μSR and neutron total scattering methods to a new class of safer solid electrolyte double perovskite materials, which the team synthetically realised and characterised using lattice-matching approaches to deliver a novel candidate solid state battery.

Having developed this extensive expertise, the team then turned its attention to successfully demonstrating the application of μSR to determining ion transport properties in polyatomic anionic cathodes containing fluoride ions. These were previously unexplored using muons due to potential muon-fluoride interactions making ion diffusion study difficult. Work then followed to uncover ion transport properties in next-generation cathodes, including doped high-nickel and disordered rock salt high-energy-density cathodes.

Most recently, the team has developed a new cell and testing protocol that will enable μSR investigations of materials within operating batteries for the first time. This technique provides new insights on crucial diffusion properties including ion diffusion in solid electrolytes and interfaces during operation.

μSR has emerged as an invaluable tool for the microscopic investigation of ionic motion in crystalline solids, e.g. in the study of intrinsic ionic conduction in electrode or solid electrolyte materials. The scientific impact delivered by the team's efforts is in determining diffusion and local structure properties of energy storage materials and in developing new in-situ methods to interrogate ion diffusion in these during operation. Their new battery cell for in-situ muon investigations was developed through an ISIS Facility Development Studentship held by Mr Innes McClelland and co-supervised by Corr, Baker and Dr Eddie Cussen, which has provided a new capability now available to (and being taken up by) the research community; for example, researchers at the Faraday Institution.

The team led by Professor Corr has demonstrated how non-destructive μSR will pave the way for following transport behaviour across emerging interfaces and provide insights to those researchers tailoring interfaces for optimising ion transport. These insights and the capability developed through her work has benefited both facility technique development and the wide community of international researchers working on next-generation battery materials.

ISIS Impact Awards 2021

2021 Economic Impact Award Winner: David Lennon – Probing the interactions of atoms and molecules with the surfaces of catalysts.

Economics

David Lennon's research involves applying a variety of spectroscopic techniques to probe the interaction of atoms and molecules with catalyst surfaces. Over the last two decades he has studied processes as varied as methane reforming to produce syngas (CO + H_2), Fischer-Tropsch synthesis to generate fuel and chemicals, the production of methyl chloride (an intermediate in polydimethylsiloxanes), understanding the formation, and the mitigation, of by-products in isocyanate synthesis (the monomers for polyurethane manufacture) and selective hydrogenation for fine chemical synthesis.

He has made a major contribution to the study of methanol-to-hydrocarbons (MTH) reaction, a reaction first commercialised in the 1970s. The reaction uses a zeolite catalyst, and while there is general agreement that the pores of the zeolite act as a microreactor, key details of what is happening inside the zeolite and how it deactivates are still debated.

The process reacts methanol, which is widely available from a variety of sources, including biomass, to a mixture of low molecular weight alkenes (mainly ethene, propene and butenes) and methylated aromatic molecules, i.e. gasoline. David's group at the University of Glasgow used neutron scattering to observe the 'vibrational fingerprint' of the hydrocarbon pool for the first time – that is, to see what is present in an active catalyst as it reacts. It also provided insight into the nature of the carbon that causes the catalyst to deactivate, which was surprisingly well-structured, resembling glassy carbon.

This project has produced fundamental insights into the process with direct industrial relevance, as demonstrated by two EPSRC industrial CASE awards provided by global science and chemicals company, Johnson Matthey, who also provided the catalysts and analytical characterisation.

David's group also applied neutron scattering to investigate how the same catalyst can be used to crack long chain alkenes to propene (propylene). This is a valuable commodity chemical that is the monomer for the vast range of products made from polypropylene. Their studies showed that the MTH and the alkene cracking reactions are strongly related, and both go by similar mechanisms, which had not been generally recognised. The work also studied the same catalyst after it had been steam de-aluminated – a process where steam at ~700°C is passed through a zeolite, greatly reducing the number of active sites by removing the aluminium. The resulting material is much more like that used in working industrial reactors and the reactivity is correspondingly modified. Surprisingly, these materials have been little studied academically and this new understanding helps explain why this is the material of choice industrially.

In addition to the specific knowledge gained about this reaction, this project has raised awareness within Johnson Matthey of the capabilities of neutron scattering and contributed to the creation of the Johnson Matthey - ISIS fellowship, which is about to be renewed for a further three years. See page 13 for more on the collaboration between ISIS and JM.

Separately, the wider ISIS user community have benefitted from a collaboration between David's group, the ISIS Pressure and Furnace section and the Molecular Spectroscopy Group. The Glasgow/ISIS catalysis rig has been developed over a number of years to prepare the large catalyst samples needed for neutron scattering (typically these are 100-1000 times larger than used in conventional micro-reactor lab-based studies). Recent major improvements to the rig include on-line quantitative analysis by gas chromatography and the ability to handle liquid products. The rig is heavily used by a variety of academic and industrial users and the recently enhanced capabilities are already popular with the user community.

ISIS Impact Awards 2021

2021 Society Impact Award Winner: Mariela Martins Nolasco on the characterisation of polymer structure and dynamics.

Society

Mariela Martins Nolasco (University of Aveiro, Portugal) has developed the ability to characterise polymer structure and dynamics, embracing both natural polymers (e.g. cellulose and bacterial cellulose) and bio-based synthetic polymers. This knowledge is critical in developing new functionalised or composite materials for use in emerging technologies such as medical devices or fuel cells.

Her approach took advantage of inelastic neutron scattering (INS) combined with discrete and periodic density functional theory (DFT) calculations to delve deeper into the structure–property correlations in polymeric materials. This combination is ideal either to assist the elucidation of measured data or, conversely, as method of validating theoretical models. The scientific impact of these projects arises from the recognition of the potential of INS spectroscopy to give answers to the questions relating the micro-structure and dynamics of polymer chains and the macroscopic properties of polymeric materials, including nano-structured and composite materials.

One class of polymers studied using INS was bio-based synthetic polymers (furandicaboxylate polyesters). These polymers are a new class of sustainable materials derived from renewable resources which are intended to gradually phase out their petrochemical counterparts.

Bio-based synthetic polymers could replace poly(ethylene terephthalate) (PET), a petro-based high performance polyester widely used as packaging material, offering good mechanical performance, comparable thermal stability, and increased barrier properties (approximately 10 times less permeable to oxygen and 20 times less permeable to carbon dioxide). Their industrial and commercial potential is already being implemented by industry stakeholders.

In addition, her comprehensive study of celluloses – in which the periodic-DFT calculations provide a detailed description of the vibrational spectra of bacterial and vegetal cellulose with different wet contents – set the grounds for the understanding of subtle interactions in cellulose-based composites and to assist the characterisation of bacterial cellulose membranes in microbial fuel cells. The comprehensive character and clarifying nature concerning the vibrational spectra of celluloses makes it possible to assess not only domains within the supramolecular structure, but also to identify the sample origin (bacterial, kraft pulp, etc) with high accuracy, a result of the resolution power of the INS technique.

Right: Beamline scientist Genoveva Burca and Tinashe Mawodza from the University of Sheffield on the IMAT instrument.

Science Highlights

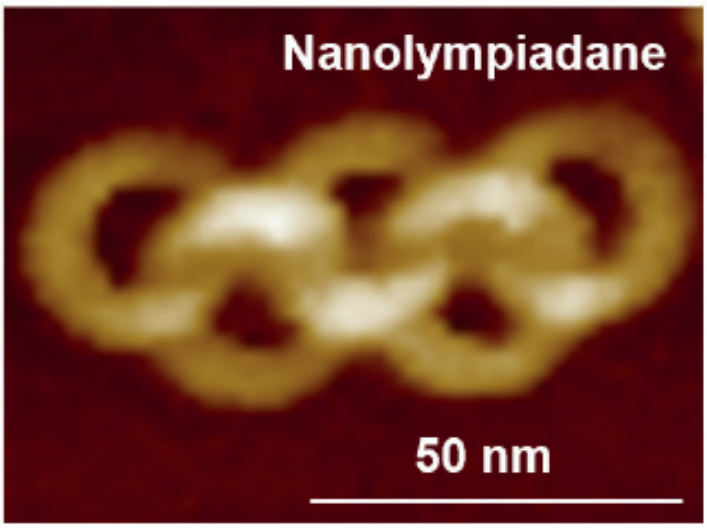
Zoom

Zoom experiment enables the formation of nanoscale Olympic rings

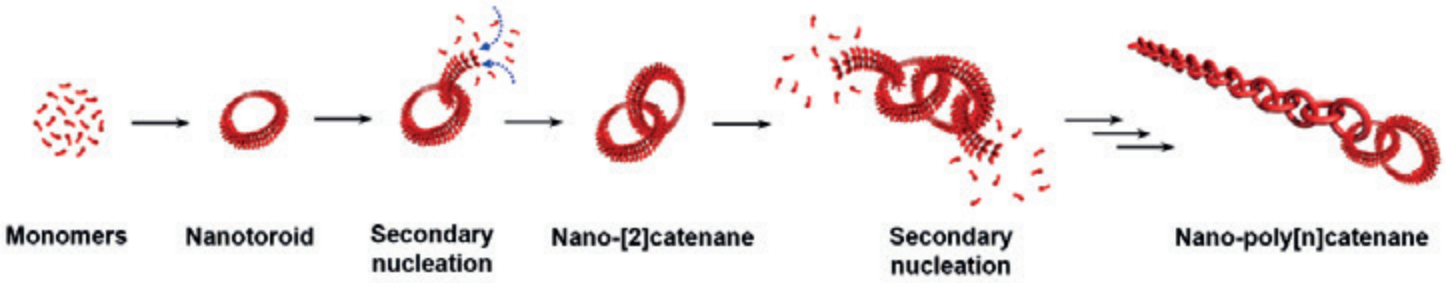
The first publication to come from an experiment on the newest ISIS instrument, Zoom, identified a nucleation mechanism that enabled a collaboration of research groups from Japan, Italy, Switzerland and the UK to form and study structures comprising of mechanically interlocked self-assembled rings, made solely from one molecular ingredient.

This work, published in *Nature*, is the first report of synthesis of nano-poly[n]catenanes via molecular self-assembly, without using an additional molecular template. By altering the self-assembly conditions, the group were able to create intricate structures of up to 22 rings, including a nano-[5]catenane with interlocked rings in a linear arrangement, which has been coined 'nanolympiadane'.

Given the size of these structures (already hundreds of nanometres), it is possible that only minor changes to the sequential addition process may build structures that are sufficiently large for purification by simple filtration. This would allow for in-depth study of the unique physical properties that a structure made up of miniscule interlocked chain links may have, and their potential for creating molecular machines.



Atomic force microscopy (AFM) image of nano-[5]catenane.



Self-assembly of a barbituric acid based molecule into nano-poly[n]catenanes.

Related publication: "Self-assembled poly-catenanes from supramolecular toroidal building blocks." Nature **583**, 400–405 (2020)

DOI: 10.1038/s41586-020-2445-z

Funding: The Japanese Ministry of Education, Culture, Sports, Science, and Technology (MEXT), Murata Science Foundation, Shorai Foundation for Science and Technology, Swiss National Science Foundation and the European Research Council. Computational resources provided by the Swiss National Supercomputing Centre (CSCS) and by CINECA

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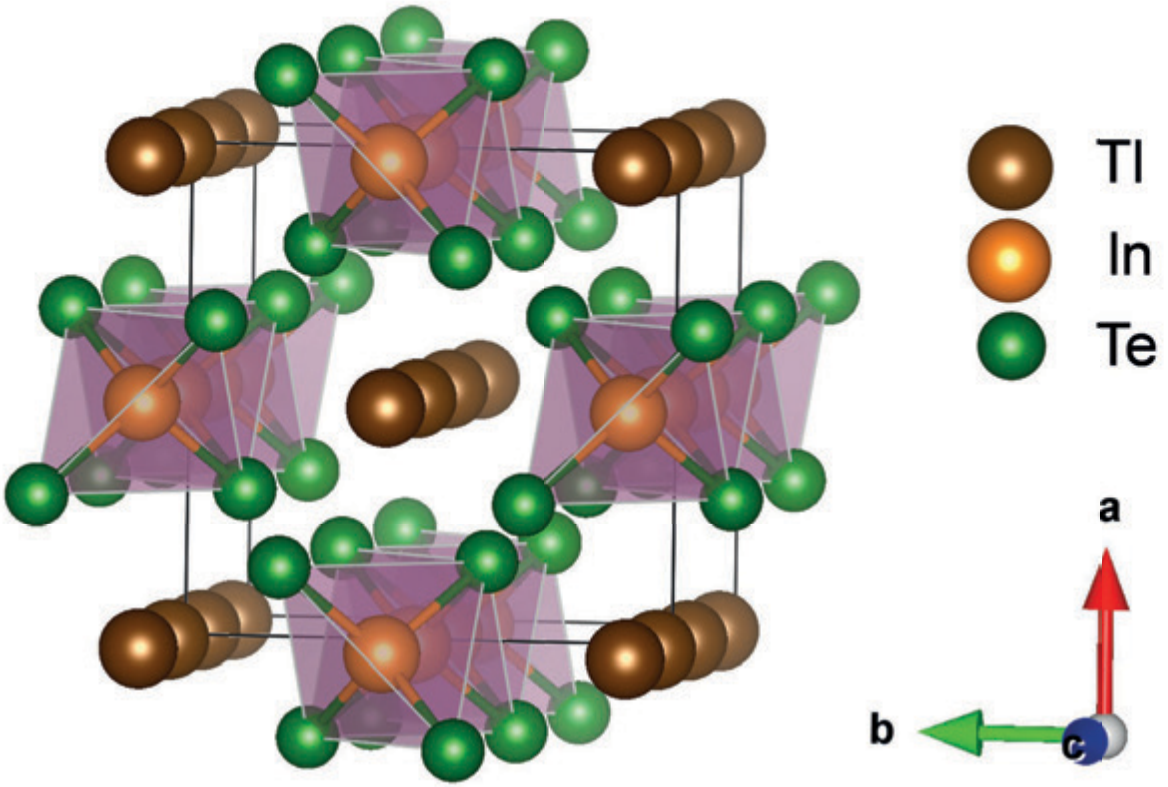
MARI

Rattling thallium explains low thermal conductivity

Understanding how heat travels through materials is important for a variety of technical applications. This includes thermoelectrics: materials that can generate electricity from the application of a temperature gradient, or vice versa. A key requirement of a thermoelectric material is that it should achieve low thermal conductivity without compromising the electrical properties, limiting the flow of heat via lattice vibrations known as phonons.

In this study, published in *Angewandte Chemie*, the researchers studied $TlInTe_2$, a material with an incredibly low thermal conductivity. They hoped to understand what causes this by studying the temperature dependent variation of the structure and vibrations of the material.

They uncovered that the vibrations of weakly bound thallium (Tl) disrupts other vibrations as they travel through the lattice. This process, described as 'rattling', is why it has such a low thermal conductivity. They hope this knowledge will be applied for designing new materials.



Structure of $TlInTe_2$ with weakly bonded Tl atom rattling along the crystallographic c-axis.

Related publication: "Evidence of Highly Anharmonic Soft Lattice Vibrations in a Zintl Rattler." Angew. Chem. Int. Ed., **60**, 8, 4259-4265 (2020)

DOI: 10.1002/anie.202013923

Funding: Science and Engineering Research Board, Department of Science and Technology, Sheikh Saqr Laboratory, International Centre for Materials Science and the University Grants Commission

Authors: M. Dutta, M. Samanta, T. Ghosh (Jawaharlal Nehru Centre for Advanced Scientific Research), D.J. Voneshen (ISIS), K. Biswas (Jawaharlal Nehru Centre for Advanced Scientific Research)

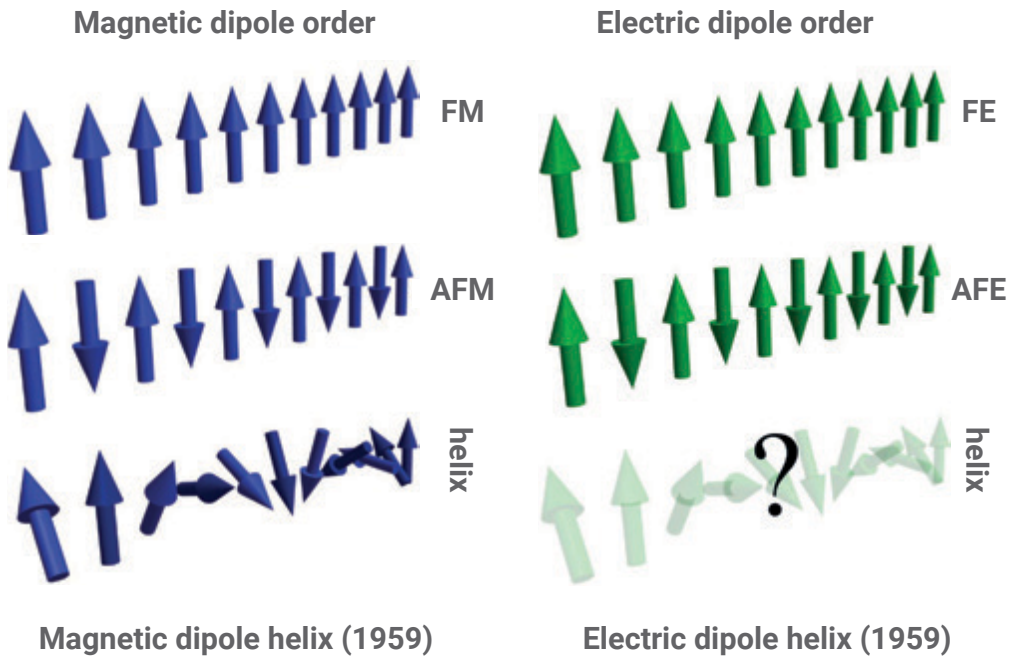
WISH

First bulk observation of helical ordering of electric dipoles

The long-range ordering of magnetic and/or electric dipoles are canonical causes of phase transitions in crystalline materials, and they are both associated with a variety of functional properties. In addition to ferromagnetism and antiferromagnetism, many types of non-collinear magnetic ordering have been found since the late 1950s, such as those in which magnetic dipoles rotate describing helical patterns.

By contrast, only parallel (ferroelectric) and antiparallel (antiferroelectric) alignments of electric dipoles have thus far been reported. This gives rise to a natural question: are there electric-dipole counterparts to the most complex magnetic structures found to date? In this study, published in *Science* nearly sixty years after the discovery of helical magnetism, the researchers describe the first example of helical ordering of electric dipoles, thus completing the analogy between ordering of magnetic and electric dipoles in the solid state.

The authors demonstrate that the helical ordering of electric dipoles occurs due to the microscopic competition between two instabilities that are present in the crystal structure of $BiCu_xMn_{7-x}O_{12}$. One of them favours a conventional ferroelectric state, while another is associated with other structural distortions that are unrelated to the local charge separation. The helical ordering of electric dipoles emerges as a delicate balance these instabilities, which is finely tuned by modifying the concentration of Cu substituted for Mn.



The different orderings of magnetic and electric dipoles.

Related publication: "Emergent helical texture of electric dipoles." Science, **369**, 6504, 680-684 (2020)

DOI: 10.1126/science.aay7356

Funding: STFC, the Royal Society and ATLA, Japan

Authors: D.D. Khalyavin (ISIS), R.D. Johnson (University College London, University of Oxford), F. Orlandi (ISIS), P.G. Radaelli (University of Oxford), P. Manuel (ISIS), A.A. Belik (National Institute for Materials Science)

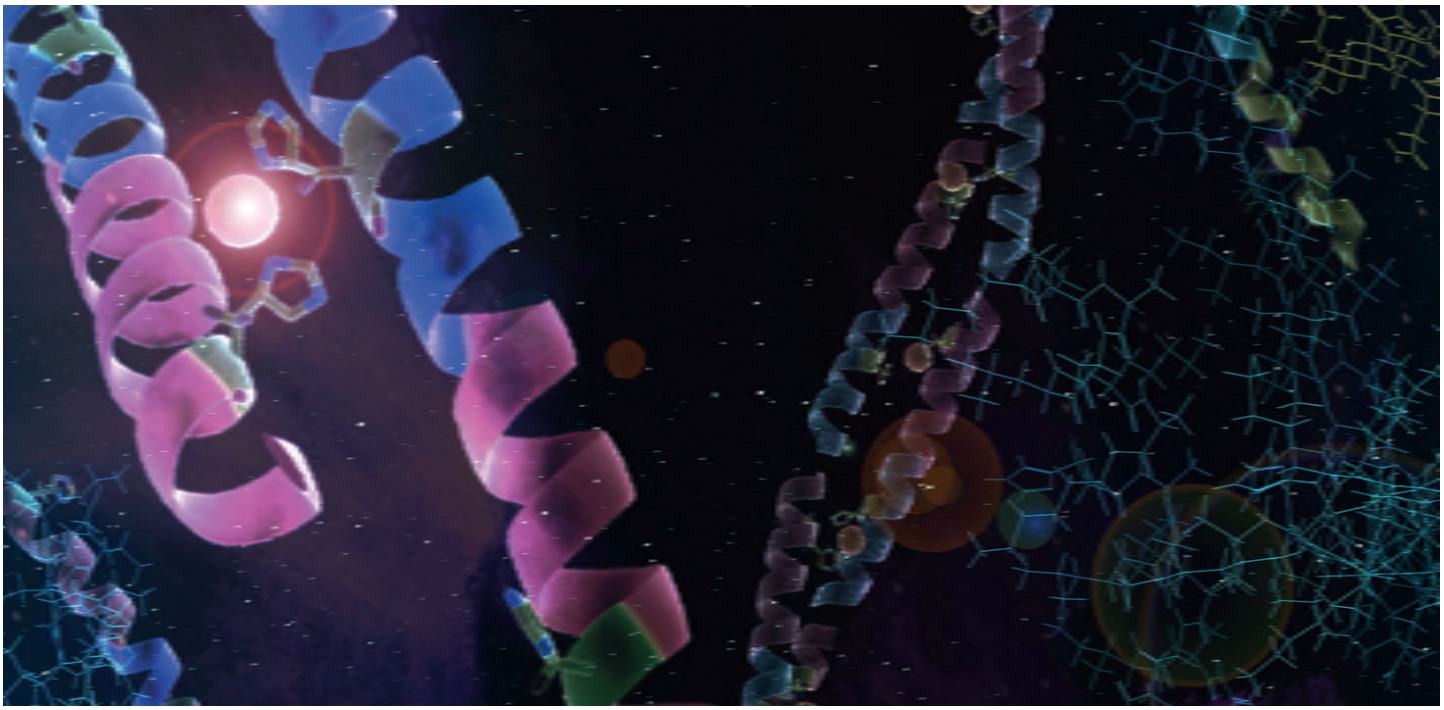
LOQ

Nanostructures formed by self-assembling peptides

In proteins, chains of amino acids known as peptides are arranged in the form of an α helix. The peptides assemble into these helices because of the favourable formation of hydrogen bonds and other non-covalent interactions. Being able to control this self-assembly could open possible applications in tissue engineering, regenerative medicine and even organic semiconductors.

In this study, published in Small, researchers designed a series of helical peptides and studied their self-assembly behaviour. Using a range of techniques, including neutron scattering, they were able to determine the effect of the different noncovalent interactions on the nanostructure formed.

The system they have developed is a straightforward and versatile self-assembly method for creating complex biomolecules. As well as developing a system that could have applications in medicine, the work also provides a convenient approach for building biologically-inspired functional architectures for potential applications in functional materials and catalysis.



The hierarchical self-assembly of the His-containing helical peptide HH driven by Cu^{2+} coordination.

Related publication: "Ordered Nanofibers Fabricated from Hierarchical Self-Assembling Processes of Designed α-Helical Peptides." Small, **16**, 45, 2003945 (2020)

DOI: 10.1002/smll.202003945

Funding: National Natural Science Foundation of China, Syngenta, University of Manchester, Innovate UK, Lonza, BBSRC and AstraZeneca

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ChipIr

Simulated moon dust on ChipIr

A research group has used ChipIr to study lunar soil analogues to investigate their potential use for radiation shielding of future lunar habitats. Establishing a manned Moon base will involve building habitats that will need shielding from meteoroids and space radiation. The practice of harnessing local resources for human or robotic exploration, known as in situ resource utilisation, is becoming increasingly important, allowing materials found at the exploration site to replace materials otherwise brought from Earth. This would reduce the costs and risks of exploratory missions.

It has been proposed that the unconsolidated solid material that covers the surface of the moon, known as lunar regolith, could be used as a general construction material on a lunar base. Through processing techniques such as sintering, a method to fuse granular material together by applying high temperature high temperature, simulants of lunar regolith can be fused together to form solid construction blocks. This study, published in *Radiation Measurements*, investigated the effect of these processes on the shielding capability of the regolith. Neutrons on the moon are produced by spallation interaction of primary cosmic rays on materials, the same process as on the ISIS neutron source. Therefore, the fast neutrons on ChipIr are representative of cosmic ray neutrons in space. By subjecting their samples to the stream of high-energy neutrons, and comparing their results with computer simulations, they were able to estimate the required level of shielding needed to cope with galactic cosmic rays and solar particle events.

Example of regolith samples derived from 3D printing of a model building block for the outer shell of a lunar base.

Related publication: "Neutron radiation shielding with sintered lunar regolith." Radiation Measurements, **132**, 106247 (2020)

DOI: 10.1016/j.radmeas.2020.106247

Funding: ESA Technology Development Element programme and the German Aerospace Center Institut für Materialphysik im Weltraum

Authors: A.Meurisse (ESA-ESTEC), C.Cazzaniga, C.Frost (ISIS), A.Barnes (ESA/ECSAT), A.Makaya, M.Sperl (Institut für Materialphysik Im Weltraum)

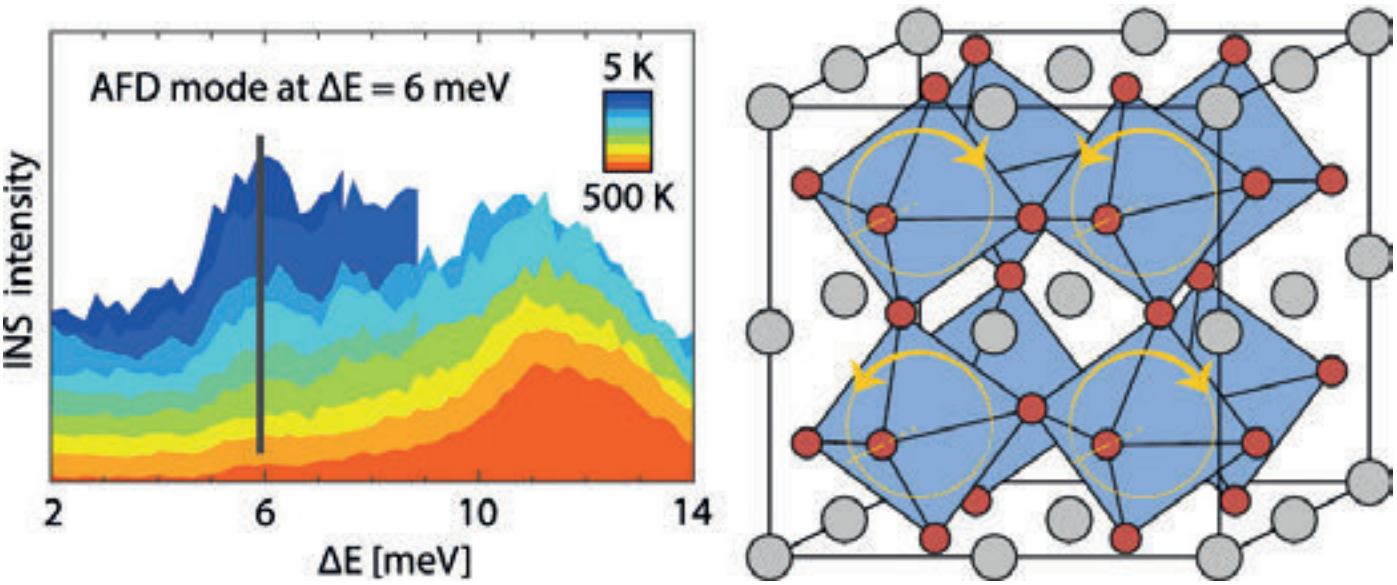
Vesuvio

Investigating perovskite ground state structures on Vesuvio

Barium zirconate, $BaZrO_3$, is a widely used material, and has the potential for application in a range of different technologies including fuel cells and hydrogen separation membranes. However, fundamental questions surrounding the crystal structure of $BaZrO_3$, especially in regard to its ground state structure, remain.

In this study, published in *Chemistry of Materials*, the researchers used a combination of high-resolution neutron powder diffraction, inelastic neutron scattering (INS), neutron Compton scattering (NCS), and first-principles density functional theory calculations to investigate the ground state structure of $BaZrO_3$.

They found that the first-principles calculations are highly sensitive to the choice of the exchange-correlation functional and that a correct description about the ground state structure requires the use of hybrid functionals. Combined analyses of neutron and computational data based on hybrid functionals showed that the ground state structure is cubic. This study illustrates that NCS is a powerful technique, not only for the study of very light atoms such as hydrogen, which is performed routinely, but also for heavier atoms in complex materials.



Inelastic neutron scattering data and structural model of the antiferrodistortive mode in $BaZrO_3$.

Related publication: "Unraveling the Ground-State Structure of $BaZrO_3$ by Neutron Scattering Experiments and First-Principles Calculations." Chem. Mater., 32, 7, 2824–2835 (2020)

DOI: 10.1021/acs.chemmater.9b04437

Funding: Swedish Research Council, the Swedish Energy Agency and the Swedish Foundation for Strategic Research. Partially supported within the CNR-STFC Agreement

Authors: A. Perrichon, E.J. Granhed (Chalmers University of Technology), G. Romanelli (ISIS), A. Piovano (ILL), A. Lindman, P. Hyldgaard, G. Wahnström and M. Karlsson (Chalmers University of Technology)

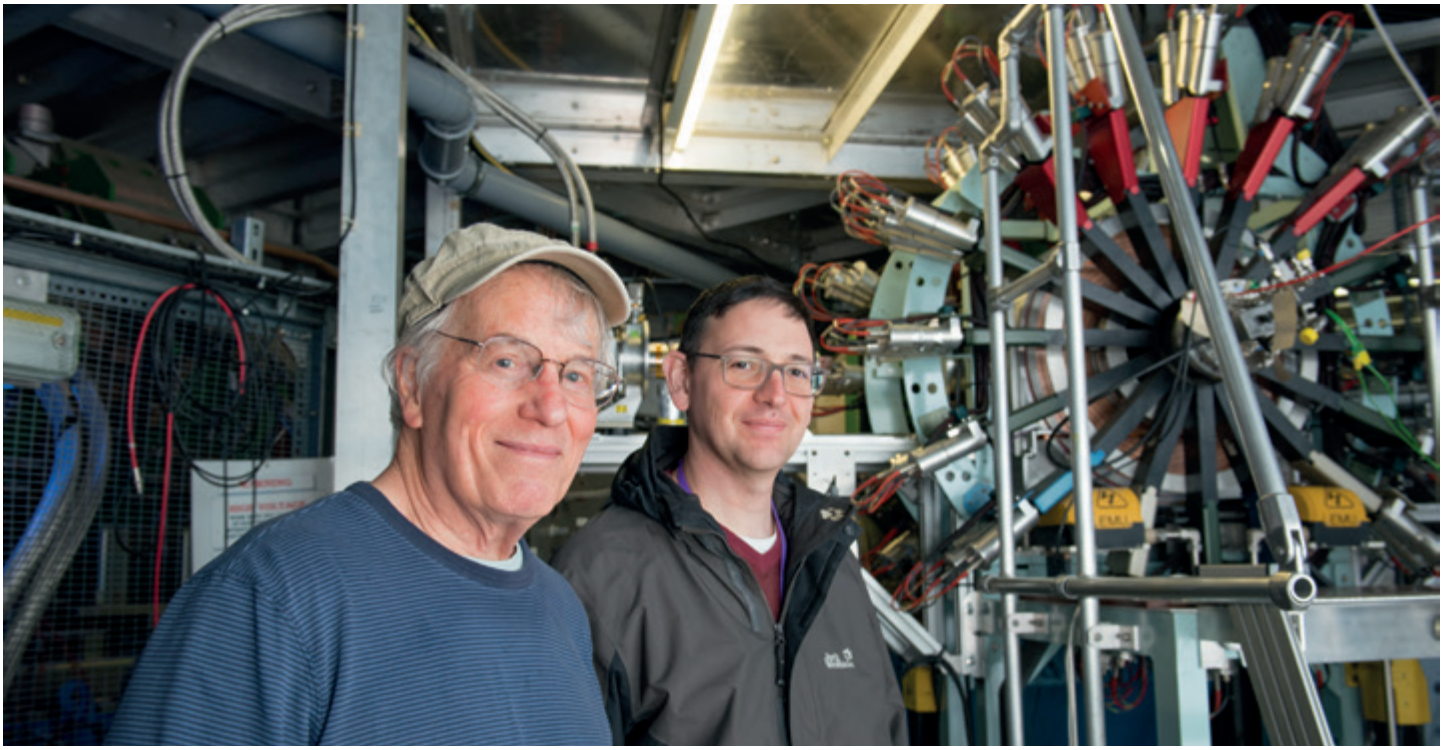
EMU

Quantum tunnelling plays a major role in muonium reactions with larger alkanes

Muonium (Mu = μ^+e^-), formed spontaneously when muons are stopped in many materials, acts as the lightest isotope of hydrogen. By measuring the kinetics of its reactions, and comparing with other hydrogen isotopes, scientists are able to quantify its kinetic isotope effects (KIEs). This study, published in *PCCP*, focuses on the abstraction of a hydrogen atom from propane and n-butane by muonium, and compares this with similar to similar reactions of the hydrogen atom.

Unlike previous experiments on the lighter alkanes, methane and ethane, their results showed that quantum tunnelling plays a much more major role than expected. Through their uniquely important experiments, these researchers showed that tunnelling had a dramatic effect on the reaction rates.

The outcome of this study posed a considerable challenge to accepted reaction rate theory on hydrogen-atom reactions in alkane systems. Recent work by Gao et. al. has partially addressed this challenge, but discrepancies between quantum theory and experiment still remain. In the future, these researchers plan on using additional techniques to fully probe both the degree and effects of this tunnelling behaviour.



Don Fleming and Abdel Jawad on the EMU instrument.

Related publications: "Rate constants and kinetic isotope effects for H-atom abstraction reactions by muonium in the Mu + propane and Mu + n-butane reactions from 300 K to 435 K: challenges for theory." Phys. Chem. Chem. Phys., **22**, 6326-6334 (2020)

DOI: 10.1039/C9CP06822H

Funding: European Commission and NSERC (Canada)

Authors: D.G. Fleming (TRIUMF and University of British Columbia), D.J. Arseneau (TRIUMF), S.P. Cottrell and J.N.T. Peck (ISIS)

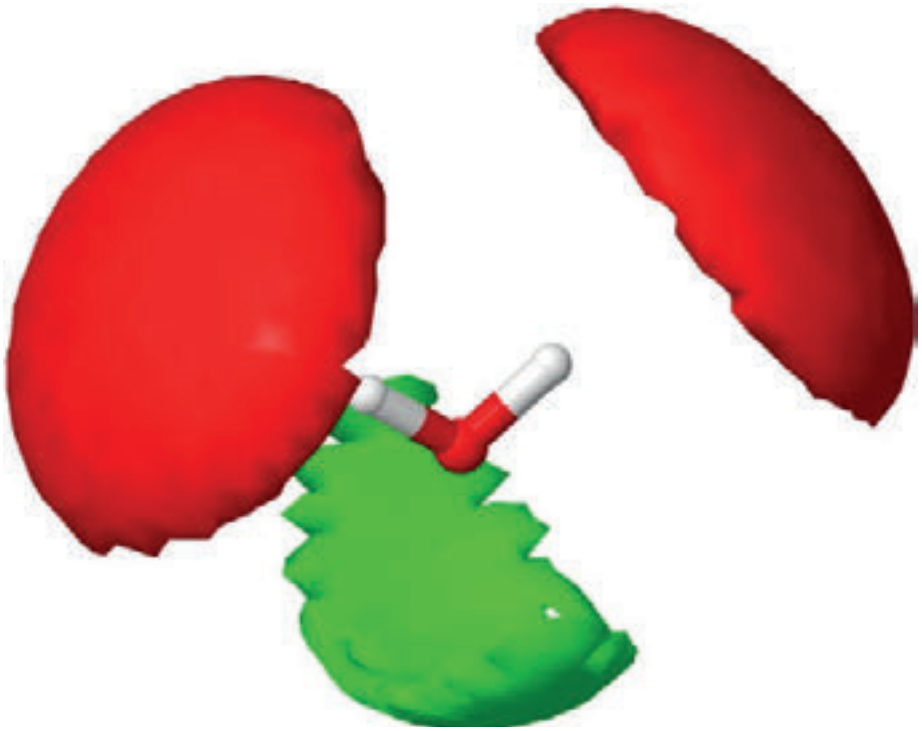
Sandals

Size of magnesium ion more important than its strength when attracting water molecules

Minerals are crucial for many organisms. Amorphous calcium carbonate (ACC) is one of the most widespread biogenic minerals and it plays a central role in the formation of skeletal elements of many animals, for example molluscs. Commonly seen in ACC is the stabilising effect of magnesium ions. This was thought to be due to magnesium's high dehydration energy causing it to bind water more strongly, but recent work suggests other factors may be at play.

By studying the effect of increasing the magnesium content in a mixed magnesium-calcium system, this study was able to show that the stabilising effect is actually unlikely to be due to the magnesium ion alone but also to the hydroxide ions that co-precipitate with it. Moreover, using a combination of neutron and X-ray total scattering with computational fitting, the researchers were able to see that the small size of the magnesium ion restricts the number of water molecules that can bind to it.

As a result, roughly a third of water molecules in the pure magnesium phase are bound exclusively to other water molecules and anions. When the larger calcium ion is introduced, this proportion goes down to closer to 10%. As the interaction of water with other water molecules and anions is a hydrogen bond, which is weaker than the coordinative interaction with cations, water is also able to diffuse faster through the pure magnesium phase than through those containing calcium.



Spatial density function showing the hydroxide, carbonate, calcium, and magnesium ions in the local water environment in the mixed phase.

Related publication: "Small Ionic Radius Limits Magnesium Water Interaction in Amorphous Calcium/Magnesium Carbonates." J. Phys. Chem. C, **124**, 11, 6141–6144 (2020)

DOI: 10.1021/acs.jpcc.9b11594

Authors: A.C.S. Jensen (Max Planck Institute of Colloids and Interfaces, Queen Mary University of London, Imperial College London), S. Imberti (ISIS), W.J.E.M. Habraken, and L. Bertinetti (Max Planck Institute of Colloids and Interfaces)

Inter

The effect of chain length and water content on ionic liquid behaviour

Ionic liquids have the potential for application in a range of industries, including green energy technologies such as fuel cells and providing lubrication by changing surface charges and reducing friction. However, the presence of water in an ionic liquid can have a big influence on its properties and, where halogens are present, it can react to produce toxic by-products.

By studying a halogen-free ionic liquid and its interactions with a gold surface under both wet and dry conditions, researchers have been able to gain an insight into how the presence of water influences these interactions. The charged nature of the ionic liquid means that its interfacial properties can be controlled using an applied potential, and the group found that this control was strongly affected by the presence of water but that it was still possible to achieve.

The researchers also studied the effect of changing the alkyl chain length of components of a non-halogenated ionic liquid. They found that, if the alkyl chain is sufficiently long, the interaction between the molecules becomes more dominant than that from the charged surface, with the longer chain liquids forming cation bilayers.

These two studies confirm the feasibility of using non-halogenated ionic liquids for lubrication, even in the presence of water. Further investigations into the wear behaviour of the system will inform its feasibility for wider use.

Georgia Pilkington, KTH, Royal Institute of Technology, Stockholm, Sweden, preparing samples for an experiment on the INTER instrument.

Related publication: "Effect of water on the electroresponsive structuring and friction in dilute and concentrated ionic liquid lubricant mixtures." Phys. Chem. Chem. Phys., **22**, 28191-28201 (2020); "Interfacial structuring of non-halogenated imidazolium ionic liquids at charged surfaces: effect of alkyl chain length." Phys. Chem. Chem. Phys., **22**, 8450-8460 (2020)

DOI: 10.1039/D0CP05110A; DOI: 10.1039/D0CP00360C

Funding: Knut and Alice Wallenberg Foundation, the Swedish Research Council and the Swedish Foundation for Strategic Research

Authors: G.A. Pilkington, A. Oleshkevych, S. Watanabe, P. Pedraz, M. Radiom (KTH Royal Institute of Technology), R.Welbourn (ISIS), S. Glavatskih (KTH Royal Institute of Technology, Ghent University) and M.W. Rutland (KTH Royal Institute of Technology, RISE Research Institutes of Sweden)

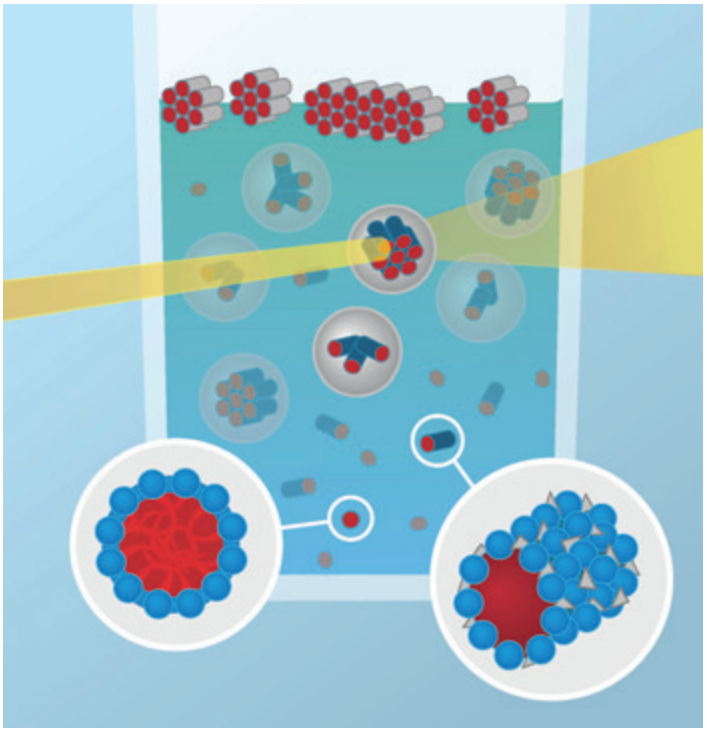
Larmor

Investigating silica-surfactant interactions: when two techniques are better than one

By combining traditional Small Angle Neutron Scattering (SANS) and Spin-Echo Modulated Small Angle Neutron Scattering (SEMSANS) for the first time, an international collaboration was able to investigate the mechanism behind the initial growth of mesostructured silica-surfactant particles at the nano- and micro-metre scales simultaneously. The study, published in *ACS Applied Materials & Interfaces*, provides valuable insights on the formation of these particles, which are the precursors to thin films that grow at the solution interface.

Two possible mechanisms for the self-assembly of these films from a silica-surfactant system have been suggested, but neither has previously been confirmed experimentally. This study used the unique combination of SANS and SEMSANS on Larmor to study the behaviour of the micelles and growing particles in solution to determine which mechanism occurs under these conditions.

The researchers were able to see the surfactant micelles elongate on addition of the silica species, before they aggregate to form droplets. After this droplet formation has occurred, the micelles inside the droplet order into large particles with an ordered mesostructure. The particles then migrate to the air/liquid interface, forming the thin film. The ability to manipulate the structure of mesoporous thin films, and the pore size within them, gives the films potential applications in a wide variety of fields including catalysis and drug-delivery.



Schematic of the surfactant-silica solution and the formation of a microporous thin film.

Related publication: "Mesoporous Silica Formation Mechanisms Probed Using Combined Spin–Echo Modulated Small-Angle Neutron Scattering (SEMSANS) and Small-Angle Neutron Scattering (SANS)." ACS Appl. Mater. Interfaces, 12, 25, 28461–28473 (2020)

DOI: 10.1021/acsami.0c03287

Funding: Dutch Research Council, Oak Ridge National Laboratory, U S Department of Energy and the US Department of Commerce

Authors: J. Schmitt (University of Bath), J.J. Zeeuw (University of Bath, Delft University of Technology), J. Plomp, W.G. Bouwman (Delft University of Technology), A.L. Washington, R.M. Dalgliesh (ISIS), C.P. Duif, M.A. Thijs (Delft University of Technology), F. Li (Oak Ridge National Laboratory), R. Pynn (Oak Ridge National Laboratory, Indiana University), S.R. Parnell (Delft University of Technology) and K.J. Edler (University of Bath)

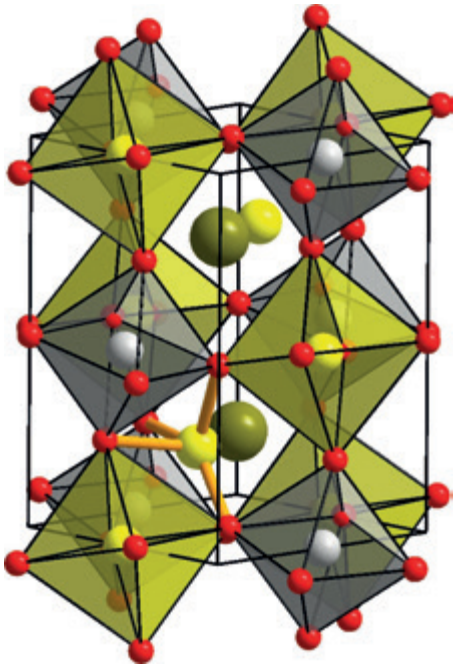
Polaris and EMU

New solid state battery material for next generation batteries

In a solid-state battery, a solid electrolyte component replaces the liquid electrolyte, improving the safety and the amount of energy that the battery can store. However, using a solid-state electrolyte brings other challenges, such as resistance and chemical incompatibility with the electrodes.

This study, published in *Nature Communications*, reports the development of a new family of materials that contains suitable candidates for both the electrode and the electrolyte. This leads to more compatible and stable interfaces between the two. The research group used computational modelling to design the materials by tweaking the chemical composition. They then brought the materials to ISIS to confirm their predictions using neutron diffraction and muon spectroscopy.

Their new materials take the perovskite structure, with one containing tungsten and the other tellurium, leading to excellent compatibility. Both contain a high concentration of lithium ions in their crystal structure, which provides fast lithium-ion diffusion. They found that, while tungsten can readily change oxidation state – ideal for an electrode – tellurium is resistant to redox cycling suitable for the electrolyte. As well as testing the materials separately, the group also combined them in a single hybrid solid-state cell, and found that the electrode functionality was maintained.



Crystal structure of $Li_{1.5}La_{1.5}MO_6$ double perovskites.

Dr Marco Amores, Austrian Institute of Technology
"Our work opens up the possibility to expand this approach to other families of materials, contributing towards the ultimate goal to speed up the realisation of solid-state batteries for a safer and increased energy storage technology."

Dr Eddie Cussen, University of Sheffield
"Our strategy to stabilise the solid/solid interface uses a shared crystal structure, with a minimal difference in composition, for electrolyte and electrode to give an ensemble with chemical and mechanical compatibility."

Related publication: "$Li_{1.5}La_{1.5}MO_6$ (M = W^{6+}, Te^{6+}) as a new series of lithium-rich double perovskites for all-solid-state lithium-ion batteries." *Nature Communications*, **11**, 6392 (2020)

DOI: 10.1038/s41467-020-19815-5

Funding: EPSRC, Faraday Institution, STFC, Diamond Light Source and the Universities of Sheffield, Glasgow, Strathclyde and Loughborough

Authors: M. Amores, H. El-Shinawi, I. McClelland (University of Sheffield), S.R. Yeandel (Loughborough University), P.J. Baker, R.I. Smith, H.Y. Playford (ISIS), P. Goddard (Loughborough University), S.A. Corr & E.J. Cussen (University of Sheffield)

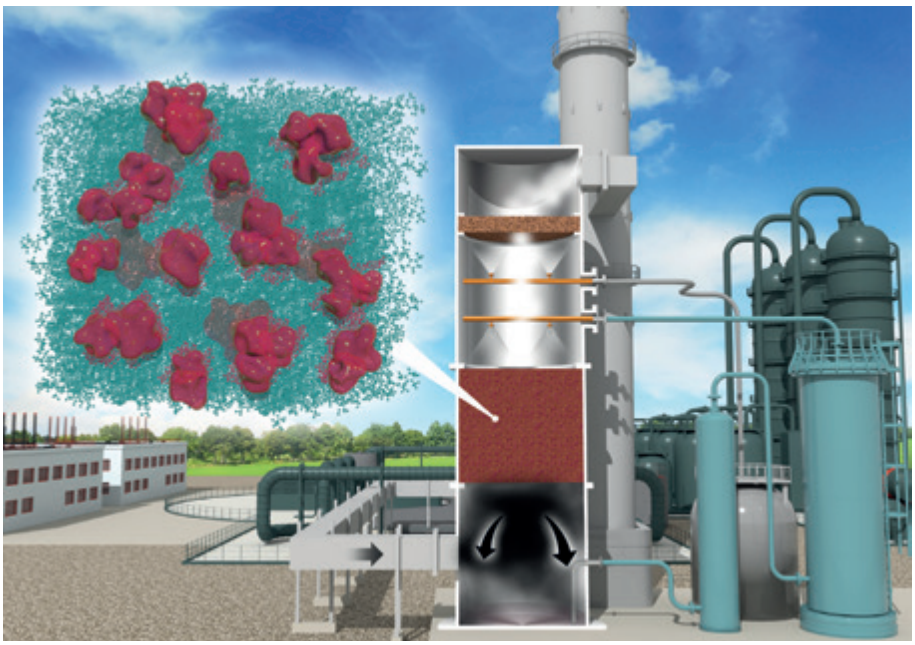
Nimrod and Larmor

Novel method of studying glassification could revolutionise future carbon capture technology

This work is the first to focus on the process of glassification in carbon capture solvents, and how working above glass transition temperature can minimise the formation of failure-causing clusters and prompt more efficient testing of carbon capture and sequestration technology.

Solvent-based technology is the most mature post-combustion carbon capture solvent technology that is undergoing testing. The advantage of using solvent-based technologies is that their formulation can be designed to reduce the amount of water, and thus the amount of energy used. This study, published in *PCCP*, looked at concentrated solvents known as CO_2-binding organic liquids, or CO_2BOLs.

Using new spectroscopic measurements on ISIS instruments Nimrod and Larmor alongside computation, they measured the changes in the CO_2BOL 1-IPADM-2-BOL under different temperatures. They found that the heating and cooling of these clusters is reversible and temperature-dependent, much like a glass transition. Crucially, they saw a first-order phase transition at 40°C, which is near to the absorption temperature for post-combustion CO_2 capture processes.



Schematic showing the CO_2BOL during application in carbon storage.

Related publication: "Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents." Phys. Chem. Chem. Phys., **22**, 19009-19021 (2020)

DOI: 10.1039/D0CP03503C

Funding: United States Department of Energy

Authors: J.L. Bañuelos (The University of Texas), M-S. Lee, M-T. Ngyuen, D. Zhang, D. Malhotra, D.C. Cantu, V-A. Glezakou, R. Rousseau (Pacific Northwest National Laboratory), T.F. Headen, R.M. Dalgliesh (ISIS), D.J. Heldebrant, T.R. Graham (Pacific Northwest National Laboratory, Washington State University), K.S. Han (Pacific Northwest National Laboratory) and S.R. Saunders (Washington State University)

Tosca

Neutrons optimise high efficiency catalyst for greener approach to biofuel synthesis

Researchers have designed a catalyst that converts biomass into fuel sources with remarkably high efficiency, offering new possibilities for manufacturing advanced renewable materials. Neutron scattering experiments played a key role in determining the chemical and behavioural dynamics of the new zeolite catalyst NbAlS-1 to provide information for maximising its performance.

The optimised catalyst converts biomass-derived raw materials into light olefins such as ethene, propene, and butene, which can then be used to make plastics and liquid fuels. Their study, published in *Nature Materials*, finds that the new catalyst has a yield of 99%, whilst requiring significantly less energy than its predecessors.

Typically, the chemical conversion of the organic matter to smaller molecules requires a tremendous amount of energy. Investigating possibilities for a greener alternative, the team doped the catalyst by replacing the zeolite's silicon atoms with niobium and aluminium. The substitution created a chemically unbalanced state that promotes bond activation and radically reduces the need for high temperature treatments.

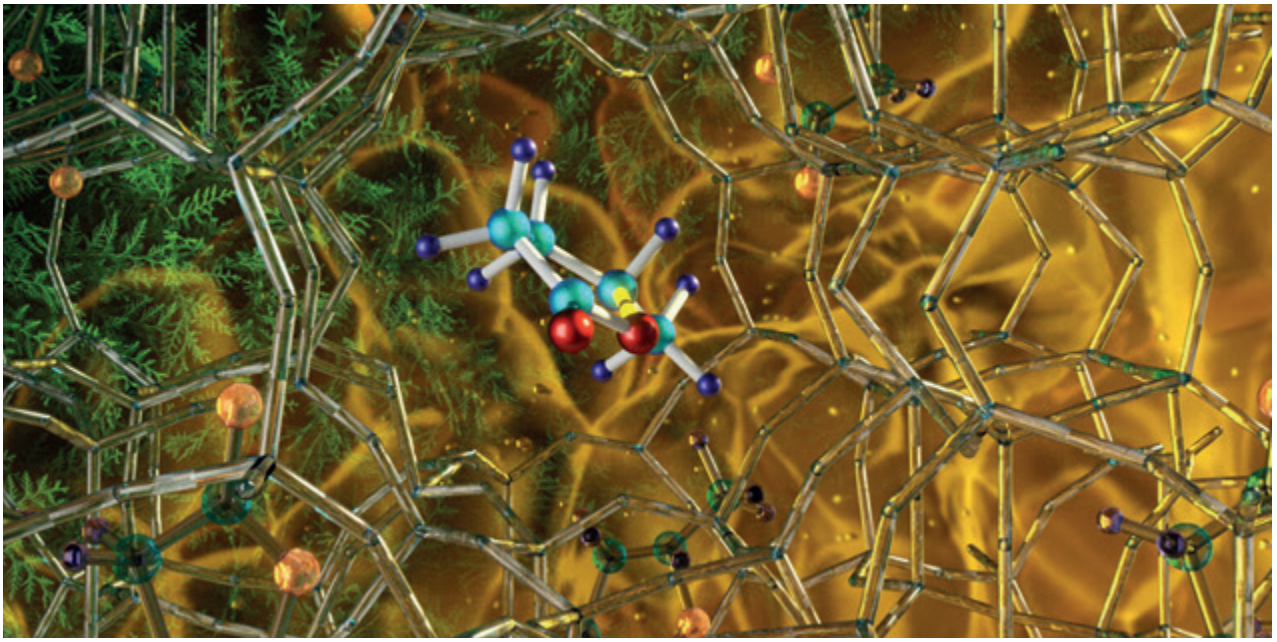


Illustration of the optimized zeolite catalyst (NbAlS-1), which enables a highly efficient chemical reaction to create butene, a renewable source of energy, without expending high amounts of energy for the conversion. Credit: ORNL/Jill Hemman.

Related publication: "Quantitative production of butenes from biomass-derived γ-valerolactone catalysed by hetero-atomic MFI zeolite." Nature Materials, 19, 86-93 (2020)

DOI: 10.1038/s41563-019-0562-6

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

Authors: L. Lin (University of Manchester), A.M. Sheveleva (University of Manchester, International Tomography Centre SB RAS and Novosibirsk State University), I. da Silva (ISIS), C.M.A. Parlett (University of Manchester and Diamond Light Source), Z. Tang, Y. Liu (East China Normal University), M. Fan, X. Han, J.H. Carter, F. Tuna, E.J.L. McInnes (University of Manchester), Y. Cheng, L.L. Daemen (Oak Ridge National Laboratory), S. Rudić (ISIS), A.J. Ramirez-Cuesta (Oak Ridge National Laboratory), C.C. Tang (Diamond Light Source) and S. Yang (University of Manchester)

ChipIr

Preparing robots to survive longer in extreme radiation environments

When carrying out tasks in environments with high radiation levels, such as in decommissioning nuclear sites, it is often essential to use robots rather than people, due to hazardous radiation. However, the radiation can also damage the electronics inside a robot, causing it to fail much more quickly than if it was used under normal conditions. Developing strategies to prevent such failures will enable the robots to be used for longer.

One such strategy is the use of scrubbing technology, which reads back data from the memory and corrects errors that have been caused by radiation damage. In this study, researchers from the University of Essex developed a self-scrubbing scheme that can be used to protect systems used in high radiation environments.

To test their new design, they brought it to the ChipIr instrument, where the high neutron flux replicates long periods of time in a high radiation environment. They found their design to be successful and reliable, achieving a high correction rate and better performance than existing solutions. Their experiments also showed that the cost of the hardware needed does not grow linearly with the available RAM size, making it suitable for devices where limited resources are available such as mobile robots.

Maria Kastriotou on the ChipIr instrument.

Related publication: "A self-scrubbing scheme for embedded systems in radiation environments." 2020 IEEE 26th International Symposium on On-Line Testing and Robust System Design (IOLTS)

DOI: 10.1109/IOLTS50870.2020.9159718

Funding: EPSRC

Authors: Y. Lu, X. Zhai, S. Saha, S. Ehsan, K. McDonald-Maier (University of Essex)

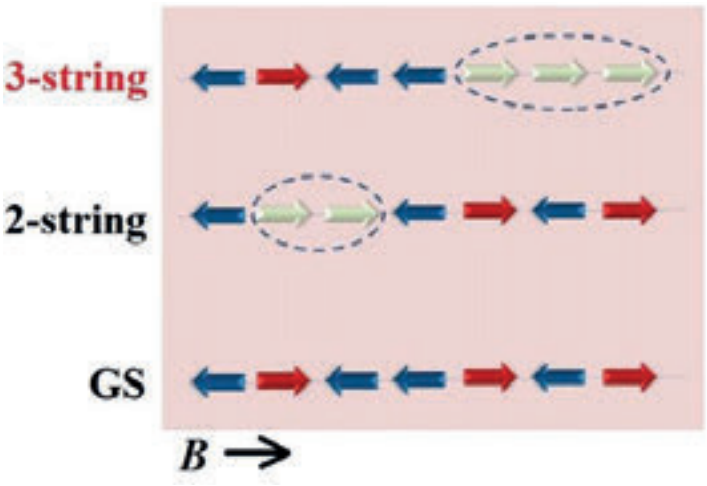
LET

Long-standing quantum physics prediction proven: Bethe strings experimentally observed

Ninety years after physicist Hans Bethe postulated the existence of unusual patterns in magnetic solids, known as Bethe strings, an international research team has experimentally detected them for the first time. Using neutron scattering and high magnet fields, the group were able to collect experimental data that are in excellent agreement with Bethe's theoretical prediction, illustrating how quantum physics can give accurate predictions of physical properties.

Previous theoretical studies have shown that Bethe strings are excitations occurring in some one-dimensional models. They are, however, very difficult to detect experimentally using, for example, a spectroscopic method, because their contribution to quantum dynamics is negligibly small and overlaps with other features. In 2018, the group found the first evidence of Bethe strings in the chain antiferromagnet, $SrCo_2V_2O_8$, using high-resolution terahertz optical spectroscopy in applied external high magnetic fields. In this system, only the cobalt atoms have magnetic moments, and they all are aligned parallel or antiparallel to a specific direction with adjacent moments cancelling each other out.

The international collaboration's latest study, published in *Nature Physics*, shows the first experimental identification and characterisation of Bethe strings. Using inelastic neutron scattering, the team resolved the dispersion of Bethe strings for the first time in high-quality single crystals of $SrCo_2V_2O_8$. The successful measurements relied on and the use of high magnetic fields to separate the Bethe strings from other excitations at a neutron scattering facility.



A snapshot of the ground state (GS), as well as the two-string and three-string excitation states (dashed ellipses).

Related publication: "Dispersions of many-body Bethe strings." Nature Physics, **16**, 625-630 (2020)

DOI: 10.1038/s41567-020-0835-7

Funding: Helmholtz Gemeinschaft

Authors: A.K. Bera (HZB and Bhabha Atomic Research Centre), J. Wu (Shanghai Jiao Tong University), W. Yang (Stewart Blusson Quantum Matter Institute), R. Bewley (ISIS), M. Boehm (ILL), J. Xu, M. Bartkowiak, O. Prokhnenko, B. Klemke, A.T.M. N. Islam (HZB), J. M. Law (Hochfeld-Magnetlabor Dresden), Z. Wang (University of Cologne) & B. Lake (HZB and Technische Universität Berlin)

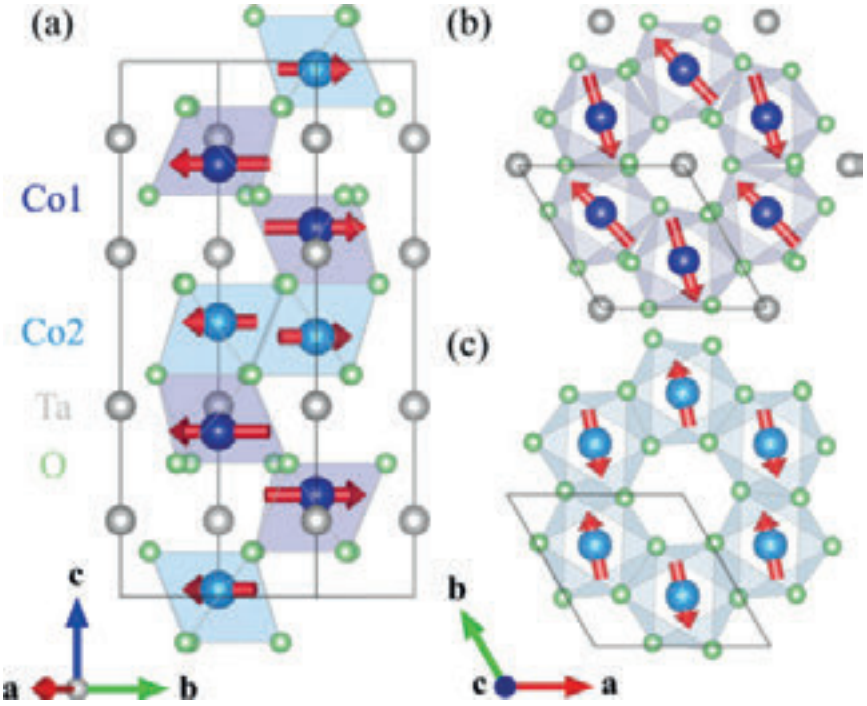
SXD

Noncollinear magnetic order of a new magnetoelectric material determined by neutron diffraction

The magnetic structure of an unusual magnetoelectric compound has been determined by combining single-crystal neutron diffraction and direction-dependent magnetic susceptibility. In magnetoelectric materials, the magnetic order can be controlled using an electric field or, conversely, the electric polarisation can be controlled using a magnetic field. Developing these materials could lead to a new generation of energy-efficient devices.

One such candidate is $Co_4Ta_2O_9$. Its magnetoelectric behaviour, however, is uncommon and not previously understood. This study, selected as an Editor's suggestion in *Physical Review B*, used single-crystal neutron diffraction on SXD combined with direction-dependent magnetic susceptibility measurements to accurately determine the magnetic structure, key information to explain its magnetoelectricity.

The international group of researchers found that, below 20.3 K, $Co_4Ta_2O_9$ exhibited unusual long-range antiferromagnetic order, where adjacent spins are pointing in opposite directions. Surprisingly, this magnetic structure is different to that observed for $Co_4Nb_2O_9$, a material that takes the same crystal structure. This could suggest that nonmagnetic Ta^{5+}/Nb^{5+} ions may also influence the magnetic property. Based on the symmetry analysis using the spin-flop model, the group were able to successfully explain the unusual magentoelectricity found in this compound.



(a) The refined magnetic structure of $Co_4Ta_2O_9$ at 15 K. (b) and (c) show the buckled and the flat honeycomb layers, respectively. The magnetic arrangement is canted antiferromagnetic in the former and collinear antiferromagnetic in the latter. The net moment of the two buckled layers in the unit cell is zero.

Related publication: "Noncollinear antiferromagnetic order in the buckled honeycomb lattice of magnetoelectric $Co_4Ta_2O_9$ determined by single-crystal neutron diffraction." Phys. Rev. B, **102**, 214404 (2020)

DOI: 10.1103/PhysRevB.102.214404

Funding: National Science Foundation, China Scholarship Council, and the National Research Foundation of Korea

Authors: S. Choi (Rutgers University, Max Planck Institute for Solid State Research), D.G. Oh (Yonsei University), M.J. Gutmann (ISIS), S. Pan (Rutgers University, Ningbo University), G. Kim (Max Planck Institute for Solid State Research), K. Son (Max Planck Institute for Intelligent Systems), J. Kim (Rutgers University), N. Lee (Yonsei University), S-W. Cheong (Rutgers University), Y.J. Choi (Yonsei University) and V. Kiryukhin (Rutgers University)

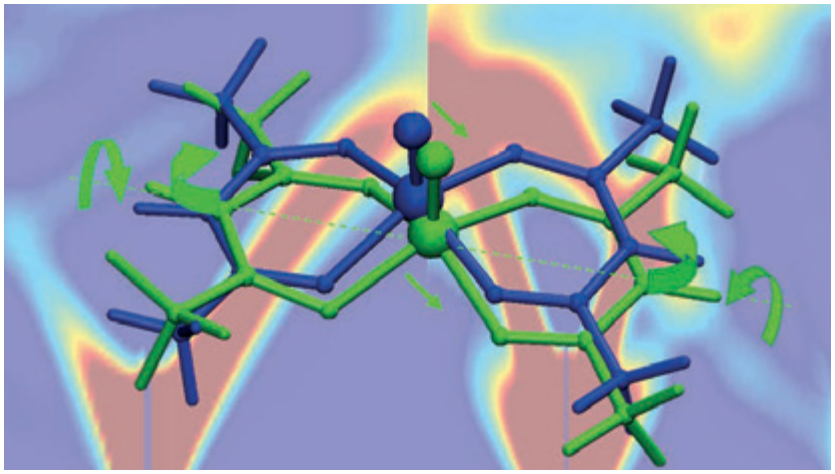
LET

Phonon dispersions measured for the first time in prototype molecular qubit

Molecular nanomagnets (MNMs) have the potential for use in quantum information processing as 'qubits', or for high-density magnetic memories as classical 'bits'. However, their exploitations for either of these applications is undermined by molecular vibrations and spin-phonon interactions. There are has been little research in the past on phonons in MNMs, and this study, published in *Nature Communications*, is the first to directly measure phonon dispersions in a molecular material with qubit applications.

The material studied in this work is a molecular crystal of VO-acetylacetonate [$VO(acac)_2$]. This molecule is a typical example of a new generation of molecular qubits with long coherence times up to high temperatures. The researchers used four-dimensional (4D) inelastic neutron scattering (INS) to study the material, a method never applied before to study phonons in molecular crystals. INS is a very powerful technique to study phonons, and the recent advent of spectrometers combining the time-of-flight technique with position-sensitive detectors makes measuring the 4D scattering function in large portions of the reciprocal space possible.

After completing their 4D-INS work, the researchers compared their results to state-of-the-art density functional theory (DFT) calculations. The simulations reproduced important features of their observed data, also providing insights into the spin-phonon couplings in the system. This comparison for molecular crystals is almost unique and it could represent a new standard in the benchmarking of DFT methods. Being able to correlate the molecular structure of these systems with their experimentally tested vibrational and phonon spectra could lead to the development of new strategies for the design of new, and optimised, molecular qubits and bits.



Structure of the molecular qubit $VO(acac)_2$ at equilibrium (blue) compared to the structure distorted by a low-energy phonon (green): molecular and lattice vibrations can cause decoherence of the quantum state of the qubit.

Related publication: "Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory." Nature Communications **11**, 1751 (2020)

DOI: 10.1038/s41467-020-15475-7

Funding: Italian MUR, QuantERA, University of Parma, Fondazione Cariparma, Fondazione Angelo della Riccia and the Science Foundation Ireland

Authors: E. Garlatti (ISIS and Università di Parma), L. Tesi (Università degli Studi di Firenze), A. Lunghi (Trinity College, Dublin), M. Atzori (Università degli Studi di Firenze), D. J. Voneshen (ISIS), P. Santini (Università di Parma), S. Sanvito (Trinity College Dublin), T. Guidi (ISIS), R. Sessoli (Università degli Studi di Firenze) and S. Carretta (Università di Parma)

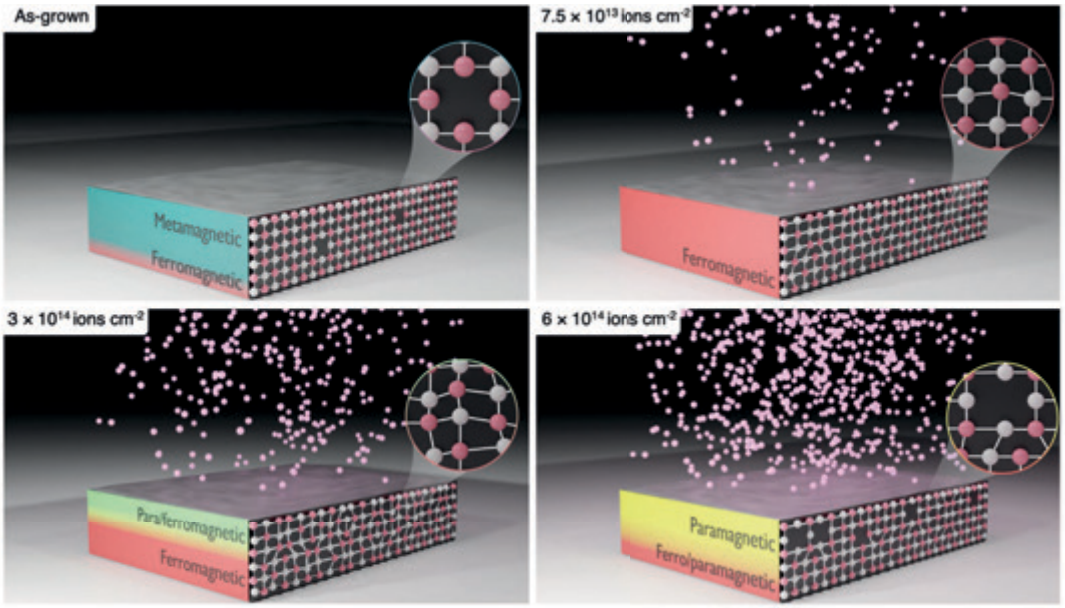
Polref

Fine tuning of the magnetic properties within thin films

FeRh thin films undergo a highly unusual magnetic phase transition, where the magnetic moment suddenly switches on. This can be carefully controlled in many ways, including temperature, fabrication methods and external strain. One method of promoting the phase transition involves disrupting individual atoms within the structure. This local manipulation can be done using beams of ions, such as Ne^+. This study, published in *APL Materials*, explores the depth-dependent magnetic state of a thin film of FeRh which has been subjected to a range of ion beam treatments.

The researchers used temperature dependent polarised neutron reflectometry to determine how the magnetic structure of a FeRh thin film changes when it is subjected to ion beams of different intensities. Despite the films being only 40 nm thick, they were able to see the layers of different magnetic structures created by the atomic displacements caused by the ion beams.

Their results show that it is possible to use radiation at specific intensities to tailor the magnetic properties of thin films. This effective method to control disorder inside these alloys provides the basis to create devices for application in spintronic devices or data storage on sub-100 nm length scales that have antiferromagnetic and ferromagnetic order in close physical proximity.



The layers of different magnetic structure types after irradiation with different intensity ion beams. The dominant defect type is also shown for each case.

Related publication: "Depth selective magnetic phase coexistence in FeRh thin films." APL Materials, **8**, 121103 (2020)

DOI: 10.1063/5.0032130

Funding: EPSRC, Helmholtz Association, the Helmholtz Energy Materials Characterization Platform and the Deutsche Forschungsgemeinschaft

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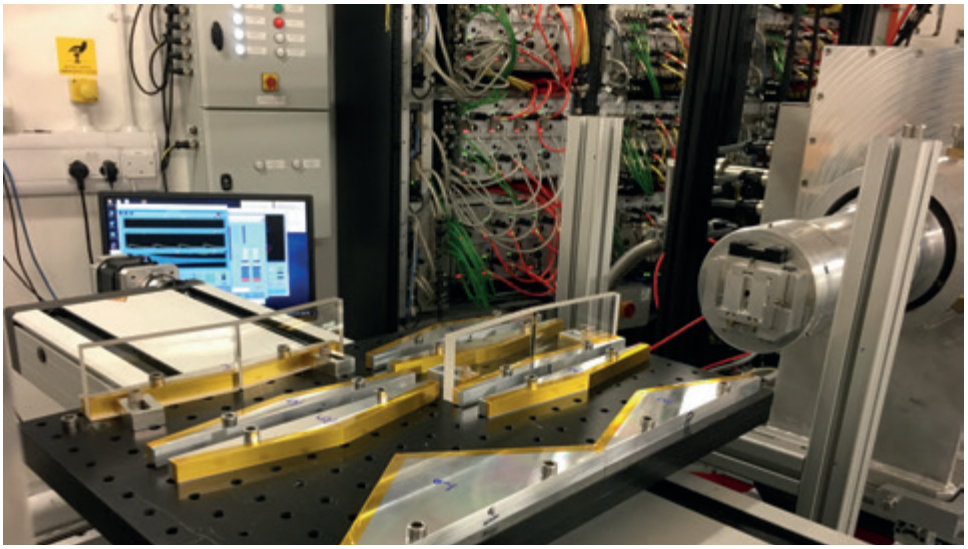
Larmor
Microscopic neutron entanglement

Researchers from ISIS and their global collaborators have proposed and demonstrated the first tuneable beam of entangled neutrons, a fundamentally new quantum probe. Individual neutrons can be entangled in spin, trajectory and energy.

The spin, trajectory and energy states of individual neutrons were independently tuned in order to reveal a uniquely quantum result that is at odds with the logic we apply in our daily lives. The trajectory of a particular neutron spin state can be manipulated using refraction through suitable magnetic fields that couple with the neutron's magnetic moment. The group's experiments used Larmor as a neutron spin-echo interferometer to show that it is possible to entangle the trajectory, spin and energy of individual neutrons on a microscopic length scale.

The development of this probe may offer new opportunities to investigate quantum phenomena in materials as well as fundamental symmetries and interactions, such as the effect of gravitation on the entangled distinguishable neutron properties, such as spin. Orbital angular momentum can also be added to the list of properties to be entangled, opening the potential for advancing applications in quantum metrology and high-precision measurement.



Using the Larmor instrument, the researchers separated the two spin states of each neutron so that they followed parallel paths. The phase difference between these paths was controlled, in part, by passing the neutron beam through blocks of single-crystal quartz which are shown here mounted on the Larmor sample table.

Related publication: "Unveiling contextual realities by microscopically entangling a neutron." Nature Communications, **11**, 930 (2020)

DOI: 10.1038/s41467-020-14741-y

Funding: National Science Foundation, US Department of Commerce, Oak Ridge National Laboratory, the office of the IU Bloomington Emerging Areas of Research program and the US Department of Energy

Authors: J. Shen, S.J. Kuhn (Indiana University), R.M. Dalgliesh (ISIS), V.O. de Haan (BonPhysics Research and Investigations BV), N. Geerits (TU Wien), A.A.M. Irfan (Indiana University), F. Li (Oak Ridge National Laboratory), S. Lu (Indiana University), S.R. Parnell, J. Plomp, A.A. van Well (Delft University of Technology), A. Washington (ISIS), D.V. Baxter, G. Ortiz, W.M. Snow (Indiana University) & R. Pynn (Indiana University, Oak Ridge National Laboratory)

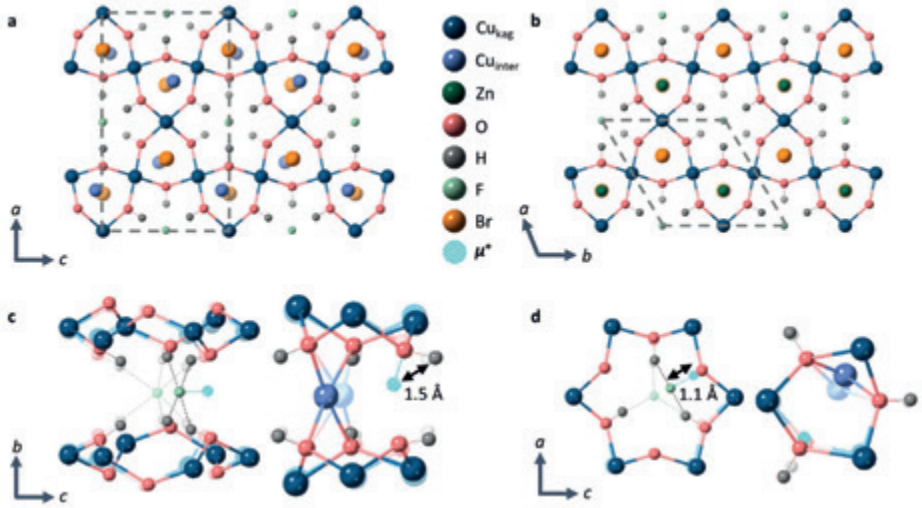
MuSR

Characterising a quantum spin liquid candidate

A group of researchers has used MuSR alongside theoretical calculations to characterise the magnetic properties of Zn-barlowite, highlighting its potential as a quantum spin liquid. Zn barlowite is zinc-doped $Cu_4(OH)_6FBr$, a naturally occurring mineral. In barlowite, the Cu^{2+} ions are arranged in kagome layers, as predicted by theory to be the starting point for a quantum spin liquid (QSL), where the magnetic moments of a material act like a liquid and remain disordered even at absolute zero. The addition of zinc ions in between these layers could trigger the formation of QSL state.

In this study, published in *npj Quantum Materials*, the group monitored the time-dependence of the muon spin polarisation by measuring the asymmetry of the emitted muon-decay positrons. This provided them with a unique insight into the local magnetic properties of the material. By using density functional theory (DFT) to calculate the muon stopping sites, the group were able to reveal the onset of the possible QSL phase in Zn-barlowite.

Their study looked at the temperature dependence of the structures formed across the full range of zinc doping in the material, from $Cu_4(OH)_6FBr$ to $ZnCu_3(OH)_6FBr$. Their measurements on the parent compound confirmed previous experimental results that static long-range magnetic order is seen below 15 K. As the zinc content was increased, the formation of this long-range order occurred at lower temperatures. No such state was seen for the $ZnCu_3(OH)_{cc}FBr$, even when going as low as 50 mK, indicating the possibility of a quantum disordered ground state.



Low temperature structure of barlowite and Zn-barlowite.

Related publication: "From magnetic order to quantum disorder in the Zn-barlowite series of S = 1/2 kagomé antiferromagnets." npj Quantum Materials, **5**, 74 (2020)

DOI: 10.1038/s41535-020-00276-4

Funding: University of Liverpool, STFC, the University of Chicago, EPSRC, French Agence Nationale de la Recherche and Université Paris-Sud

Authors: K. Tustain, B. Ward-O'Brien (University of Liverpool), F. Bert (Université Paris-Saclay), T. Han (University of Chicago, Argonne National Lab), H. Luetkens (Paul Scherrer Institute), T. Lancaster, B.M. Huddart (Durham University), P.J. Baker (ISIS) and Lucy Clark (University of Birmingham)

Polref and the Materials Characterisation Laboratory

Uncovering the cause of surprise superconductivity

Conventional theory about superconductors requiring pairs of electrons with their spins pointing in opposite directions meant that superconductivity and ferromagnetism were previously thought to not be able to co-exist within the same material. However, in samples of bilayers of nickel and bismuth, However, in samples of bilayers of nickel and bismuth, despite the ferromagnetic nickel, a superconducting state has been observed.

A group of researchers from the University of Leeds used polarised neutron reflectometry on Polref alongside SQUID magnetometry and X-ray diffraction in the ISIS materials characterisation lab, to measure changes in Bi/Ni samples to determine the cause of this surprise superconductivity. Their results, published in *Physical Review Research*, show that even under ambient conditions a layer of $NiBi_3$ is formed, and that this is the source of the superconductivity.

When freshly prepared, their layered samples were non-superconducting. However, when left at room temperature for several days, or heated up to 50°C, the layers mix to form a $NiBi_3$ layer. This shows the importance of storage conditions to maintain the integrity of Ni/Bi layers, but also opens up possibilities for both ferromagnetism and superconductivity to be present in the same system.

Gavin Stenning from the ISIS materials characterisation lab with one of the ISIS X-ray diffractometers.

Related publication: "Origin of superconductivity at nickel-bismuth interfaces." Phys. Rev. Research, 2, 013270 (2020)

DOI: 10.1103/PhysRevResearch.2.013270

Funding: EPSRC and European Union H2020

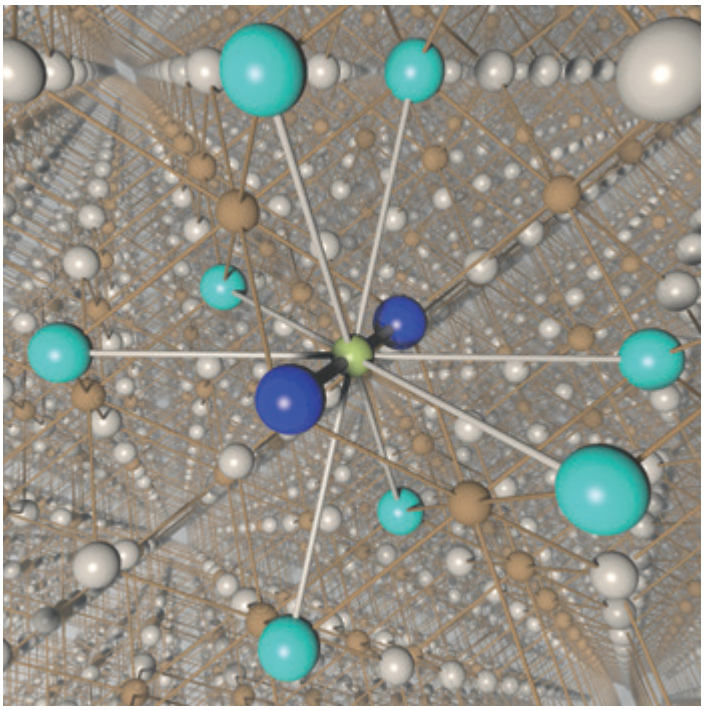
Authors: M. Vaughan, N. Satchell, M. Ali (University of Leeds), C.J. Kinane, G.B.G. Stenning, S. Langridge (ISIS), and G. Burnell (University of Leeds)

MuSR
Decoding decoherence

Using MuSR, researchers have observed the decoherence process that occurs within quantum mechanical systems. Despite the many potential advantages of quantum computation, the integrity of any quantum mechanical system is vulnerable to interactions with its environment which cause any stored information to be slowly lost - a process known as decoherence.

In their paper, published in *Physical Review Letters*, the group has shown that an interesting realisation of decoherence occurs when a spin-polarised muon, an unstable radioactive particle, is implanted inside a crystal of an inorganic fluoride. The positively-charged muon nestles between two negatively-charged fluoride ions, pulling them towards it, creating an interacting bound F-μ-F unit, with the spins of the muon and the two fluorine nuclei creating a coherently evolving quantum system. Weak interactions between this system and the other fluoride ions in the crystal decohere the quantum information stored in the muon. This process can be followed by watching the quantum interference oscillations in the muon spin polarisation as a function of time.

The degrading of quantum information can be understood by calculating the entropy in the entangled muon and fluorine spins, and the group have developed a method to describe the decohering effect of the environment in detail in a way that provides excellent agreement with their experimental data.



The muon (green sphere) strongly coupled to two fluorine nuclei (dark blue spheres), and weakly coupled to next-nearest neighbour fluorine nuclei (cyan spheres), embedded inside the fluorite structure of CaF_2.

Related publication: "Information and decoherence in a muon-fluorine coupled system." Physical Review Letters, **125**, 087201 (2020)

DOI: 10.1103/PhysRevLett.125.087201

Funding: EPSRC

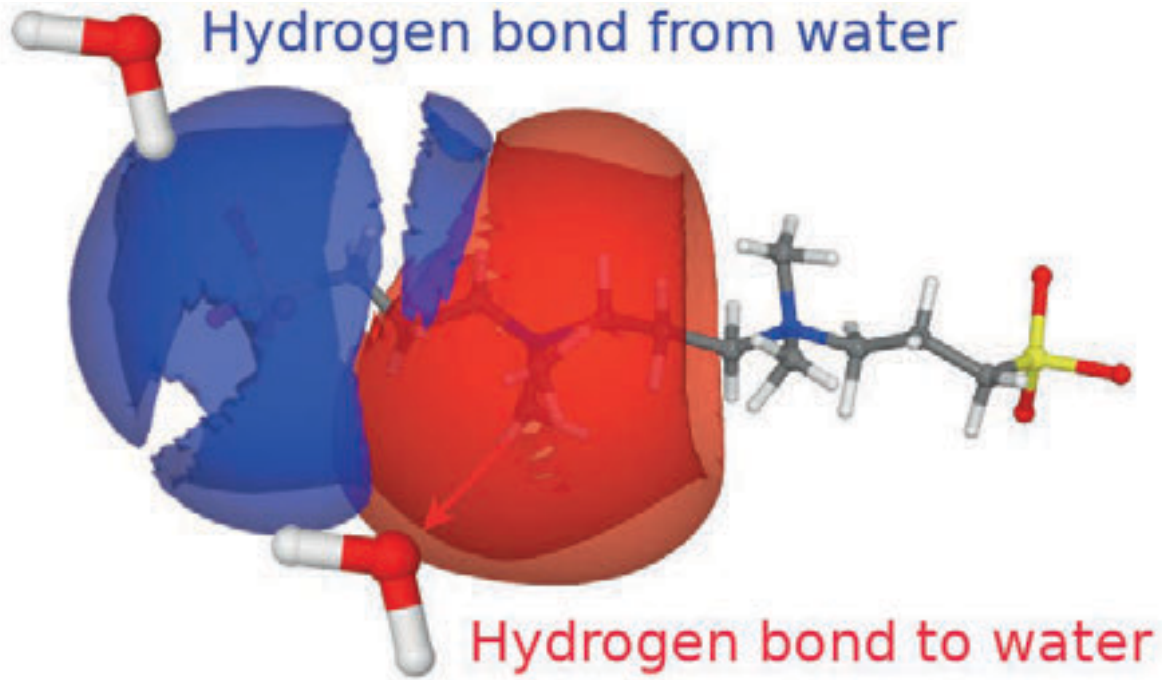
Authors: J. Wilkinson and S. Blundell (University of Oxford)

Sandals
Zwitterions as protein repellents

Understanding the ability of a protein to stick to a surface is important in many industrial and biological applications. The ability to create a protein-repellant surface and prevent biofouling is of great interest in areas such as marine coatings and design of diverse medical devices. One approach to enable this would be to create a surface system where the interactions with water are so favourable that proteins are excluded and not bound.

One possible option is to use zwitterionic materials: molecules that contain both a positive and negative charge. This study, published in *PCCP,* studied dizwitterionic molecules, incorporating two zwitterionic sections at each end of an alkyl-chain spacer. The researchers investigated what happened to the water molecules surrounding the dizwitterionic molecule when the length of the alkyl-chain spacer was changed.

They found that, for all chain lengths, each zwitterion end attracted a shell of about fifty water molecules. This high hydration activity suggests that this type of system may be suitable in applications where a protein-repellent is required.



Water molecules strongly hydrate tethered sulfobetaine dizwitterions directed by electrostatic interactions and retain strong affinity for water even with a hexyl-groups separating the zwitterion.

Related publication: "Hydration of sulfobetaine dizwitterions as a function of alkyl spacer length." Phys. Chem. Chem. Phys., **22**, 16040-16050 (2020)

DOI: 10.1039/D0CP02654A

Funding: EPSRC and the Royal Academy of Engineering

Authors: O.S. Hammond, L. Moura, G. Level (Queen's University Belfast), Silvia Imberti (ISIS), J.D. Holbrey and M. Blesic (Queen's University Belfast)

Iris and Tosca

Neutron experiments have been used to study the effect of bleaching on human hair at the atomic level

Although neutron spectroscopy is rarely used in this area of science, it is an ideal tool to study the structure and dynamics of confined water and proteins in hair, and the strength of the hydrogen-bond interactions present. This study, published in *The European Physical Journal Special Topics*, investigated how the oxidative damage that occurs during chemical bleaching is caused.

A single hair is made up of a central cortex surrounded by the cuticle. Inside the cortex is a crystalline helical phase embedded in a matrix of proteins. The group studied the changes to both the central helix and the matrix around it to see what effect the bleaching had. Their results showed that the lighter hair actually weighed less, as the process of bleaching reduced the mass of the hair. Loss of the crystalline material, proteins and lipids caused the hair to weaken.

The researchers then delved deeper into the structural changes to look at the hydrogen atoms on the surface of the hair. They found that, for bleached hair, the hydrogen atoms are able to move more freely, indicating that the structure is more flexible. This is caused by the chemical bleaching attacking the thioester groups that bind lipids to the cuticle, promoting the cleavage of cystine amino acids of the cuticle and cortex. This chemical modification makes the structure less rigid and, in turn, the proton mobility increases.

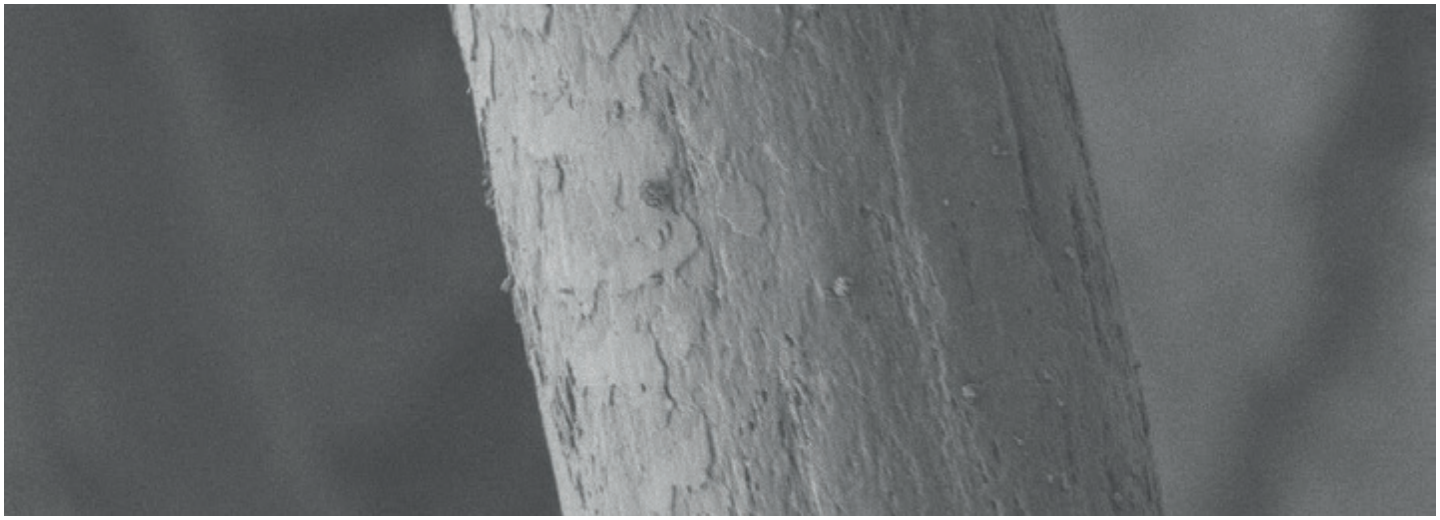


Image of a bleached hair fibre.

Related publication: "Human hair: subtle change in the thioester groups dynamics observed by combining neutron scattering, X-ray diffraction and thermal analysis." The European Physical Journal Special Topics, **229**, 2825–2832 (2020)

DOI: 10.1140/epjst/e2020-900217-4

Funding: CAPES, the National Institute of Science and Technology Complex Fluids, Conselho Nacional de Desenvolvimento Científico e Tecnológico , FAPESP, São Paulo Research Foundatio and Danscatt, the Danish Agency for Science, Technology and Innovation

Authors: C.R.R.C. Lima (University of São Paulo), R.J.S. Lima (University of Campina Grande, University of Copenhagen), L.D.B. Machado (Nuclear and Energy Research Institute), M.V.R. Velasco (University of São Paulo), L. Lakic, M.S. Nordentoft, L. Machuca-Beier (University of Copenhagen), S. Rudić, M.T.F. Telling, V. García Sakai (ISIS), C.L.P. Oliveira (University of São Paulo) and H.N. Bordallo (University of Copenhagen, ESS)

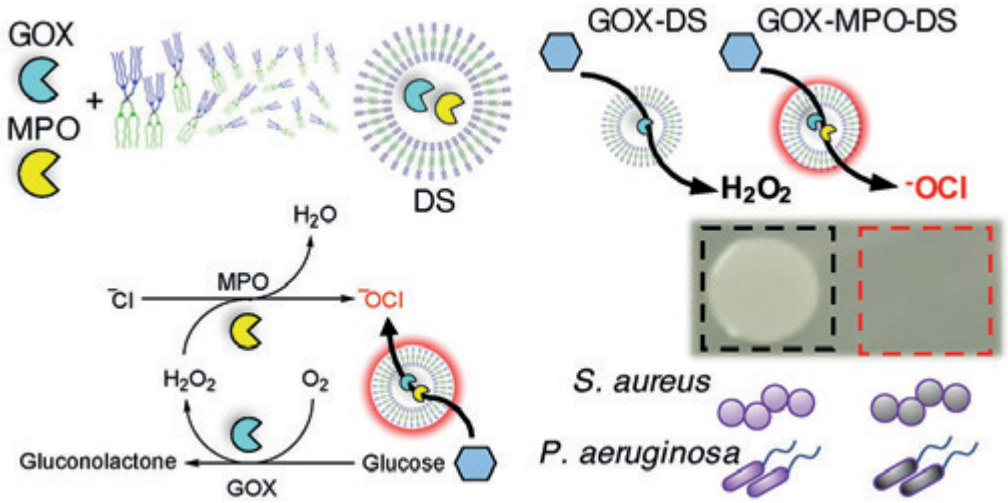
Sans2D

White blood cell inspired nanoreactor created to tackle antibiotic resistance

With a rise in antibiotic resistance, alternative treatment methods are becoming increasingly important. This study, published in *ACS Nano*, created an artificial nanoparticle system, known as a nanoreactor, which adapts certain functions of white blood cells.

To create their nanoreactor, they encapsulated two enzymes, myeloperoxidase and glucose oxidase, inside a nanocompartment called a dendrimersome. This nanoreactor converted glucose to hypochlorite (otherwise known as bleach), which was then shown to be an excellent bacterium killer, destroying two WHO-listed pathogens without using antibiotics.

Dendrimersomes have interesting properties including enhanced stability and programmable self-assembly. Small angle neutron scattering was crucial for characterisation of the dendrimersome assembly during this work; experiments on the Sans2D instrument determined properties such as size and membrane thickness with excellent resolution.



A schematic showing the creation of the nanoreactor, and its bactericidal properties.

Related publication: "Controlled Dendrimersome Nanoreactor System for Localized Hypochlorite-Induced Killing of Bacteria." ACS Nano 2020, 14, 12, 17333–17353 (2020)

DOI: 10.1021/acsnano.0c07459

Funding: EPSRC, Swiss National Science Foundation, Wellcome Trust, German Research Foundation, the European Union's Horizon 2020, Rosetrees Trust, China Scholarship Council, Shionogi & Co. Ltd and the National Institute for Health Research Imperial Biomedical Research Centre

Authors:M. Potter, A. Najer, A. Klöckner, S. Zhang (Imperial College London), M.N. Holme (Imperial College London and Karolinska Institutet), V. Nele, J. Che, L. Massi, J. Penders, C. Saunders (Imperial College London), J.J. Doutch (ISIS), A.M. Edwards, O. Ces, and M.M. Stevens (Imperial College London and Karolinska Institutet)

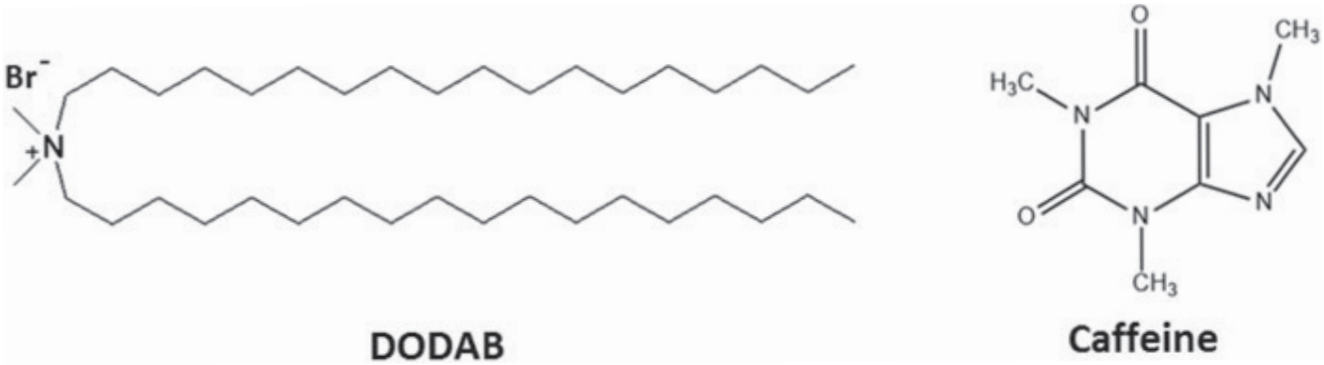
Iris

Using QENS to investigate why caffeine gives you a boost

Caffeine is the world's most widely consumed legal psychoactive substance. As well as being used to avoid fatigue, it has been investigated for its potential antioxidant activity that could lead to protection against diseases such as Alzheimer's. Despite its widespread use, the exact mechanism of caffeine is not well understood. This study, published in *Journal of Applied Physics*, used quasi-elastic neutron scattering on the Iris instrument to investigate the interaction between caffeine and a model lipid membrane.

The lipid used was dioctadecyldimethyl-ammonium bromide, known as DODAB, which forms a structure in solution that is analogous to biological membranes. Depending on the molecular arrangements of the lipids within the membrane, it can form a crystalline or fluid phase. The influence of the caffeine was found to be different for each of these two phases.

In the fluid phase, the addition of caffeine restricted the movement of the lipid molecules, whereas the opposite was true in the crystalline phase. These changes to membrane dynamics can impact the fluidity and permeability of the whole membrane, which could affect the functionality of embedded membrane proteins and transport properties of the cell membrane and could be the key to understanding the science behind the boost you get from your morning coffee.



Chemical structures of the DODAB lipid and caffeine.

Related publication: "Caffeine modulates the dynamics of DODAB membranes: Role of the physical state of the bilayer." Journal of Applied Physics, **128**, 154701 (2020)

DOI: 10.1063/5.0027953

Funding: Government of India

Authors: V.K. Sharma, H. Srinivasan (Bhabha Atomic Research Centre, Homi Bhabha National Institute), V. García Sakai (ISIS), and S. Mitra (Bhabha Atomic Research Centre, Homi Bhabha National Institute)

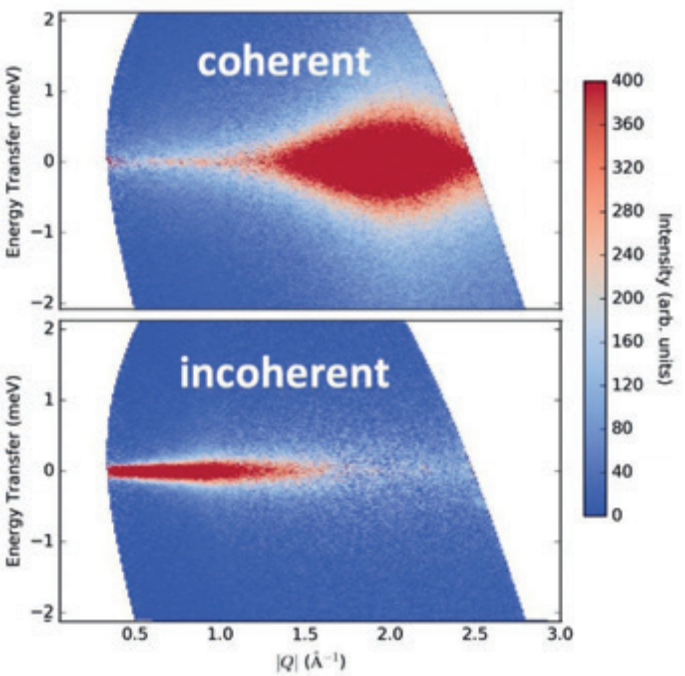
LET

LET distinguishes coherent and incoherent low energy scattering in water for the first time

Combining polarisation analysis with the unique capabilities of the LET spectrometer has enabled the distinction between the single-particle and collective dynamics of water for the first time. In this study, published in *Physical Review Research*, the incoherent and coherent contributions to the neutron intensity scattered by deuterated water (D_2O) were separately measured in a wide range of length scales covering from intermolecular distances to the mesoscale.

By using polarised neutrons, the researchers were able to distinguish the diffusive motions of the D_2O molecules from other dynamical contributions. This was not previously possible when approaching the relevant regime of the mesoscale, where the incoherent and coherent scattering intensities are roughly equal. They found that in this region, incoherent scattering is due to the diffusion of single D_2O molecules, whereas coherent scattering hardly depends on the length scale of observation. This verifies molecular dynamics simulations of D_2O at intermediate length scales and is in agreement with the so-called viscoelastic model.

This work offers new insights into the origins of density fluctuations occurring from meso- to intermolecular scales, not only in water under different conditions but also in hydrogen-bonded liquids, glass-forming liquids, and biological systems where water plays an important role. It also convincingly proves the power of recently implemented neutron-scattering polarisation analysis capabilities, which can hugely impact the progress of microscopic dynamics investigations in fields such as soft matter or biology.



Coherent (top) and incoherent (bottom) dynamical structure factors of D_2O measured at 295 K with an incident neutron energy E_i = 3.84 meV.

Related publication: "Coherent structural relaxation of water from meso- to intermolecular scales measured using neutron spectroscopy with polarization analysis." Phys. Rev. Research, **2**, 022015(R) (2020)

DOI: 10.1103/PhysRevResearch.2.022015

Funding: Eusko Jaurlaritza and the Ministerio de Economía y Competitividad

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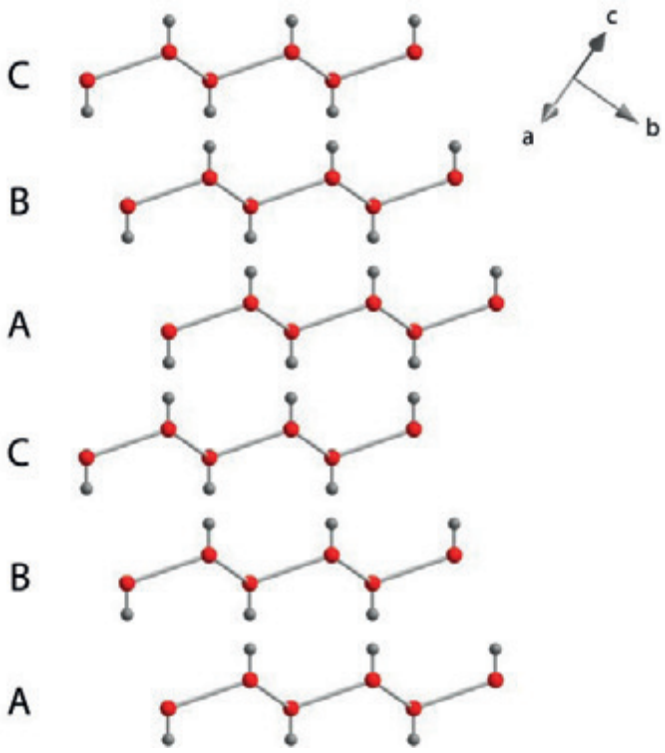
HRPD

HRPD helps find a way to make ice cubic

As shown by snowflakes, water does not freeze naturally into a cubic structure but, instead, into a hexagonal one. But, by developing a novel synthesis method, a group of researchers have been able to synthesise and characterise pure cubic ice on the HRPD diffractometer.

Inside ice, the water molecules are arranged in layers, which can be stacked in different ways to form hexagonal ice Ih, which is common on Earth, and in a cubic structure forming cubic ice Ic. This second form of ice is much more difficult to make. It usually forms by vapour deposition of water at very low temperatures, and it is likely to form in the Earth's polar stratosphere, although without being fully cubic. The researchers' work, published in *Nature Materials*, details a novel synthesis method that allows the formation of 100% cubic ice, with no measurable hexagonal stacking sequences.

The group started with a high-pressure form of hydrogen hydrate called C_0 filled ice, a crystal in which there is a framework of water molecules arranged in such a way as to create cavities in which the hydrogen is located. By means of an annealing treatment, it was possible to remove the hydrogen from the structure of the hydrate crystal on the HRPD beamline, forming a very low-density form of ice called ice XVII that, on warming, transforms to pure cubic ice. Their synthesis method now allows bulk preparation of pure cubic ice so that details of its thermodynamics, thermal expansion and possible proton ordering can be explored in more detail and compared with the well-known anomalous properties of hexagonal ice.



Stacking sequence of the layers in cubic ice Ic.

Related publication: "Cubic ice Ic without stacking defects obtained from ice XVII." Nature Materials, **19**, 663–668 (2020)

DOI: 10.1038/s41563-020-0606-y

Funding: Italian Ministero dell'Istruzione, dell'Università e della Ricerca, and Fondazione Cassa di Risparmio di Firenze

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Chris Lawson

Technical manager for ISIS ultra-low temperature (ULT) experiments

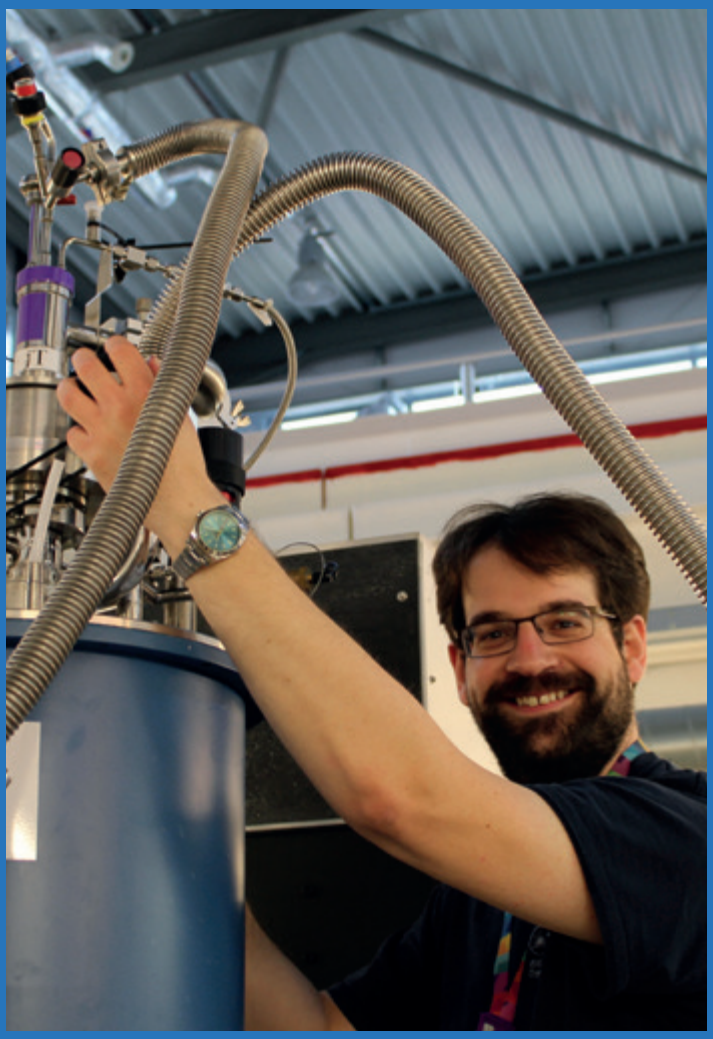
> “Working here brings the freedom to run with a good idea: the attitude is very positive and encouraging.”

After completing his PhD in the low temperature group at Lancaster University, Chris Lawson completed a post-doc and then joined a company in the Netherlands that makes ultra-low temperature cooling devices for, mainly, the quantum computing market. After meeting ISIS’ Oleg Kirichek, Chris because aware of the work going on here, and joined the cryogenics group in 2016.

Each year about 500 experiments at ISIS require cryogenic cooling, and the number of experiments that require ULT conditions has grown from around 20 in 2008 to over 100 in both 2019 and 2020. The ULT experiments take samples down to 25-30 mK using dilution fridges that rely on quantum mechanical effects. “We are limited by how many we can run by the amount of equipment, and number of people trained to use it.” Chris adds, “We are currently investing in new kit, and actively recruiting new people, so I’m hopeful we can expand beyond our current limits.”

Despite being on call over evenings and weekends, Chris finds the job challenging and fun. “As well as the day to day experiment management, we also have a number of development projects ongoing: we are hoping to image the dilution fridge mixing chamber using IMAT to see what’s going on inside. Working here brings the freedom to run with a good idea: the attitude is very positive and encouraging.”

In addition to his work in the cryogenics team, Chris plays an active role in the ISIS Public Engagement programme. His liquid nitrogen show has engaged many visitors to ISIS, getting people involved in super low temperatures that they would otherwise not be exposed to.



Right: Science Minister Amanda Solloway MP signing the ISIS visitor book.

ISIS News and Events

ISIS News and Events

ISIS staff join ventilator development project

As part of ISIS' COVID-19 response, software engineers from the facility were part of an STFC-led team that was awarded funding to develop a robust, low-cost ventilator to help patients in low and middle-income countries.

Mechanical ventilation is a small but important part of the management of pandemic virus infections that affect the lungs, including flu and COVID-19. Ventilators are typically expensive to purchase and maintain, and need considerable training to use. A team, led by STFC, has produced and tested an affordable, reliable and easy-to-operate ventilator that does not rely heavily on compressed gases and mains electricity supply, both of which are not readily available in many countries.

The project, known as the High Performance Low Cost Ventilator (HPLV), is coordinated by the STFC's Daresbury Laboratory. Tiago Sarmento from the Ion Source group, and Sarah Medley and Mihnea Romanovschi from the ISIS Controls Group volunteered to be part of the project. All three are part of the work package related to the controls software on the ventilator. The project builds on the original designs for the High Energy physics Ventilator, which was developed at CERN. The aim of the project is to bring the prototype up to a standard where it can be applied in a medical setting.

Although usually dealing with accelerating particles, their work on this project gives them the opportunity to use their programing and electronics skills in another field, and be part of an international development project that could impact the lives of many people around the world.

The High Energy physics Ventilator. Image credit: CERN

> "The project is a collaboration not just within STFC but also with universities and medical professionals. The aim is to move the prototype up the technology readiness levels to a stage where it can be ready for industry."
>
> **Sarah Medley, ISIS Software Engineer**

User Meetings

Due to COVID-19, the annual UK Neutron and Muon Science and User Meeting (NMSUM) took place online on the morning of Friday 30 April 2021. Along with updates from ISIS, ILL and ESS, we welcomed plenary talks from Dr Valeska Ting and Dr Wuge Briscoe. 191 people attended from 16 countries.

Science meetings for the user community were also taken online during the year. ISIS held three webinars during Summer and Autumn 2020, on Chemistry & Catalysis, Soft Matter & Bioscience, and Functional Materials, with the latter attracting 165 participants.

ISIS also hosted a series of subject-based webinars to learn more about the Endeavour programme of large instrument upgrades and new instrument builds that we hope to carry out at ISIS over the next few years. See pages 8-9 for more on the Endeavour programme.

Dr Valeska Ting presenting at the virtual NMSUM.

Science Minister Visit

On 8 July 2021, the UK science minister Amanda Solloway MP visited RAL for a tour of ISIS and discussions with staff. After meeting with STFC's Executive Director for the National Laboratories to discuss the work of STFC, ISIS' Director of Operations Zoë Bowden took the minister on a tour of ISIS. During the tour she visited the IMAT and ChipIr beamlines, speaking to the instrument scientists. She also spoke to an ISIS graduate scheme member to learn about ISIS' contributions to training. The most challenging part of the visit was getting her back out of the target station!

Sara Karbassi and Albin Nilson

New Duty Technicians in the Main Control Room

> There is so much to learn, but it's a really good group of people, who are all willing to help.

Sara and Albin joined ISIS in August 2020 as Duty Technicians. "I always want to try new things, and so when I saw the opportunity to work at STFC become available, I applied," Sara explains.

For Albin, it was a similar experience. "During my undergraduate degree at Lund University (Sweden), I did a summer placement at Diamond Light Source, which meant I knew about RAL. I had also worked on the Max IV accelerator in Sweden during its commissioning, so this role looked like a really good option."

Despite joining in the middle of a pandemic, both Albin and Sara are required to be on site, as a member of one of six shift teams that monitor the facility around the clock. As new starters, they were initially the fourth member of an existing shift team, so they could learn from the experience of others. By working some shifts with different crews, they were able to meet more people and see how they approach the tasks.

The Main Control Room (MCR) crew act as a hub, preparing equipment for use and keeping track of who is in the restricted areas of the accelerator. They are also the alarm investigation team, and first aiders. "Our role is to maintain the machine," Sara explains. "We monitor all the alarms and are first on the scene if anything goes wrong. We do a lot of routine checks to equipment and safety procedures, and things can get really busy when there is a maintenance day or the beam is being switched on."

While the beam is off, the team are busy carrying out routine checks, and scheduling other work that is due. When the beam is on, Albin explains, "it's the same thing, but more can go wrong! An accelerator has one on switch and a million different off switches - on some shifts we will have little to do, but others you can go the full 12 hours without sitting down."

The team's goal is to keep the beam on as much as possible. "If we can solve the problem, we will," says Sara, "but we might need to call in an equipment expert: from where they are working on site, or from home if it's during the night. We can then help them fix the issue, and learn from what they do for the future."

When it comes to fixing a particle accelerator; knowledge comes with time in the job. Albin says, "We get trained up, but sometimes we have to wait for a fault until we can be taught how to fix it. After a couple of months I felt like I could deal with the simple stuff alone, but there is always someone on the end of the radio if needed."

As there are very few opportunities around the world to work in a similar environment, the crew are used to new starters coming in without specific experience. "There is so much to learn, but it's a really good group of people, who are all willing to help," says Sara. Sara is also the first female member of the MCR crew, although this is not the first time she has been the only woman in a team at work. "I seem to always be the first one! But I want to be there so that other women can see that it's possible."

During the long shutdown, it's likely that MCR staff will be seconded to other groups around ISIS. This will be an opportunity for them to meet more people across ISIS, something that COVID-19 restrictions have prevented.

International

International

ISIS has significant, long-standing agreements with several countries which provide support for ISIS instruments for all users whilst allowing particular access for researchers from the partner countries.

ISIS and Italy

ISIS has continued its long-standing partnership with Italy, including involvement in the Vespa instrument at ESS, and is anticipating signing a new collaboration agreement with the Italian research council (CNR) later this year.

Antonella Scherillo prepares samples for study on the INES instrument, created under the ISIS-Italy partnership.

The partnership between the UK and Italy in neutron scattering has reached a new exciting milestone, the creation of the new ISIS@MACH ITALIA (IMI), the first distributed research infrastructure (RI) hub of ISIS sited in Italy. First experiments at ISIS included investigations on the beneficial effects of minor polar components in extra-virgin olive oil, a study of ancient Roman bones from a sepulchral site, and the characterisation of shielding materials for radiation-protection applications. IMI extends the project ISIS@MACH (MAterial Characterisation) which was started in 2019 as an initiative of the University of Roma Tor Vergata funded by Regione Lazio in Italy. The RI is distributed across research centres, universities and enterprises, and offers open access for public and private users in Italy to a complementary set of tools of light and particle probes. It also provides a dedicated Neutron Gate access route to ISIS to tackle issues in life science, physical and engineering sciences, as well as in arts and heritage.

Daniele Leodori (vice president of Regione Lazio) visiting ISIS.

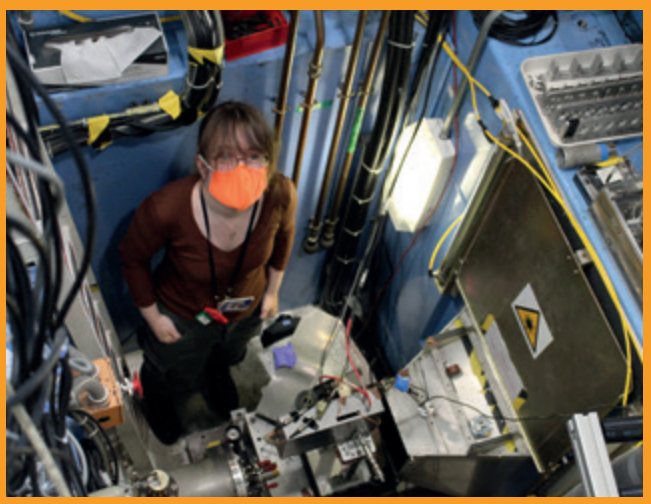
The ISIS – Sweden partnership

The collaboration between ISIS and Sweden is ISIS' longest-standing international partnership.

In January 2021 ISIS Director Robert McGreevy signed an agreement for a further 5 years with Swedish research council Vetenskapsrådet (VR). The new agreement will create new opportunities for Swedish researchers at ISIS and provide resources to benefit all the ISIS user community.

A delegation from Sweden's Council for Research Infrastructures visited ISIS in September 2018. Pictured is the Swedish delegation at the IMAT instrument with ISIS director Robert McGreevy.

The ISIS-Sweden partnership has lasted over 30 years, enhanced recently by ISIS' contributions to the European Spallation Source, currently being constructed in Lund.



Industrial placement student Arianna Wintle on LOQ testing the NitroGEM detector for the ESS LoKI instrument.

Left: Dr Yu Lu, Postdoctoral Researcher at the University of Manchester, on ZOOM.

30 years of ISIS – RIKEN Collaboration

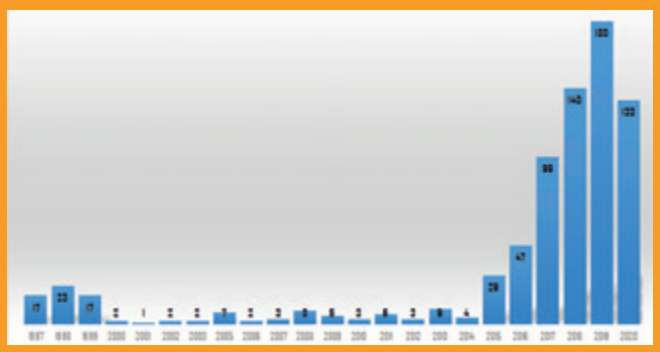
September 2020 marked 30 years of continuous agreements between ISIS and RIKEN in Japan. This partnership has seen the creation, development and operation of the RIKEN-RAL Muon Facility at ISIS. Since its creation in the early 1990s, the facility has produced over 500 publications and had researchers from over 90 Japanese institutes come to use it; collaborations with a further 40 institutions worldwide have also been formed, as well as the creation of agreements between RIKEN and Indonesian, Malaysian and Korean institutes for muon studies.

The milestone was marked by the daily release of a congratulatory video during the 30 days of September 2020, along with a science highlight from the facility. A celebratory song was also created!

30 years of the RIKEN-RAL Muon Facility being celebrated in song over Zoom.

ISIS – India partnership

The Indian Department of Science and Technology signed a £2 million, 5-year agreement with ISIS in November 2016 through its Nanomission programme. This enables Indian scientists to gain access to ISIS, and allows Indian early-career researchers to be based at ISIS. The agreement has been extended to March 2022 due to Covid, with discussions on a continuation due to happen in 2021. A very successful Indian user meeting was held in March 2021, jointly with DESY in Germany and KEK in Japan, who are also partners with India for facility-based science.



Graph of Indian proposals vs. year.

Koji Yokoyama

Beamline scientist on the muon instrument EMU

> It's extremely fruitful seeing the user community engaging with our research and then coming to ISIS to use the techniques we have developed.

After high school, Koji attended Shizuoka University in Japan to study physics. "In my early years at university, I hoped to become a scientist and have been on that path ever since."

His PhD was based in a laser lab, studying optical physics in semiconductors. In 2007, a collaboration with RIKEN took him to ISIS to carry out photo-excited μSR experiments. He joined RIKEN in 2009 as a postdoctoral researcher working on slow muon generation, known as 'low-energy muons'.

Low energy muon generation at the RIKEN facility at ISIS requires the use of muons and a laser. Koji explains, "Surface muons commonly used for material studies have a defined momentum, so their energy cannot be changed and they become deeply implanted into materials. However, with slow muons, we can change their energy by re-acceleration and therefore their implantation depth." Because slow muons can stop near the surface, a wide range of μSR experiments can be conducted on the surface-subsurface range of materials.

After joining the European Research Council funded muon group as a postdoctoral researcher, to build a laser system for the ISIS muon instrument HiFi and carry out photo-excited μSR experiments, Koji is now a full-time beamline scientist on the EMU instrument.

"Currently I'm focusing on studying charge carrier kinetics in semiconductors with photo-excited μSR, which has a wide range of applications from photovoltaics to power semiconductors." Understanding the charge carrier dynamics ultimately helps to optimise device performance and feeds into developing better models and designs. Koji's pioneering research has shown that muons can be used to probe the carrier density and give us an idea of how they move around in bulk, which previous research hasn't been able to do.

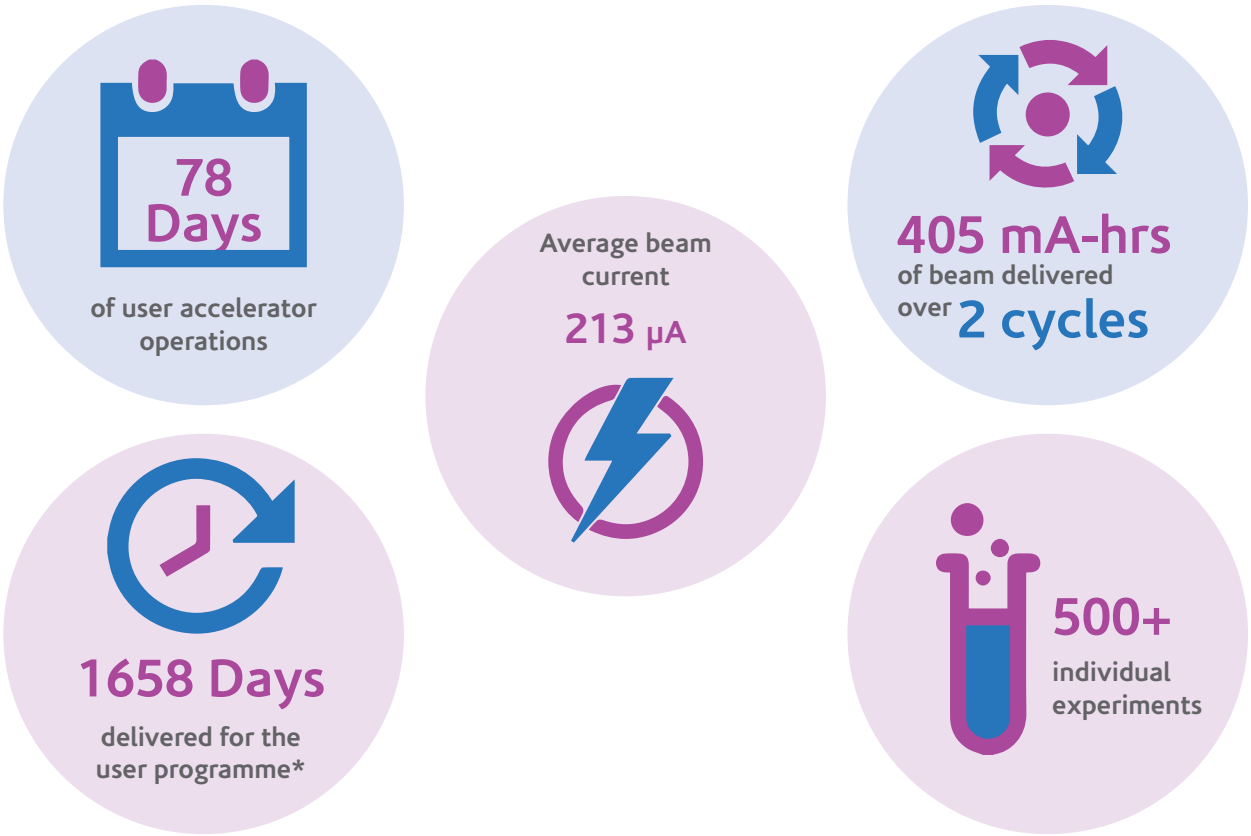
"It's extremely fruitful seeing the user community engaging with our research and then coming to ISIS to use the techniques we have developed."

Technology

Technology

Cutting edge science at ISIS must be underpinned by cutting edge technology. ISIS has an ongoing programme of developments on its accelerator complex and instruments, extending capabilities and improving performance.

Despite the lockdown restrictions, ISIS successfully ran two user cycles during 2020. In order to allow for this method of working, and to take into account Covid working practices, additional days were added to experiments and more space left between experiments. Even with these requirements in place, over 500 experiments were run across these two cycles. During the run cycle in September 2020, ISIS broke the record for daily beam current delivery on several days.



*Taking into account instrument down-time, plus calibration and commissioning time.

Table 1.1: Performance in 2021 Cycle by Cycle

Cycle	2020/2	2020/3
Beam on time (h)	928.9	747.5
Availability (%)	92.1	86.5
Total Beam (mAh)	225.7	178.9
Mean current when beam on		
Synchrotron (uA)	243	239
TS1 (uA)	203	202
TS2 (uA)	40	38
Highest daily beam total (mAh)	5.87	5.8

Left: Helen Popland and the new target assembly for TS1.

Major Projects

The 2021/22 Long Shutdown

In June 2021, ISIS entered a long shutdown period to enable two large projects: refurbishment of the first target station (TS1) and replacement of a tank in the linear accelerator.

TS1 Project

The new target, reflectors and moderators (TRaM) assembly was built up on the new cantilever support frame, flow tested and its alignment measured.

Trials were carried out for the removal of the current TRaM and support frame; its size means that this will have to be removed in pieces after being cut up by remote handling.

The large radiologically shielded flasks that will house the components being removed from the remote handling cell, some of which weigh up to 20 T, were delivered, tested and prepared for use.

This year has seen the completion of the water circuits, the associated compressed air lines and cabling in the new modular services trolley. A full programme of pre-installation commissioning has also been carried out.

The two cryogenic cold boxes that will provide the moderating fluids for the hydrogen and methane moderators were also delivered and installed. Pipework to connect these cold boxes up to vacuum, gas and cryogenic fluid transfer lines is also in production.

Underpinning all these technical activities is the documentation needed to ensure safe and correct strip-out, installation and commissioning. There has been a great effort over the year to ensure that this documentation is written, reviewed and communicated to the team.

Andy Robinson and Justin Miles adjusting the pipework on the service trolley.

Helen Popland working on the new TRaM assembly.

Chris Russell carrying out cutting trials.

Graham Wallace and Henry Russell with some of the large flasks.

Robin Burridge and Rajesh Gupta with the testing controls system.

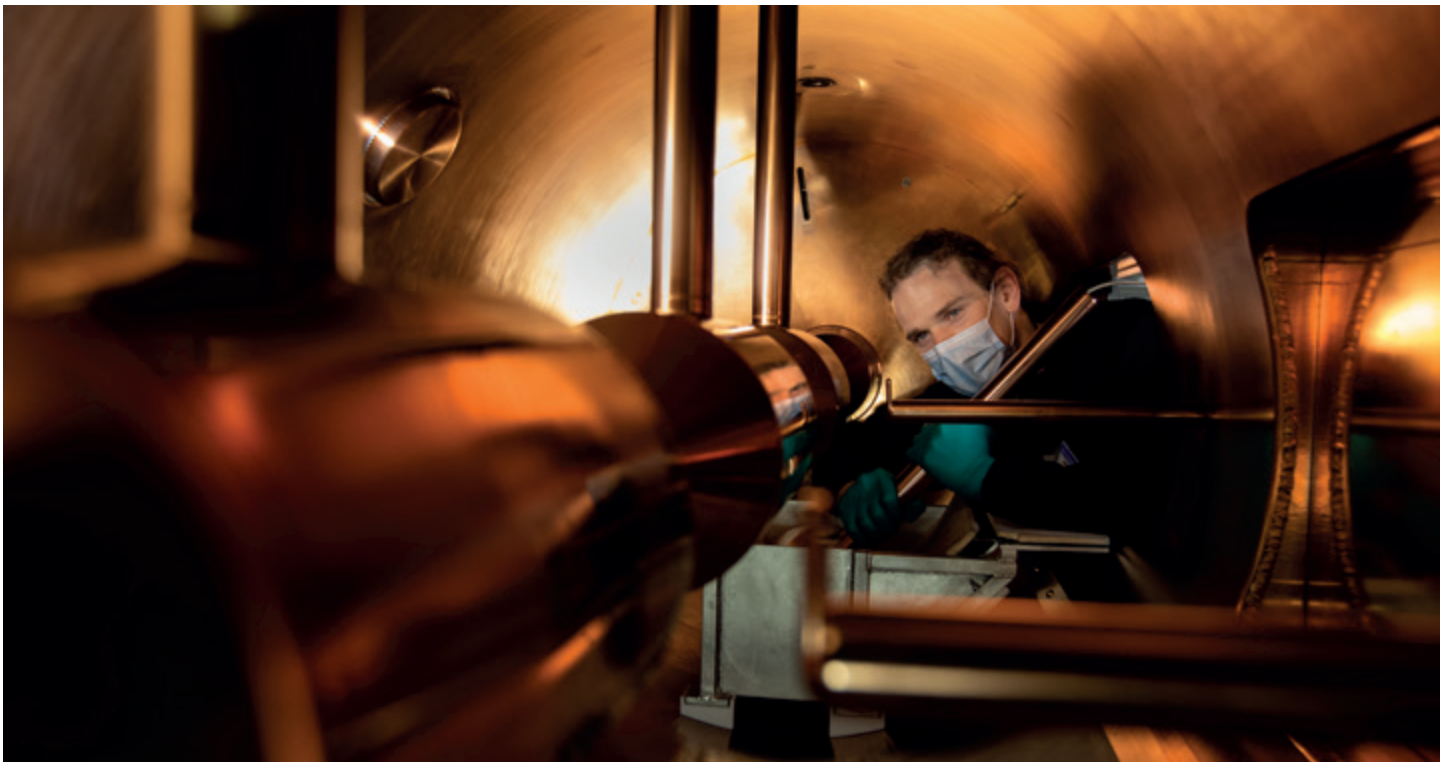
Linac Tank IV

A 12 metre section of the linear accelerator will be replaced during the 2021/22 long shutdown. It has required several years to build the structure and all of the components and, in March 2021, the final components, the drift tubes, were all delivered to site to be installed.

Before being tested at high power, the team needed to ensure that the field along the tank has the shape they need it to have. To test this, they ran a 'bead pull' test, where a small hollow metal bead is pulled through the centre of the drift tube whilst field measurements are taken.

After the bead pull test was complete, the team have been carrying out high power testing prior to installation.

Preparations are also being made for the removal of the old tank.



William Spencer installing the drift tubes in the new Linac tank IV.

The bead pull test being carried out in the new tank.

Nick Terzino and Mark Keelan in the Linac tank 4 modulator room testing the new tank.

Stuart Edmonds, operations manager of the ISIS Plant section, and the old Linac Tank IV.

ISIS and the European Spallation Source

ISIS are making a major contribution to the European Spallation Source (UK-ESS), one of the largest science and technology infrastructure projects being built today, on the outskirts of Lund in southern Sweden. The unique capabilities of the ESS will complement those of leading neutron sources such as ISIS, enabling new opportunities for researchers across the spectrum of scientific discovery.

ISIS staff have been vital in delivering two of the multimillion pound instruments, Loki and Freia, as well as detector electronics, data reduction and streaming, the latter of which supported the ESS instrument data streaming and processing framework which has been successfully completed. Justin Greenhalgh, UK-ESS programme manager, says, "This has been an interesting year, as it has for everyone, but there's been a real shift in focus, from planning and procuring components to building and delivering."

The Labs Advice project, led by Marek Jura at ISIS, is also coming to a close. This project focused on delivering user labs within the experimental halls at the ESS facility, to provide users access to labs in order to prepare samples for neutron scattering experiments. Marek says, "I have really enjoyed working with the ESS Lab Group over the last five years. It has been a real team effort, where all members of both ISIS and ESS lab groups have been involved in the sharing of ideas and experiences, and it's great to see it come to fruition."

ISIS' James Prince with one of the choppers for Loki, built at ISIS.

Over the past 12 months, components for the Loki instrument have been constructed both at ISIS and with external contractors.

Finally, in June 2021, the Loki detector vessel was delivered to Lund, having been manufactured in Spain by STFC partner AVS engineering.

The Loki detector vessel arriving at the ESS site on 29 June 2021.

> This is a really inspiring international project, which has progressed really well over the last year despite Covid, and it's great to be a vital part of that.
> **Justin Greenhalgh, UK-ESS programme manager.**

ISIS–II

ISIS-II is the proposal for a next-generation neutron source as the successor for ISIS. Although ISIS will continue to operate for many years to come, plans for a new facility will be developed over the next decade in order to be ready for construction sometime after 2030. This will maintain and enhance the UK's neutron provision, in a way complementary to the ESS, in order to continue to support the UK research community.

A project has been established to consider the requirements for an ISIS-replacement facility, and to explore the technologies that might underpin this. This work includes considering the science drivers for neutrons and muons over coming decades and how these will influence the design of new instrumentation. In turn, these considerations affect the nature of the source and hence the accelerator characteristics. Feasibility work on accelerator possibilities is ongoing, with the aim of ramping this up over coming years.

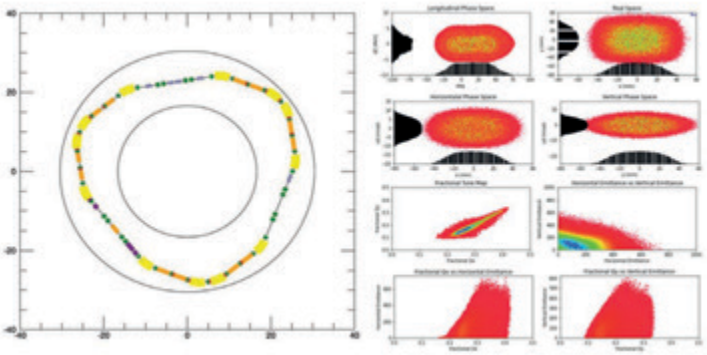
In July 2021, the UKRI Infrastructure Fund awarded £1.5M towards feasibility work for ISIS-II. This will enable development of the plans for the accelerator, including assessment of relevant technologies. Professor Robert McGreevy, Director of ISIS, said, "For over 30 years ISIS has been a world renowned UK research facility, used to study everything from anti-bacterials to batteries. But the present facility won't last forever. This investment enables us to start the early design for a new facility."

ISIS-II green field site option.

Accelerator design work

Accelerator physicists in the synchrotron group are designing Accumulator and Rapid Cycling Ring options for the next generation ISIS-II facility. These options require state of the art understanding of beam dynamics to achieve the best possible designs at 1 MW beam power levels with suitably low loss levels of 0.1%. Working designs for the most difficult options, where the new ring is constrained to fit in the existing ISIS hall, have now been identified.

Key issues for the design have been high temperatures of the injection stripping foil, identifying suitably flexible magnet lattice designs and optimal injection painting schemes. Developments of the PyORBIT high-intensity simulation code have been required, and now indicate well controlled beams with suitably low loss. Detailed work continues to optimise all aspects of the design: the injection straight layout, longitudinal dynamics, transverse dynamics and resonances, correction and tuning systems, collimation, and extraction. The next stage of the study is focussing on green field options. Much of the advanced beam dynamics required for these designs is benefitting strongly from high-intensity research and developments on the existing ISIS ring.



[left] layout of the proposed lattice for a 1.2 GeV rapid cycling synchrotron in the ISIS and [right] simulated beam properties after injection. Top left to bottom right: longitudinal phase space, real space, horizontal phase space, vertical phase space, fractional tunes of individual particles, horizontal vs vertical emittances, horizontal emittance vs tune, vertical emittance vs tune.

Zoë Clark

Zoë is a mechanical design engineer at ISIS on the Graduate scheme, but her route here was not straightforward, going via research, consultancy, and the powerlifting world championships.

> I enjoy doing the public engagement, as it's when you tell someone about working at ISIS that you realise how cool it is!

During her MEng degree at the University of Oxford, Zoë Clark did a summer placement at ISIS working on the commissioning of the new ISIS instrument ZOOM. She finished her degree, specialising in a project on systematic wear testing, and then was unsure as to what to do next.

"I had a job offer from a consultancy company, but they'd made an error with their resourcing and didn't want us to start for 9 months. My masters' project supervisor was very persuasive, so I ended up continuing with them and starting a PhD."

However, after six months of research, Zoë realised it wasn't for her. "I transferred to an MSc course, completed my experiments, and took up the delayed job offer with the consultancy firm. This job involved a lot of travelling: sometimes I wouldn't even know where I would be going that week until a Monday morning."

This way of working was a struggle for Zoë, as she was also a competitive powerlifter and, after eight months of trying to balance these two parts of her life, she realised it wasn't worth it, and left the role. "I looked back at the different jobs I'd done: I'd done three placements during university, as well as working in research and consultancy, and realised my favourite time was working at ISIS."

She started the scheme in September 2019, and feels like she is finally where she belongs. "I'm glad I tried all the wrong things before I came here, as it makes me more comfortable that I made the right choice in the end."

Zoe is based in the ISIS design division, where the graduates rotate every six months. She started it the sample environment team, designing sample cells to handle high pressures and her next placement was in the targets division, working on the TS1 Project. The project, taking place during ISIS' long shutdown, will involve safely removing large pieces of the, now radioactive, target assembly.

As well as her day-to-day role, Zoë is also involved in the ISIS public engagement activities, including the Engineering Education Scheme, where she and two other ISIS graduates have designed a project for A-level students. "It's been really interesting and a good opportunity to manage other people. I enjoy doing the public engagement, as it's when you tell someone about working at ISIS that you realise how cool it is!"

Taking part in public engagement activities has given Zoë the inspiration for her graduate placement: as part of the STFC scheme, graduates have the chance to be placed in another department for three months and, for Zoë, she will be joining the central public engagement team. "It will be nice to try something new, and have the time to develop new materials and activities."

Instrument Updates

Sans2D front end

The Sans2D flexible collimation setup consists of five two metre long, two tonne, blocks that need to be positioned with micron accuracy and repeatability. The current drive system has been running at the limits of its capability since being installed on the beamline and the recent IBEX commissioning has shown that this setup is no longer fit for purpose. The first unit of a new Stober drive system was tested successfully on Sans2D during a recent shutdown. A further five units are now being purchased and will be installed and commissioned over the long shutdown. This work will remove the issues of obsolescence and restricted capability of the current system and will give the Sans2D instrument, and its user community, the required reliability and flexibility that will last for the foreseeable future.

Bana Shriky, University of Bradford, on the Sans2D instrument.

Delft Quench Furnace

A quench furnace for the measurement of simultaneous SANS and diffraction has been developed by the group of Erik Offerman at the Technical University of Delft. The technical details of the furnace and some examples of data from a steel sample can be found in the publication referenced. The furnace is intended for use on Larmor and is available for use by other groups in consultation with the Delft team and ISIS scientists.

Related publication: A. Navarro-Lopez et. al. Rev. Sci. Inst., 91, 123903 (2020), https://doi.org/10.1063/5.0022507

NUrF – In-situ UV-Vis and fluorescence with SANS

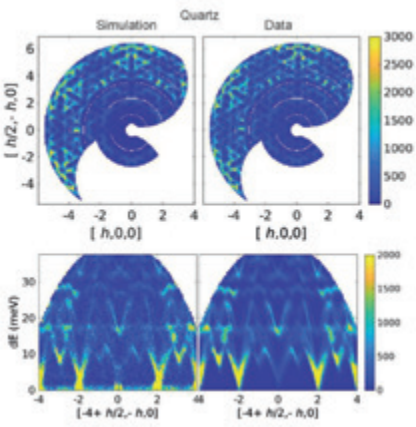
A simultaneous UV-Vis and fluorescence spectroscopy setup is now available for use on the ISIS SANS instruments. The equipment was developed by Cedirc Dikko from Lund University with assistance from ISIS and the ILL. Further development of the apparatus is ongoing to reduce the required sample volumes and to improve performance. The setup is available for use on request in consultation with the ISIS SANS group.

Related publication: C. Dicko et. al. Rev. Sci. Inst. 91, 075111 (2020), https://doi.org/10.1063/5.0011325

PACE software project

Proper Analysis of Coherent Excitations, or PACE, will be a software application that enables a step change in the rapidity and quality of analysis of neutron experiments on the ISIS spectrometers in the Excitations Group. The goal is to provide an integrated visualisation, simulation and fitting environment on massively parallel and distributed computing, and which interfaces to third party modelling codes. It will:

- Allow realistic simulations to be performed before and during the beam time to make the most effective use of neutron beam.
- Enable quantitative analysis of the full set of data collected during the experiment, with proper account of instrument resolution.
- Lower the barrier for users to analyse their data, so increasing the number of publications and reducing the time between experiment and publication.



Modelling inelastic neutron scattering due to phonons, incorporating a DFT model and a full instrument resolution to allow a comprehensive comparison between theory and experiment for quartz.

EMU Illumination

Recent work has restored a long-lost capability on EMU for running pulsed sample illumination experiments. A Xe flash lamp is now available, providing broadband illumination coincident with the implantation of the muons. Sample environment is provided by the Closed Cycle Refrigerators, and sample temperatures from 30 K to over 600 K are possible together with 'flypast' operation. The system complements the pulsed laser facility already available on HiFi, and various possibilities for pulsed illumination on the RIKEN beamlines.

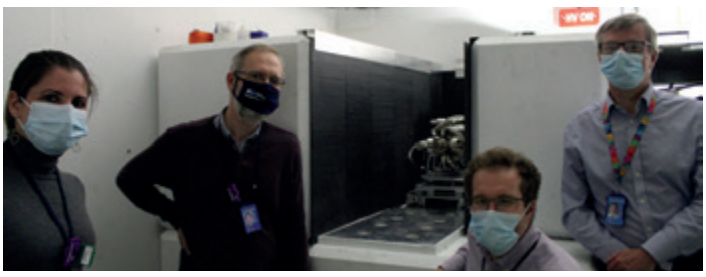
NILE

Two new desktop fusion devices are being installed at ISIS for testing the effects of cosmic rays and space weather on electronics, and supporting the search for dark matter. The new neutron sources will be housed in the new Neutron Irradiation Laboratory for Electronics (NILE) and will work alongside the ChipIr instrument.

The first new source will produce neutrons with an energy of 14 MeV, compared to the up to 800 MeV neutrons produced by the ISIS targets. The second accelerates deuterium atoms on to a deuterium target, producing 2.5 MeV neutrons.

"The new facility further extends and complements the existing irradiation capability at ISIS. This makes it an even more attractive centre for the many global electronic companies already working with ISIS on ChipIr to ensure the cosmic ray threat is understood and its effects dealt with," explains Chris Frost, the scientist leading the irradiation work at ISIS.

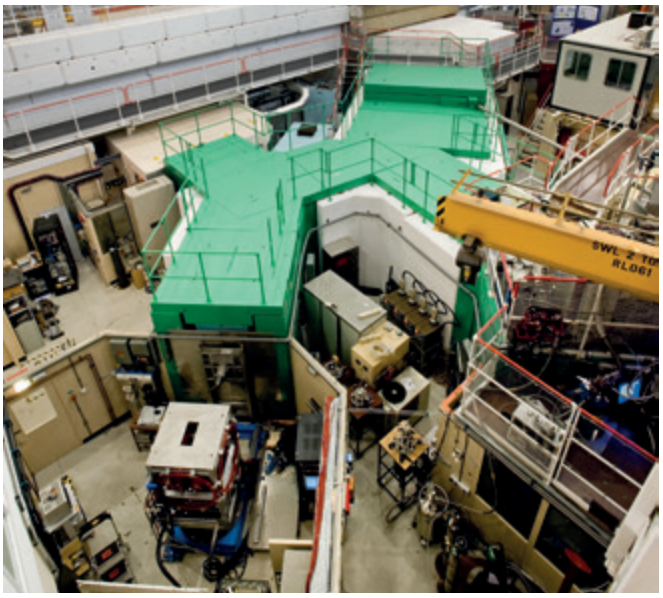
Other departments at STFC's Rutherford Appleton Laboratory are also collaborating with ISIS on the project. A group at RAL Space who are one of the lead partners in the SWIMMR programme, a major UK project that will improve the UK's capabilities for space weather monitoring and prediction, are helping to fund irradiation studies at ISIS, as well as a team from STFC's Particle Physics Department, who will be using the reactors to test their dark matter detectors.



Maria Kastriotou, Pawel Majewski, Carlo Cazzaniga and Chris Frost with the compact neutron source.

RIKEN-RAL Muon Facility Refurbishment

A major project to refurbish the RIKEN-RAL Muon Facility is now underway. The Facility has been operating for 27 years, and the refurbishment project will see its primary power supplies, cabling, water and vacuum circuits, shielding and other components replaced. The aim is to ensure the ongoing life of the facility for many years to come. The project is being undertaken in partnership with RIKEN in Japan. The Facility has just celebrated 30 years of continuous agreements between ISIS and RIKEN (see the international section on page 54 - 57 for more details).

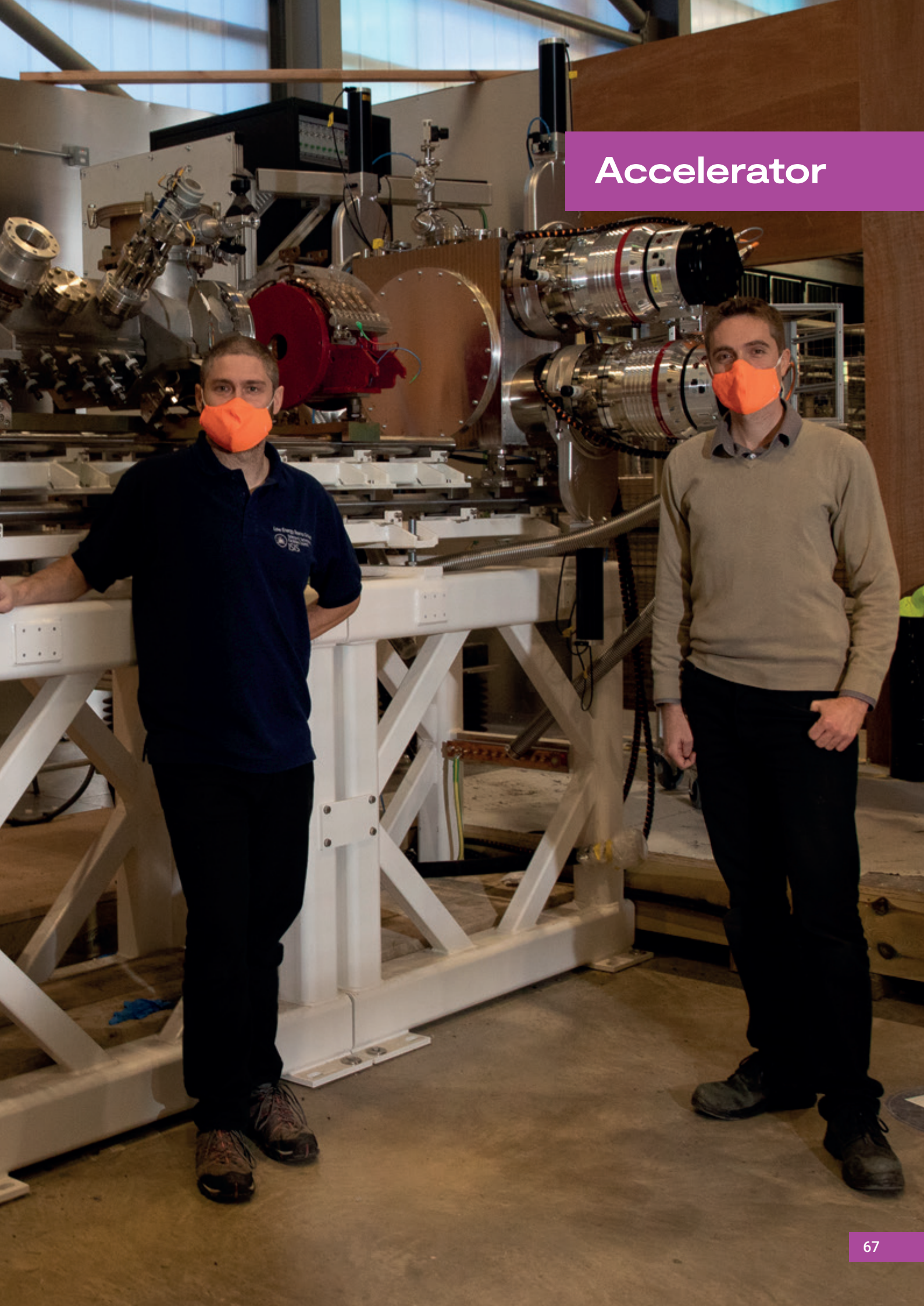


The RIKEN-RAL Muon Facility.

Beth Hampshire, PhD student from Warwick, using Port 4 of the RIKEN-RAL Muon Facility for elemental analysis of a Bronze Age Votive Boat from Tuscany.

Right: Rob Abel (RF engineer) and Scott Lawrie (ion source section leader) assembling the radio frequency (RF) matching box, which will transmit RF power to the new ion source plasma.

Accelerator



Accelerator and Electrical Systems

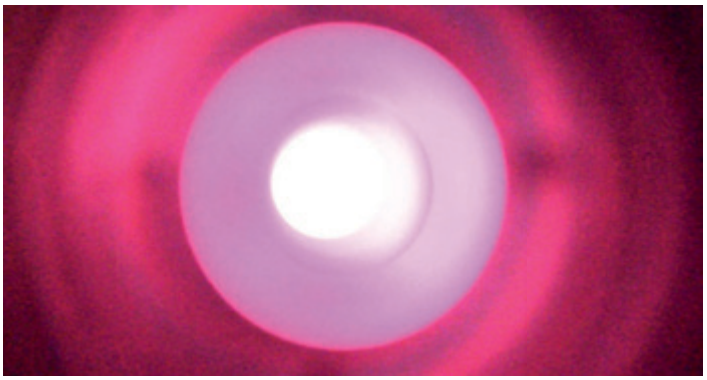
First Plasma in the RF Ion Source Project

A project is underway to upgrade the existing source of ions in the ISIS accelerator with state-of-the-art technology: the RF ion source. When fully functional, it will bring major operational reliability and flexibility improvements to the accelerator. Being constructed and tested along with the rest of a new pre-injector, the RF ion source has required fine-tuning of many enabling technologies. These include a compact microwave ignitor, an RF matching network, an array of strong permanent magnets, high vacuum pumping speed, hydrogen delivery pipework and a solenoid antenna.

Over the last year, the ISIS Low Energy Beams Group has been assembling the RF ion source and testing its sub-systems, resulting in the first plasma being struck on the 8th of April 2021. This is a big milestone for the project and confirms the physics simulations and engineering designs are correct. The team is now working toward extracting an ion beam from the plasma, which requires a comprehensive personnel protection system as high voltages are involved. First beam is anticipated toward the end of 2021.

Developments in Accelerator Design Engineering

As a facility operating for nearly 40 years, ISIS requires constant refurbishment and development of new equipment to maintain and improve upon its performance and reliability. In June 2020, ISIS received the last pair out of a set of 25 new coils to replace aging coils in the main dipoles on the synchrotron. These coils provide the magnetic bending field to steer the beam around the synchrotron, and the new coils contain mica insulation that performs better than the glass insulation in some of the older coils. The coils are now partway through being installed in the synchrotron.

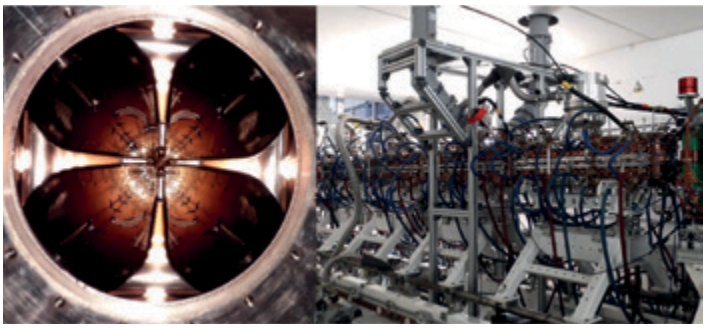


The plasma observed through a viewing window into the RF ion source. The pink colour comes from the visible light emission of hydrogen gas.

FETS RFQ Achieves Full Field Level

The Front End Test Stand (FETS) is a research and development project to build the front end of a linear accelerator that can be used for testing new techniques, physics and other components. This could eventually feed into larger experiments and contributes towards the development of future high power accelerators such as the ISIS-II facility upgrade project. The FETS beamline has recently been completed and high power testing of the Radio Frequency Quadrupole (RFQ) is underway. The RFQ is a low energy accelerator designed to accelerate an H-minus ion beam to 3 MeV with high efficiency and beam quality. The FETS RFQ incorporates many innovative features, most notably it uses separable components for easier inspection and repairs after testing.

Following months of preparatory work, in April 2021, RF power was delivered to the RFQ from the FETS high power klystron system for the first time and, after approximately one week of RF conditioning, the full design field level was achieved at an RF power of 545 kW. Once high power testing of the RFQ is complete, the entire FETS beamline will be turned on to run beam.



[Above left] an internal view of the RFQ during construction and [right] the full 4m long RFQ installed on the Front End Test Stand and ready for commissioning.

Upgraded Injector Profile Monitors

Profile monitors are essential tools for the ISIS accelerator, being used for setup and R&D operations. They provide valuable information about the beam quality, allowing precise adjustments of the accelerator components.

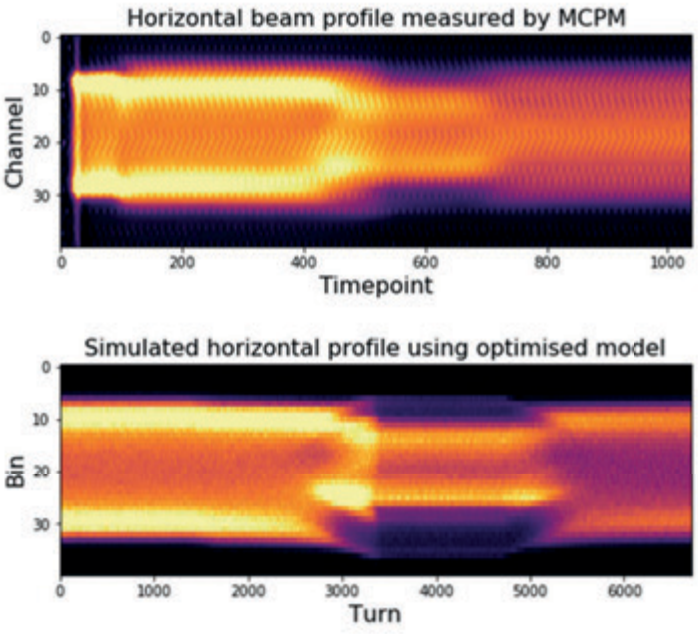
As part of the sustainability and R&D programmes, the whole set of injector profile monitors are being replaced with new, upgraded, versions. The new design will provide faster and more accurate measurements, reducing the time and number of beam pulses required for measuring a beam profile. The linear actuator has also been completely redesigned to facilitate the adjustment and replacement of the detector head assembly.

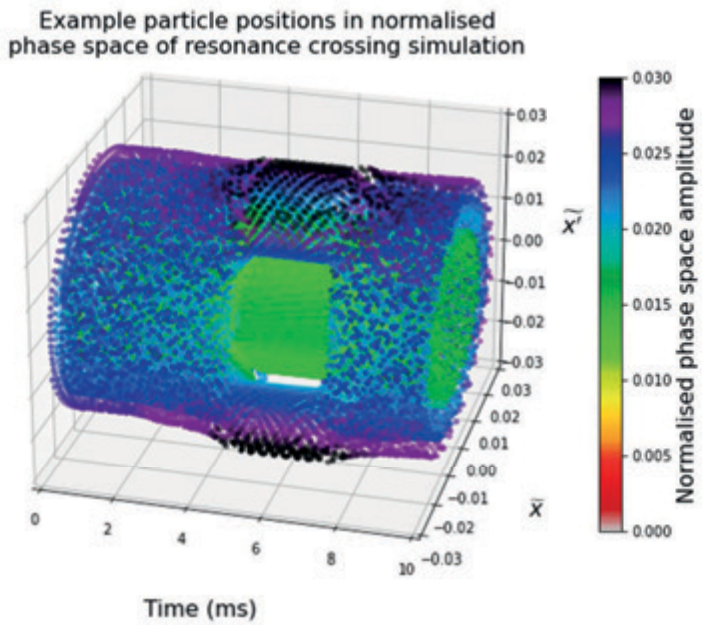
David Posthuma De Boer and Adam Filip with the new injector profile monitor.

Third Order Resonance Explored

Beam loss is an important consideration for high-intensity particle accelerators such as ISIS. Therefore, it is vital to study the mechanisms by which particles are lost to correct or mitigate them. One such mechanism is the resonant loss caused by the periodic interaction of particles in the beam with non-linear magnetic fields that are either introduced on purpose for correction of other non-linear effects or arise through magnet imperfections.

Advances in tune control at ISIS have enabled experiments probing strong third order resonances using a non-linear sextupole magnet. Clear resonant behaviour was observed using the multi-channel profile monitors. A non-linear model of ISIS was developed to simulate the experiments, and the model was optimised to match the beam profile: there was good agreement between simulation and measurement. Analysis of the individual particles in the simulation show the creation and manipulation of stable islands in phase space when on-resonance. These are the most advanced experimental observations of the third order resonance yet achieved at ISIS, and an important step in the study of resonances in the synchrotron.





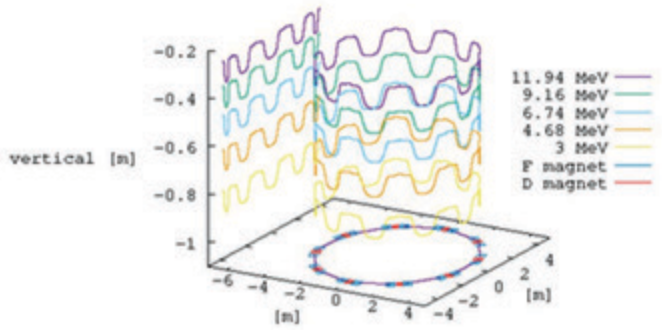
Simulation of single particle motion in the synchrotron compared to beam profiles measured during experiments. The creation of three stable regions of phase space around the beam core show clear evidence of third order resonance behaviour at ISIS.

Design of a vertical excursion Fixed-Field Alternating Gradient Accelerator

The future of proton accelerators for neutron and muon production is likely to be different from the picture we see now. Experiments will become more complex, and the accelerator infrastructure will need flexibility to supply the beam characteristics most suited to experimental needs. Sustainability of accelerator operations is key and must be incorporated from the very beginning of the accelerator design.

Physicists in the Intense Beams Group have been designing a Fixed-Field Alternating Gradient Accelerator (FFA) as a possible alternative proton accelerator for ISIS' future infrastructure. Having fixed-field magnets, the time structure and intensity of the output beams are easily controlled via the RF. The use of superconducting magnets increases energy efficiency.

The group's preferred design is based on a vertical FFA, or vFFA, in which the beam rises as it accelerates. This is a completely novel idea but one that is potentially well suited to high power proton acceleration, particularly when space is limited.



3D view of the beam orbits for different energies in the 12 MeV prototype vFFA model. The beam orbit moves upward with acceleration. The projections of the orbits onto the horizontal plane are all the same. The lattice has a triplet focusing structure: focusing magnets (blue) and defocusing magnets (red) are shown as boxes on the horizontal plane.

Sarah Fisher

Diagnostics software section leader

Sarah joined ISIS 15 years ago after seeing a local advert in the run up to the construction of Target Station 2. "I came in as diagnostics support, installing and commissioning diagnostics for TS2 as well as keeping the TS1 diagnostics operational," she says.

The beam diagnostics constantly monitor the beam losses and intensity in the accelerators and the proton beams to ensure the beam is in the correct position in the beam pipe and that the beam's position on the targets is optimised. If an issue occurs that is operationally critical, where the beam loss is too high, or too much intensity is lost, the beam turns off automatically and the main control room is alerted. This is essential to prevent damage to components of the accelerator and to keep activation of the machine to a minimum so maintenance tasks can be undertaken during shutdowns.

There are also diagnostic monitors for other parameters of the beam such as profile and position within the beam pipe. These are generally used by the accelerator physicists to help diagnose problems with the beam and to investigate the behaviour of the beam during machine physics studies outside of user runs.

Much of the software needed to monitor these diagnostic data is written in the BASIC programming language, some of which is almost 30 years old. When Sarah arrived, she was given the task of developing the use of LabVIEW code for data acquisition, and this is now widely used.

There is still a lot of old software that needs updating. "We use the time when the accelerator is off to go through the BASIC scripts and re-write them." She adds, "The upcoming long shutdown will give us plenty of time to make and test improvements. We also want to increase the frequency of the data points we record: ideally we would record every pulse, but at the moment we sum and save the data once a day."

After getting more involved with LabVIEW, Sarah discovered there were a lot of people on site who were using the code. "I set up a LabVIEW user group in 2008, and people now join us from across STFC and the Harwell campus more widely. Our quarterly meetings give us a chance to see what other people are using it for, and to share best practice." Sarah is also on the committee for an international LabVIEW conference, which she uses as another opportunity to learn more about its possible applications.

Right: Chris Russell and the remote handling training set up, for the EDT Industrial Cadets Gold Project.

Skills

Placements and visits

ISIS engages in training activities in a variety of ways, with placements and training opportunities provided to a range of staff and students, from apprentices to graduates and those working for a PhD. Although in-person work experience placements were cancelled due to Covid, the 46 confirmed ISIS work experience students took part in the online RAL work experience programme.

34 Graduates

52 Co-sponsored PhD students

3 Vacation students

15 Apprentice placements

27 Undergraduate sandwich students

The pandemic has had a huge impact on our visits programme, with most visits and tours of the facility being cancelled. However, despite the lack of in-person events, ISIS has reached many school and university students, teachers and members of the public through our online programme of events.

Total number of visitors 2961

2762 School students, teachers and public visitors

105 Business visitors

94 Higher education

Inspiring the next generation

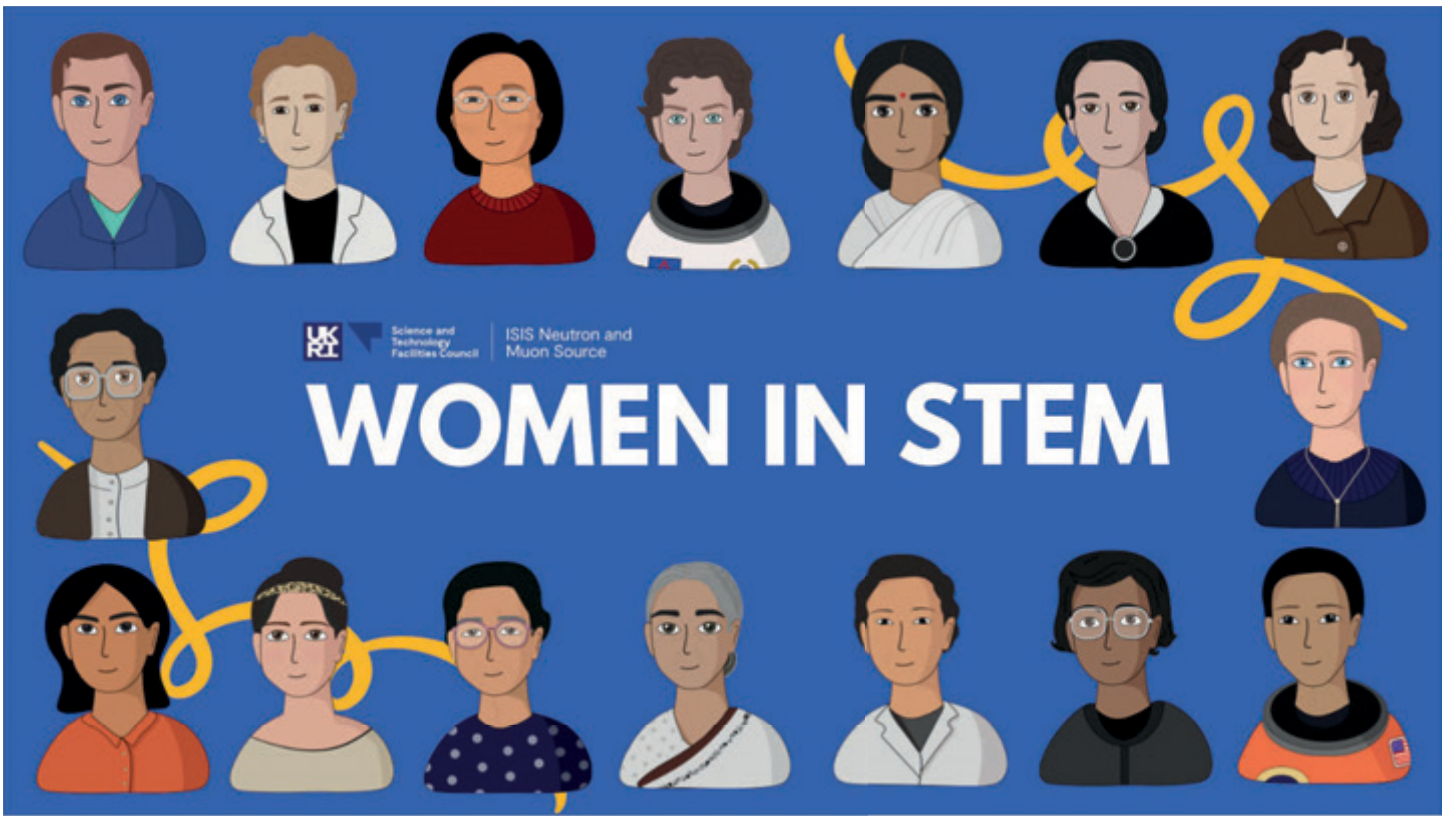
2020-21 was another successful year for public engagement at ISIS, despite the challenges the pandemic created.

ISIS frequently opens its doors to schools and the general public, receiving thousands of visitors annually. At the start of the pandemic, ISIS made a rapid transition to online events, allowing schools, universities, and members of the public to explore the facility remotely. A 360 degree tour of the facility and new hands-on "science at home" activities were developed. Through virtual tours, online talks and workshops, ISIS engaged with over 2750 school and university students, teachers and members of the public in 2020-21.

Long-standing events, such as RAL Stargazing and Particle Physics Masterclass, were adapted for online audiences, increasing our reach to more remote and diverse audiences than our usual onsite offering. Engaging diverse and under-represented audiences is an essential part of the ISIS public engagement programme, and this year ISIS created new online events and activities highlighting diversity in Science, Technology, Engineering and Maths (STEM), linking into national campaigns including Women in STEM Week and Race Equality Week.

ISIS also hosted 46 work experience students as part of the online RAL work experience programme. ISIS continues to play a leading role in the EDT Industrial Cadets Gold Project (formerly known as the Engineering Education Scheme), during which ISIS staff mentor a group of local school students for six months on a real engineering challenge. This year, A-level students from Willink School in Reading were tasked with designing a lifting device that could remove a highly radioactive component from the ISIS target assembly. The project was inspiring for both students and mentors.

Zoe Clark, Jon Cawley, Chris Russell and Conor Budd and the remote handling training set up, for the EDT Industrial Cadets Gold Project.

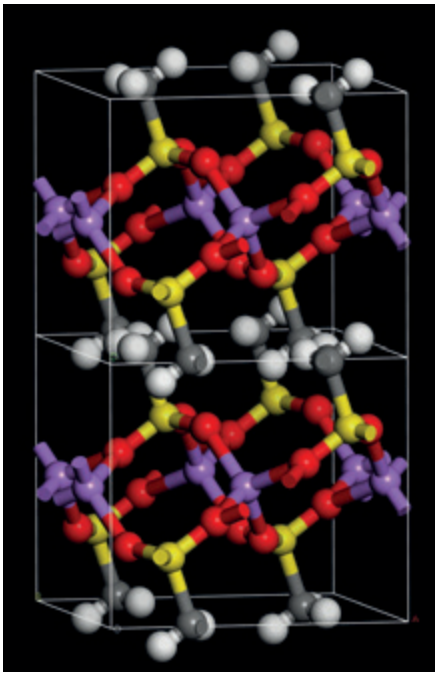


Women in STEM - see the 'For schools' section of the ISIS website for details.

From placement to publication

During a work experience placement at ISIS in 2019, Europa school student Emilie Revill-Hivet made and characterised the compound lithium methanesulfonate, leading to the publication of an article in Royal Society Open Science.

Emilie spent a two week placement with Stewart Parker, an ISIS Individual Merit scientist. Her time was split between two projects: one based on the computer, and one in the support laboratories that led to her work being published in Royal Society Open Science.



Two unit cells of the C2/m structure of $Li(CH_3SO_3)$, which was made and characterised by Emilie.

> "I made two compounds from scratch during my placement: one of these was used for a structure determination and has since been added to the Cambridge Crystallographic database," explains Emilie. "It's surreal to see my name on the publication next to Stewart's. My older siblings who are at university are very jealous!"

Apprenticeships

STFC wins the 2020 Institute of Physics' Apprentice Employer Award

STFC's Apprentice scheme was recognised in the 2020 Institute of Physics Awards for providing a wide range of apprenticeships across the country, giving young people and adults the opportunity to expand their knowledge and confidence whilst being trained in exceptional facilities. What makes this award even more special is that it was given thanks to nominations from ISIS' own apprentices.

Technician and ex-apprentice Katie Mordecai inspecting a component for the ESS.

Remote summer placements

Despite COVID-19 lockdown restrictions, ISIS still took on summer placement students in 2020. This included Ellie Dempsey, who spent 12 weeks working in the Materials Characterisation Laboratory. For Ellie, 2020 was the summer between the fourth and fifth year of her chemical physics degree at the University of Edinburgh. "Early in the year I had an email from one of my lecturers about the STFC summer placement scheme. I thought the one in the MCL looked interesting and really relevant to my studies," she says.

"When I applied for the placement, it would have been based in the lab," she explains, "But I had my interview over Zoom and when I started everyone was still working remotely. It was really good that it was able to go ahead given the circumstances."

Ellie's placement used measurements on the X-ray diffractometers in the lab to develop instrumental parameters needed for future data analysis using a piece of software called GSAS. Thanks to the ability to connect to the lab computers remotely, she was able to run the experiments herself once the samples had been loaded by Daniel, the lab's X-ray technician.

As well as keeping in touch regularly to talk about her work, the wider ISIS Support Lab group maintained informal meetings during remote working, and as some began to go back into the lab more regularly. They also gave her a video tour of the labs so she could see what it was like.

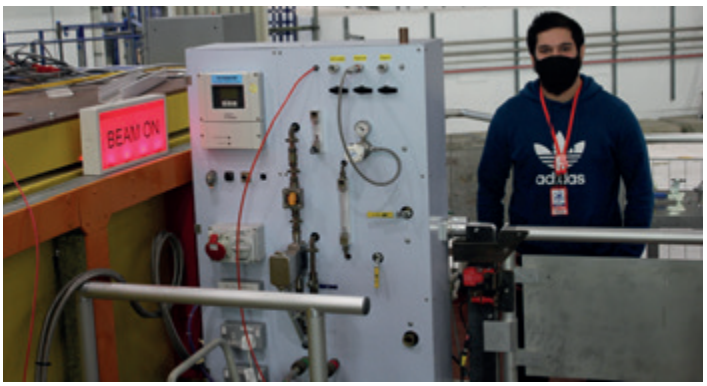
"As everyone else was working remotely too I didn't feel isolated. The regular meetings meant that we could all keep in touch." She adds, "there were also new industrial placement students who started just after me, so we were all able to go through the same processes together."

The ISIS Materials Characterisation Lab.

Student conferences

In September 2020, the ISIS Student Meeting went ahead online, featuring presentations and posters from ISIS student users, and a professional development workshop run by Vitae. 50 PhD and industrial placement students attended the two-day event, from across the UK, and internationally.

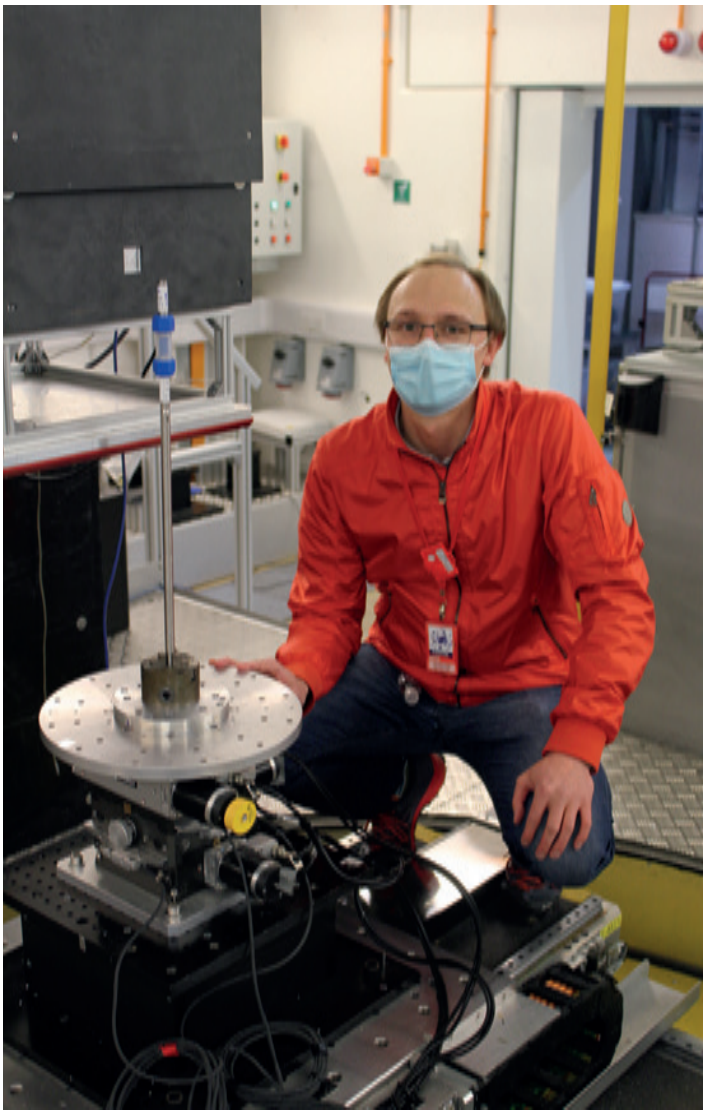
In April 2021, joint with ILL, ISIS ran a one-day conference for students using neutrons and muons in their work. The day was split between talks on common techniques and student research presentations, with students acting as chairs for the sessions. 82 students attended from the UK, France, India, Indonesia, Spain, Germany, Portugal, Slovenia, Switzerland and China.



ISIS Facility Development student and user Harrison Laurent, from the University of Leeds, on NIMROD.

Facility Development Studentships

ISIS continues to part-fund students to work on aspects of facility development. One graduate of the programme said, "The programme was amazing and I still feel giddy when I have the chance to come down to ISIS and perform experiments. The conversations I have had about science with the professionals at ISIS are irreplaceable." Over the 7 years that the programme has been running, ISIS has awarded 78 studentships so far.



ISIS Facility development student Ralf Ziesche on IMAT.

LENS Machine Learning school

From 15 – 19 February 2021, over 80 participants attended the online League of European Neutron Sources (LENS) Machine Learning School. The school, which was targeted towards neutron and muon facilities staff, offered a gateway for beginner and intermediate coders to get into machine learning, providing an overview of modern and traditional machine learning techniques alongside neutron or muon based applications.
The hands-on lectures covered a range of topics, from the very basics of how a neural network operates, to training a neural network.

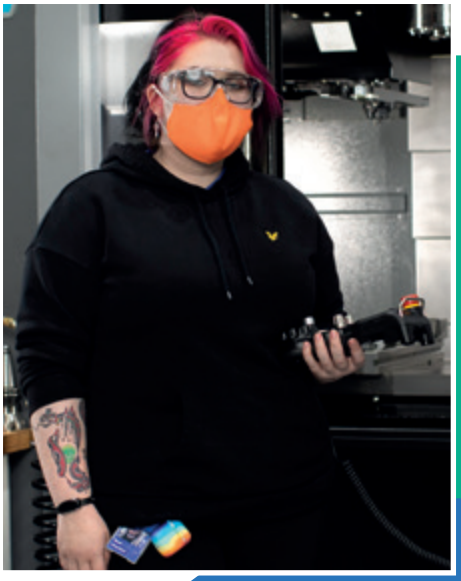
Rutherford International Fellowship Programme

ISIS has been coordinating the EU-funded Rutherford International Fellowship Programme (RIFP) over the past five years. The programme has employed 35 post-doctoral researchers across STFC departments plus Diamond, including eight based at ISIS, three of whom have been employed at ISIS after their fellowship ended. RIFP researchers, between them, produced around 180 journal articles during their fellowships, gave 135 conference talks and were involved in over 75 public engagement activities. The programme was funded by a Horizon 2020 EU Cofund award to STFC (Marie Skłodowska-Curie grant agreement No 665593), and has now reached the end of its 5-year grant.

RIFP researcher Anna Fedrigo aligning a sword specimen on the ISIS INES beamline.

Madi Woollard

Apprentice in the mechanical workshop



> We get along well and help each other out. Although we all have some background knowledge, there are some areas that are new to all of us, and it's good to talk to each other to work our way through.

Madi Woollard joined ISIS in September 2020 as an apprentice in the Mechanical Workshop. After studying machining at college, she initially went into music, getting a Level 3 performance and production qualification before deciding to pursue her engineering career. Unlike the usual apprenticeship structure that includes a rotation around different teams, Madi will be based in the workshop throughout her apprenticeship. "I really like this structure as it means I get to know my team a lot better, and allows me to really get stuck in to the jobs I'm working on," she says.

Despite the pandemic causing the college days of her apprenticeship to be put on hold for 3 months, the on-site work has been going ahead as planned. "My time has been split between training jobs that I can use to learn new skills, and working on jobs that are needed for ISIS work. It's not repetitive; all the jobs are new and interesting."

Three of the other apprentices on the scheme are also based at RAL. "We get along well and help each other out. Although we all have some background knowledge, there are some areas that are new to all of us, and it's good to talk to each other to work our way through."

The skills she's using weren't necessarily the ones she was expecting. "I've been surprised at how much maths is needed for my role; my friends joke about how I've found the only job that requires trigonometry! You also need to be a really hands-on person. Even though we're using machines, they don't do it all for you and you need to be keen to get stuck in. It's also really important to be patient, and not be too hard on yourself when things go wrong."

When she was looking at apprenticeships, she was warned that it was a very male-dominated environment. "It was a bit daunting to be told this. Not because of being treated badly, but in case people would tip-toe around me, which is something I really wanted to avoid. Also, in school, people would make comments saying we would only get accepted onto a scheme because we were 'a girl', which is another thing I didn't want to be known for, or for people to think."

However, she's learnt that at ISIS "it's not a problem at all. I'm not treated any differently and I think it's a really great working environment for anyone to be in."

"The stereotype of being an apprentice and being given all the awful jobs no-one wants is definitely not the case here either. In fact, it's almost the opposite! My colleagues will approach me if there is a particularly interesting job to do, or if there is a task where I'll be able to learn a new skill."

Publications 2020

In 2020, 644 journal articles were published resulting from work performed at ISIS.

AH Abdeldaim, T Li, L Farrar, AA Tsirlin, W Yao, AS Gibbs, P Manuel, P Lightfoot, GJ Nilsen, L Clark, Realizing square and diamond lattice S = 1/2 Heisenberg antiferromagnet models in the alpha and beta phases of the coordination framework, $KTi(C_2O_4)_2 \cdot xH_2O$, *Physical Review Materials*, **4**, (2020), 104414, Instruments: HRPD, WISH, MAT-CHAR-LAB

IB Adilina, F Aulia, MA Fitriady, F Oemry, RR Widjaya, SF Parker, Computational and Spectroscopic Studies of Carbon Disulfide, *Molecules*, **25**, (2020), 1901, Instrument: TOSCA

DT Adroja, SJ Blundell, F Lang, H Luo, Z Wang, G Cao, Observation of a neutron spin resonance in the bilayered superconductor $CsCa_2Fe_4As_4F_2$, *Journal of Physics: Condensed Matter*, **32**, (2020), 435603, Instrument: MERLIN

DT Adroja, S Sharma, C Ritter, AD Hillier, D Le, CV Tomy, R Singh, RI Smith, M Koza, A Sundaresan, S Langridge, Muon spin rotation and neutron scattering investigations of the B-site ordered double perovskite Sr_2DyRuO_6, *Physical Review B*, **101**, (2020), 94413, Instruments: GEM, MERLIN, MuSR

S Afroze, N Torino, MS Reza, N Radenahmad, Q Cheok, PF Henry, AK Azad, Structure-conductivity relationship of $PrBaMnMoO_{6-\delta}$ through in-situ measurements: A neutron diffraction study, *Ceramics International*, **47**, (2020), 541, Instrument: POLARIS

S Afroze, N Torino, PF Henry, MS Reza, Q Cheok, AK Azad, Neutron and X-ray powder diffraction data to determine the structural properties of novel layered perovskite $PrSrMn_2O_{5-\delta}$, *Data in Brief*, **29**, (2020), 105173, Instrument: POLARIS

S Afroze, D Yilmaz, MS Reza, PF Henry, Q Cheok, JH Zaini, AK Azad, A Issakhov, M Sadeghzadeh, MH Ahmadi, Investigation of Structural and Thermal Evolution in Novel Layered Perovskite $NdSrMn_2O_{5+\delta}$ via Neutron Powder Diffraction and Thermogravimetric Analysis, *International Journal of Chemical Engineering*, **2020**, (2020), 6642187, Instrument: POLARIS

KE Agbovi, J Fajoui, B Girault, D Gloaguen, S Kabra, J Kelleher, W Kockelmann, Investigation of α-Ti plastic anisotropy under thermomechanical loadings: temperature influence on deformation mechanisms, *MATEC Web of Conferences*, **321**, (2020), 7004, Instruments: ENGIN-X, GEM

SNA Ahmad, S Sulaiman, DFH Baseri, LS Ang, NZ Yahaya, H Arsad, I Watanabe, Density Functional Theory Studies of Muon Stopping Sites and Hyperfine Interaction in $[Au_{25}(SR)_{18}]^0$ Nanocluster, *Journal of the Physical Society of Japan*, **89**, (2020), 14301, Instrument: RIKEN

D Ahmadi, N Mahmoudi, RK Heenan, DJ Barlow, MJ Lawrence, The Influence of Co-Surfactants on Lamellar Liquid Crystal Structures Formed in Creams, *Pharmaceutics*, **12**, (2020), 864, Instrument: LOQ

D Ahmadi, N Mahmoudi, P Li, K Ma, J Doutch, F Foglia, RK Heenan, D Barlow, MJ Lawrence, Revealing the Hidden Details of Nanostructure in a Pharmaceutical Cream, *Scientific Reports*, **10**, (2020), 4082, Instruments: LOQ, SANS2D

V Akrivos, RC Wimpory, M Hofmann, B Stewart, O Muransky, MC Smith, J Bouchard, Neutron diffraction measurements of weld residual stresses in three-pass slot weld (Alloy 600/82) and assessment of the measurement uncertainty, *Journal of Applied Crystallography*, **53**, (2020), Instrument: ENGIN-X

A Al Mamun, C Simpson, D Agius, TL Lee, S Kabra, C Truman, M Mostafavi, D Knowles, A novel insight into the primary creep regeneration behaviour of a polycrystalline material at high-temperature using in-situ neutron diffraction, *Materials Science and Engineering* A, **786**, (2020), 139374, Instrument: ENGIN-X

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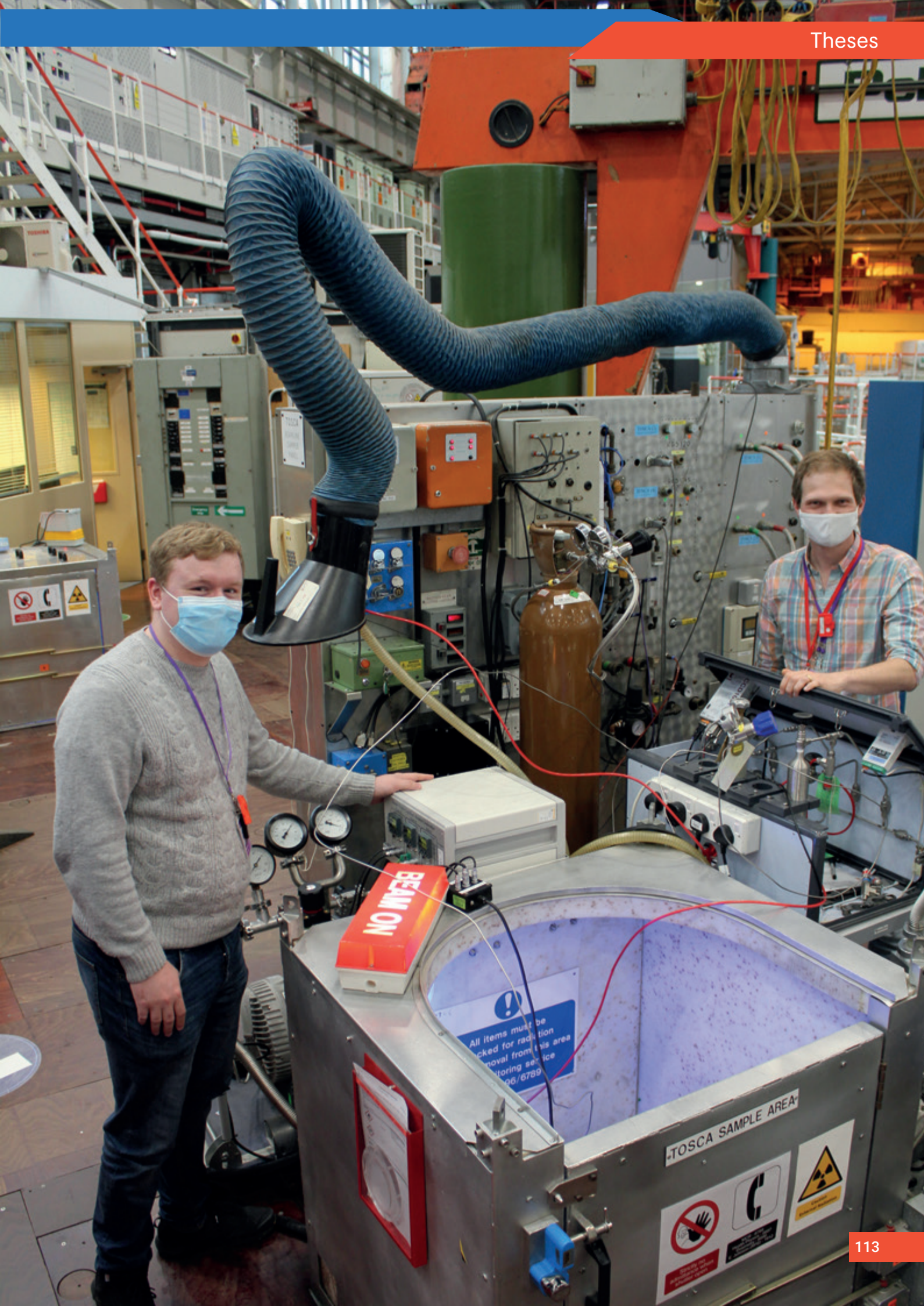
Right: Dr Simon Kondrat and Ed Jones from Loughborough University on Tosca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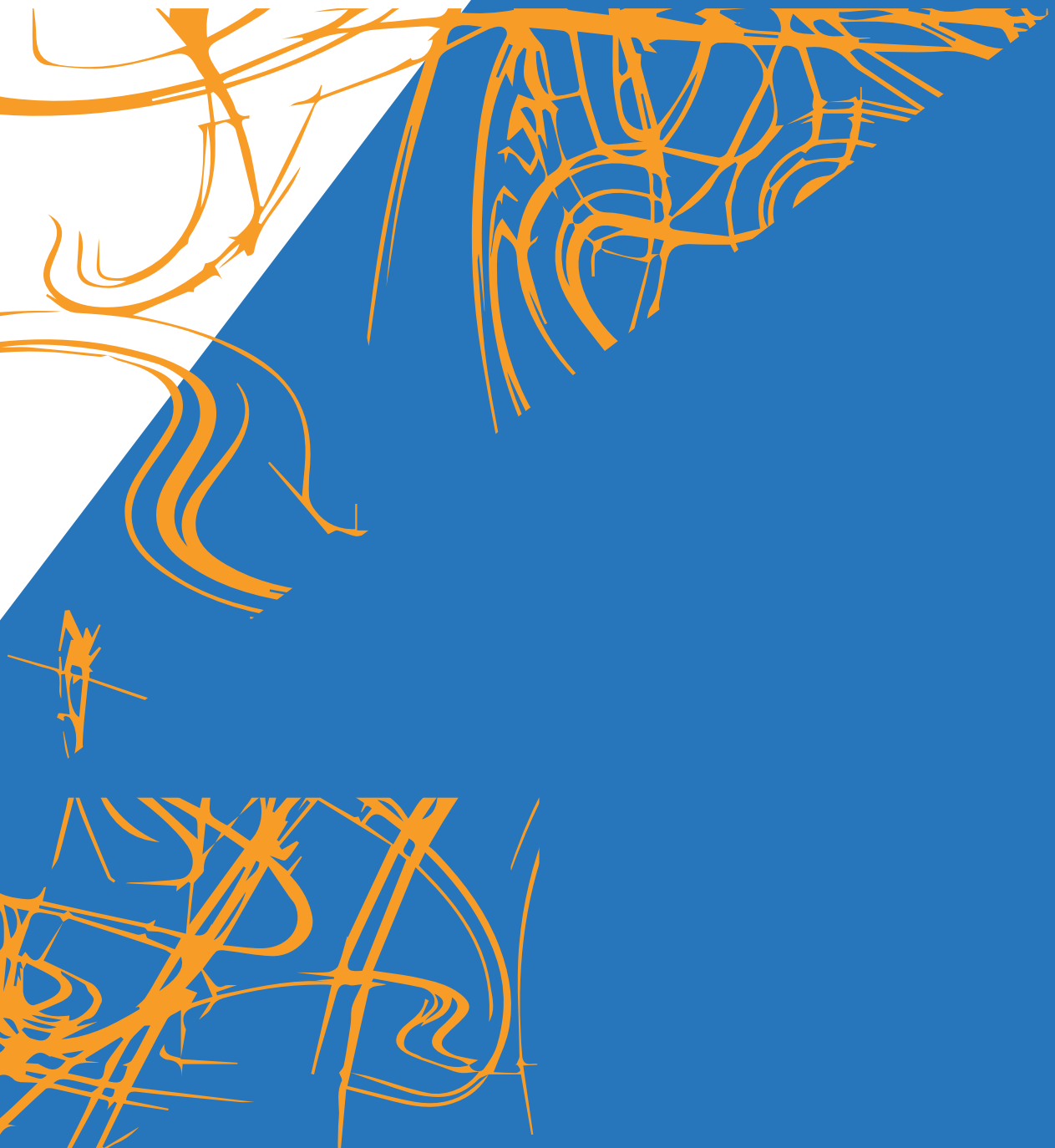

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