



Science and  
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Facilities Council

# ISIS Neutron and Muon Source: Annual Review 2022



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*Front cover: Beatrice Anna Maria Boggio Robutti and Dr Thomas McCoy,  
University of Cambridge*

# Contents

<b>Foreword</b>	<b>5</b>
<b>Overview</b>	<b>6</b>
<b>Science at ISIS</b>	<b>8</b>
Impact Awards	11
Science Highlights	15
Case Study – Professor Jacqui Cole	43
<b>Source, Instruments and Technical Development</b>	<b>44</b>
Sustainability	46
Major Projects	48
Accelerator Developments	55
Case Study – Haroon Rafique	59
Enabling Technology and Facilities	60
Instrument Updates	65
Case Study – Gemma Draper	71
Future Projects	72
<b>Partnerships</b>	<b>80</b>
<b>People</b>	<b>88</b>
Case Study – Robert McGreevy	90
Case Study – Zoë Bowden	91
Technicians Commitment and Committed Technicians	95
Case Study – Richard Waite	97
<b>Publications</b>	<b>98</b>
<b>Theses</b>	<b>129</b>

# Foreword



# Foreword

The final stanza of T S Eliot's Four Quartets contains the lines "the end of all our exploring, will be to arrive where we started, and know the place for the first time". These lines have come to mind regularly since I became ISIS Director last October, returning to the place where my scientific and professional career started, and the scientific environment that inspired me as a placement student. There is much that is familiar about ISIS, but ISIS has developed and changed so much that, in many respects, the process of settling in has been one of getting to know a new and exciting organisation rather than reacquainting myself with an old one.

I am fortunate to have succeeded Robert McGreevy as Director of ISIS at an exciting time. ISIS is in great shape, which is a testament to Robert's leadership, the excellent team I inherited and particularly the incredible commitment and expertise of the ISIS staff. I also could not write this foreword without mentioning Zoë Bowden, who retired in the spring. Zoë has worked at ISIS for more than 40 years and her contribution has been enormous. Somehow Zoë manages to embody both continuity and a relentless drive to improve.

Within this report you will find a small sample of the outstanding science delivered by ISIS users and staff. Our programme is broad, provides new insights into fundamental questions and addresses global challenges, including the drive to net-zero and improving healthcare.

During the last year, several significant and challenging projects have been completed, including the replacement of linac tank 4, a major upgrade of the synchrotron RF system and the replacement of the muon collimator at relatively short notice. In addition, the Target Station 1 Project is nearing completion. It is the biggest and most complex project we have undertaken since the construction of Target Station 2. The skill and expertise of our engineers,



technicians and scientists is incredibly impressive, as is the teamwork required to deliver such a technically demanding and complex portfolio.

The business case for Endeavour, our 10-year programme comprising 4 new instruments and 5 major upgrades, has made good progress this year and we are optimistic about being able to secure the investment required to enhance the capacity and capability of the ISIS instrument suite. ISIS's innovative approach to the development of the source, instrumentation and ancillary activities, and the incredible partnership we have with our user community, ensures ISIS continues to be world-leading in terms of both scientific productivity and technical innovation.

## Professor Roger Eccleston ISIS Director

“

There is much that is familiar about ISIS, but ISIS has developed and changed so much that, in many respects, the process of settling in has been one of getting to know a new and exciting organisation rather than reacquainting myself with an old one.

–Professor Roger Eccleston, ISIS Director

”



Please tell us what you think  
about our annual review!

# Overview

The ISIS Neutron and Muon Source: neutrons and muons to advance knowledge and improve lives.

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

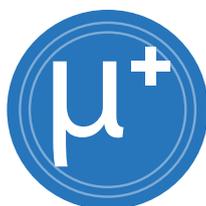
The ISIS science programme spans a wide range of areas including clean growth, advanced materials, quantum matter and life sciences. Neutrons and muons are used to address important scientific challenges across these areas and deliver societal and economic benefit: ISIS research maps strongly onto UK government science and technology priority areas, for example as described in the Net Zero, Quantum Technologies, Hydrogen and Innovation Strategies, as well as the Life Sciences Vision. ISIS attracts industrial users from a broad range of sectors including automotive, pharmaceuticals, food, petrochemicals, engineering, catalysis and biosciences, who work with ISIS scientists and in collaboration with university user groups to develop materials and processes and to address real-world problems.

ISIS is the UK's national neutron and muon source, but our reputation and impact are international. Researchers come from all over the world to use our instruments and collaborate with our scientists, engineers and technicians. We work in partnership with

neutron and muon sources in Europe, Japan, China and the US in a wide range of technical areas; and we have bilateral agreements with other countries who make use of the capabilities of ISIS and its staff and collaborate in the development of source and instrumentation.

Our public engagement programmes inspire the next generation of scientists. We support the training of early career scientists, engineers, technicians and software developers through apprentice, industrial placement, vacation project, work experience, graduate and PhD programmes.

This annual review includes recent science from ISIS, including work by industry; updates on our long-term development projects as well as recent technical work; our partnerships and collaborations; and our people, including support for early career staff.



**5 Muon instruments**



**Neutron instruments**

## In a typical year...



**1200 experiments**

*by*



**3000 users**

*from*



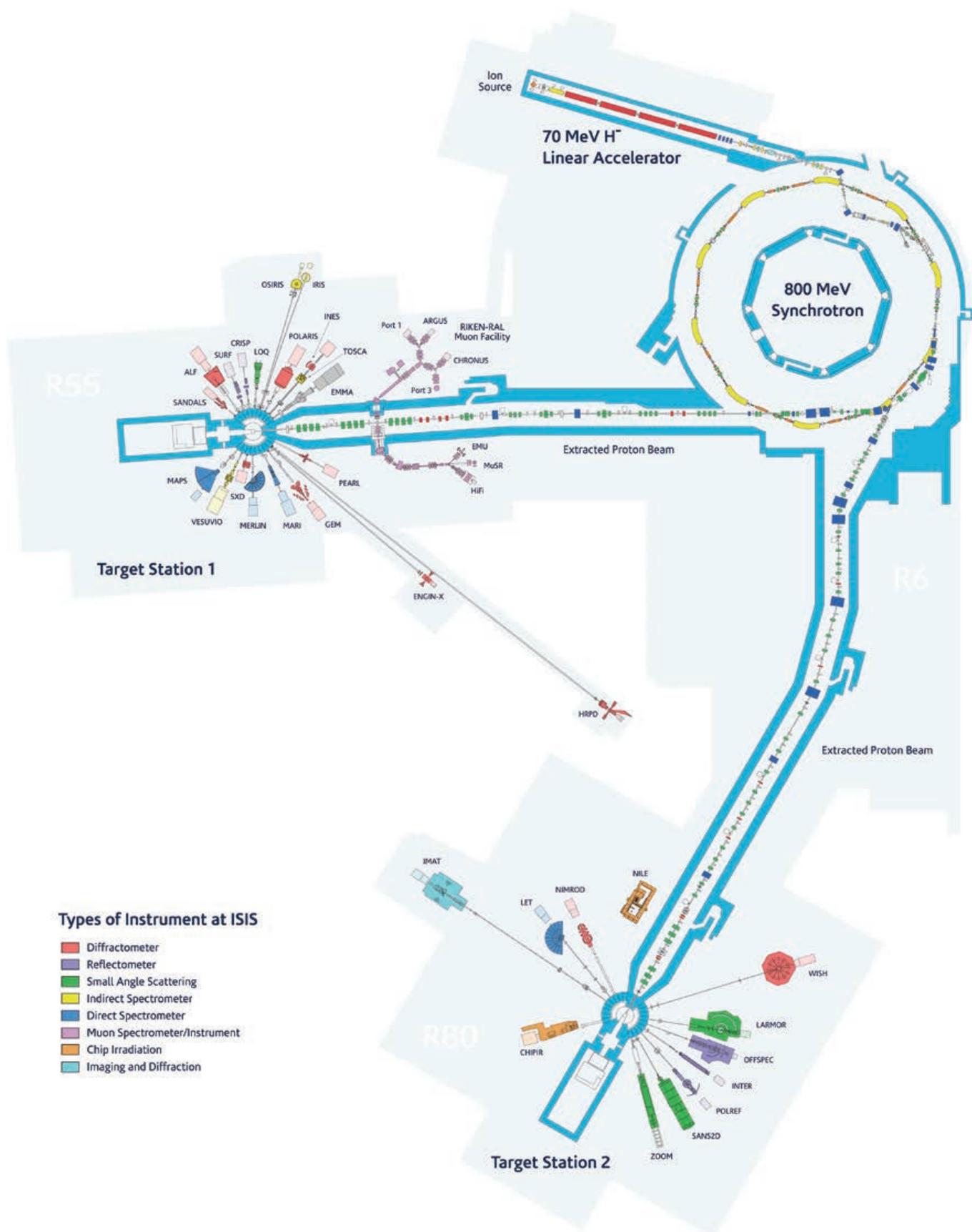
**30 countries**

*generating*



**600 publications**

# The ISIS Neutron and Muon Source

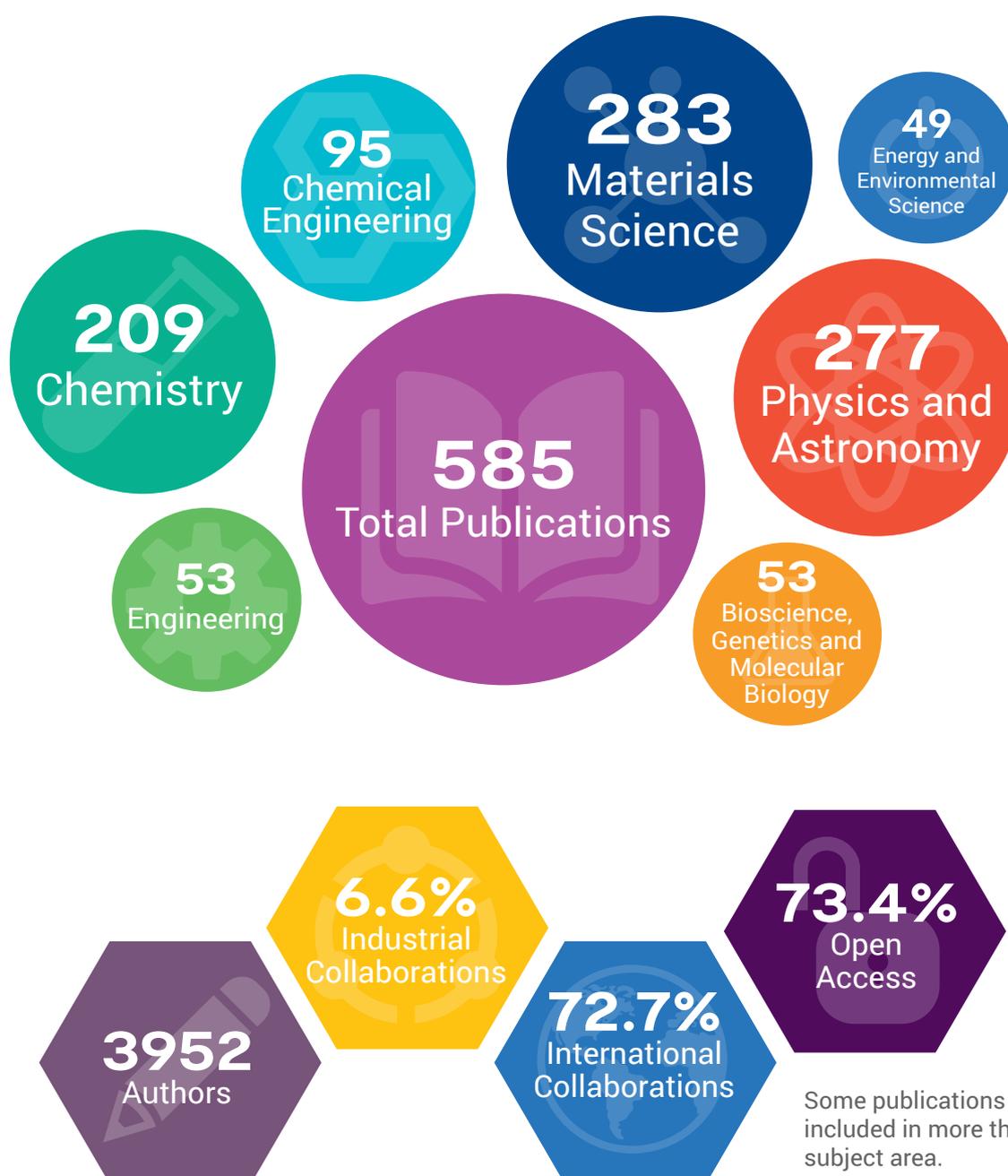


# Science at ISIS

A great strength of the ISIS source and its academic and industrial community is the breadth, depth and quality of research that is delivered. 2022 has seen another year of impactful discoveries across a diverse range of science and technology areas, from fundamental studies to those directly addressing societal challenges.

Recent times have seen the publication of a range of national and international strategic priorities around Net Zero, sustainable growth and healthcare, which draw significantly on industry and the physical and life sciences. ISIS brings together leading academics and industrialists to accept and advance these challenges, exploiting the unique insight that neutrons and muons provide.

In the following sections, we present highlights that showcase the utility and strategic importance of neutrons and muons to an incredibly broad range of science. That science spans from fundamental studies of quantum matter to applications that include sustainable growth, food science, cultural heritage, healthcare and clean energy.



## ISIS's unique industry access scheme provides major economic benefit

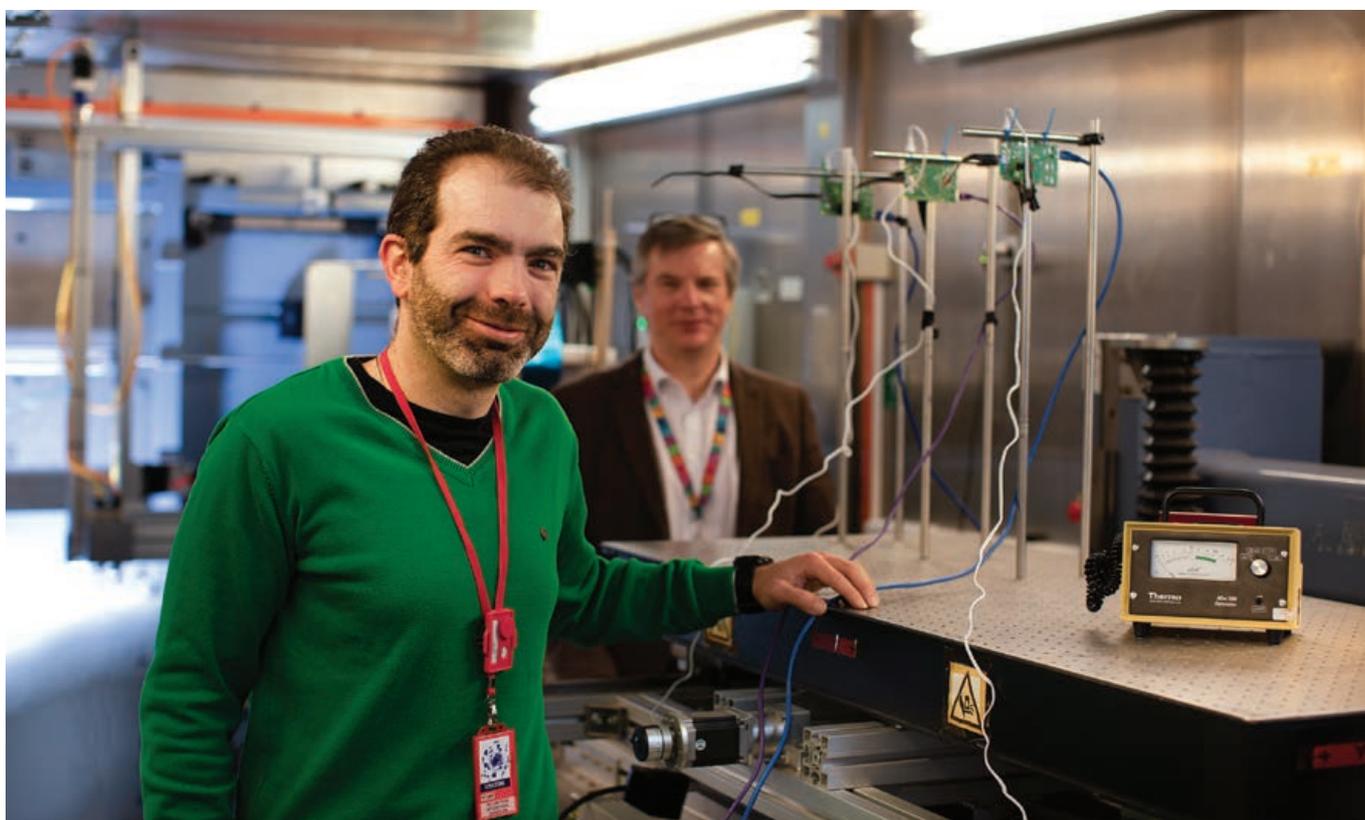
**Investigation of materials using neutron and muon techniques provides unique and key insights into their structure and behaviour. In addition to the global academic community, a diverse range of industry sectors has used and developed these techniques to understand and optimise commercial products and processes.**

The ISIS Industrial Collaborative Research and Development scheme (ICRD) was established in 2012 and provides a lower risk, more flexible access route for industry. This is because the decision to publish the results or purchase the beamtime comes after the experiment, rather than beforehand. In addition to benefitting the industrial user, the ICRD route provides qualitative and quantifiable information about the economic impact of ISIS's industrial research.

This invaluable economic data was used by the Technopolis Group in its "ISIS Lifetime Impact Study" published in 2018, and more recently in the development of the business case for the Endeavour programme.

This includes the work of a petrochemical company who used Small Angle Neutron Scattering (SANS) in the commercialisation of a new surfactant structure, which now generates income of ~\$300M per year. They also used neutron reflectometry to understand the molecular phenomena that control friction, which will lead to improved fuel economy and hence reduced gaseous emissions into the environment. Another example, from a different industry, is a pharmaceutical company who used inelastic neutron scattering to study dissolution rates in a nanoscale pharmaceutical delivery system, which has boosted the development and commercialisation of this technology.

ICRD is not just for purely commercial users but is suitable for any ISIS beamtime proposal featuring strong industry involvement. For example, if a member of the experimental team is a company employee, if the materials to be analysed are supplied by industry, or if an involved PhD student or post-doc is funded by industry.



Paolo Rech on Chiplr with Chris Frost. The Chiplr beamline at ISIS attracts significant industrial usage.

Right: Alberto Viani, Centre of Excellence Tech, Czech Republic, and Heloisa Bordallo, University of Copenhagen, Denmark, on the IRIS instrument.

# ISIS Impact Awards

The ISIS Impact Awards celebrate the socio-economic impact generated by our diverse user community. The awards have been running for five years and the quality of the nominees continues to be exceptionally high. Congratulations to this year's winners!



# ISIS Impact Awards 2022

2022 Society Impact Award winner: Heloisa Bordallo, Niels Bohr Institute, University of Copenhagen, Denmark

*Awarded for her work on developing smarter materials by tuning physio-chemical properties using Tosca and Iris*

## Society

**Dr Heloisa Nunes Bordallo uses neutrons and other complementary techniques to study a range of materials that are relevant to our daily lives including dental cements, food, drug molecules and hair bleach. The common theme that runs through these examples is the presence of water confined in porous polymer frameworks. She uses a range of spectroscopy techniques to study the dynamics of hydrogen bonding in these frameworks, and how the polymers that are held together by these bonds change under different conditions.**



In a dental cement, a glassy component is mixed with an aqueous solution, creating a mixture in which strong hydrogen bonds form. Using Quasielastic Neutron Scattering (QENS) on the Iris instrument at ISIS, Dr Bordallo was able to study the hydrogen bonding network as it formed. To study faster reactions, down to the femtosecond timescale, she used the Tosca beamline. Combining the results from experiments on different spectrometers, she was able to study how a framework behaves over a large range of timescales.

Another feature of Tosca that Dr Bordallo has used is the ability to do simultaneous Raman spectroscopy. She applied this during a study of psychotic drugs, which meant she could better define the peaks caused by the vibrations in the complex drug molecules. This knowledge of the way the individual drug molecules move could be used in the future by those developing new medicines.

By using complex sample environments, her group studies porous polymers in the presence of different gases. This includes the investigation of a material that can capture the toxic gas ammonia from the atmosphere, with potential applications in face masks. By combining neutron spectroscopy experiments with DFT calculations using the STFC computing clusters, she was able to determine exactly how the ammonia was binding to the polymer framework. This understanding will inform the design of future materials with tuneable functionality.

As well as progressing her own research, Dr Bordallo has also introduced many students to the benefits of neutron scattering. These students then take their knowledge of neutrons with them into academia, industry, or teaching.

She is a vocal advocate of using neutrons and continues to raise awareness of the uniqueness of neutron spectroscopy among communities that would otherwise not use the technique, such as cosmetic scientists, dental researchers and, more recently, food scientists.

### Related publications:

Human hair: subtle change in the thioester groups dynamics observed by combining neutron scattering, X-ray diffraction and thermal analysis, CRR de Castro Lima, RJS Lima, LDB Machado, MVR Velasco, L Lakić, MS Nordentoft, L Machuca-Beier, S Rudić, MTF Telling, V Garcia-Sakai, CLP de Oliveira, HN Bordallo, Eur. Phys. J. Special Topics (2020) 229, 2825-2832.

Ammonia Storage in Hydrogen Bond-Rich Microporous Polymers, RJS Lima, DV Okhrimenko, S Rudić, MTF Telling, V Garcia Sakai, D Hwang, GN Barin, J Eckert, J-W Lee and HN Bordallo, ACS Appl. Mater. Interfaces (2020) 12, 58161–58169

## 2022 Economic Impact Award winner: Adam Michalchuk, Federal Institute for Materials Research and Testing, Germany

*Awarded for his work on the in-silico design of safer energetic materials*

### Economics

**The economic impact award recognises research into the effect of impact in a different sense of the word. Energetic materials that release energy when a force is applied are widely used across a range of industries from defence and demolition to fireworks and Christmas crackers. However, some of the materials that are commonly used are toxic, with others causing environmental damage, and so there is a drive to find alternatives that are less damaging.**



Despite these materials having been used for many years, there is little understanding of what causes mechanical impact to prompt the chemical reaction behind an explosion. Knowing what is happening on the atomic scale is key to developing new, more environmentally-friendly energetic materials.

Dr Adam Michalchuk and his collaborators aim to address this issue using computers. They have developed a computational model, based on vibrational spectra, that predicts the properties of energetic materials. To ensure their model was giving realistic answers, they needed to benchmark it against experimental results.

After attending the ISIS neutron training course, Dr Michalchuk realised that neutrons could provide critical information that cannot be gathered using laboratory-

based techniques. Using the results of inelastic neutron scattering to validate their model, they have shown that their method is able to accurately describe the properties of a diverse range of energetic materials.

As well as using spectroscopy, he has expanded his work to using neutron diffraction on the Pearl beamline to study the crystal structure of these materials, and how they behave under high pressures. This will help him understand how mechanical force influences the activity.

The next stage of his research will see Dr Michalchuk collaborate with experimental chemists to design the energetic materials of the future. In addition, the understanding of how mechanical force can drive a chemical reaction is not only useful for this area of chemistry but can also be applied more widely.

#### Related publications:

Predicting the reactivity of energetic materials: an ab initio multi-phonon approach, AAL Michalchuk, M Trestman, S Rudić, P Portius, PT Fincham, CR Pulham and CA Morrison, *J. Mater. Chem. A* (2019) 7, 19539-19553

Predicting the impact sensitivities of energetic materials through zone-center phonon up-pumping, AAL Michalchuk, J Hemingway and CA Morrison, *J. Chem. Phys.* (2021) 154, 064105

Predicting the impact sensitivity of a polymorphic high explosive: the curious case of FOX-7, AAL Michalchuk, S Rudić, CR Pulham and CA Morrison, *Chem. Commun.* (2021) 57, 11213-11216

Vibrationally induced metallisation of the energetic azide  $\alpha$ -NaN-3, AAL Michalchuk, S Rudić, CR Pulham and CA Morrison, *Phys. Chem. Chem. Phys.* (2018) 20, 29061-29069

A Pathway to the thermal Impact Initiation of Energetic Azides, AAL Michalchuk, PT Fincham, P Portius, CR Pulham and CA Morrison, *J. Phys. Chem. C* (2018) 122, 34, 19395-19408

## 2022 Science Impact Award winner: Andrej Zorko, Jožef Stefan Institute and University of Ljubljana, Slovenia

*Awarded for the first realization of a quantum spin liquid on a triangular spin lattice with dominant Ising antiferromagnetic exchange interaction using WISH, Mari and MuSR.*

### Science

**A significant obstacle to the realisation of quantum computing is the fragility of the qubit where information would be stored. Developing a system that can store information and remain robust to interference is key to having fault-tolerant quantum computations.**



Quantum spin liquids (QSLs) occur when the magnetic moments of a material become entangled but remain disordered even at absolute zero. They can form stable complex topologies, making them a potential candidate for quantum computing materials.

Dr Andrej Zorko has been awarded the Science Impact Award this year for his work on one particular QSL material neodymium heptatantalate,  $\text{NdTa}_7\text{O}_{19}$ . This compound was anticipated to behave as a QSL after a theoretical prediction made seventy years ago, but, until recently, this had not been experimentally confirmed.

Using a combination of muon spectroscopy on MuSR, inelastic neutron scattering (INS) on Mari and neutron diffraction on WISH, as well as other experimental techniques in the laboratory and at large-scale facilities around the world, the team were able to show for the first time that a QSL is formed in  $\text{NdTa}_7\text{O}_{19}$ .

Although a few other QSL candidates have been characterised, this compound is the first of its kind: a triangular spin lattice with dominant Ising antiferromagnetic nearest-neighbour spin correlations.

Using INS, they were able to confirm that the magnetic species had effective spin 1/2 at low temperatures. They then used neutron diffraction to characterise the ground state, finding that there was no magnetic ordering even down at the lowest experimental temperature, while spin correlations were found to develop. Following up these studies with experiments on MuSR meant they were able to confirm the absence of magnetic order, and show that there were spin dynamics present in the ground state, revealing the quantum nature of the ground state.

His group's results show the community that the family of rare-earth heptatantalates is a potential source of candidate materials for quantum computing applications.

#### Related publication:

The Ising triangular-lattice antiferromagnet neodymium heptatantalate as a quantum spin liquid candidate, T Arh, B Sana, M Pregelj, P Khuntia, Z Jagličić, M D Le, P K Biswas, P Manuel, L Mangin-Thro, A Ozarowski and A Zorko, *Nature Materials* (2022) 21, 416–422

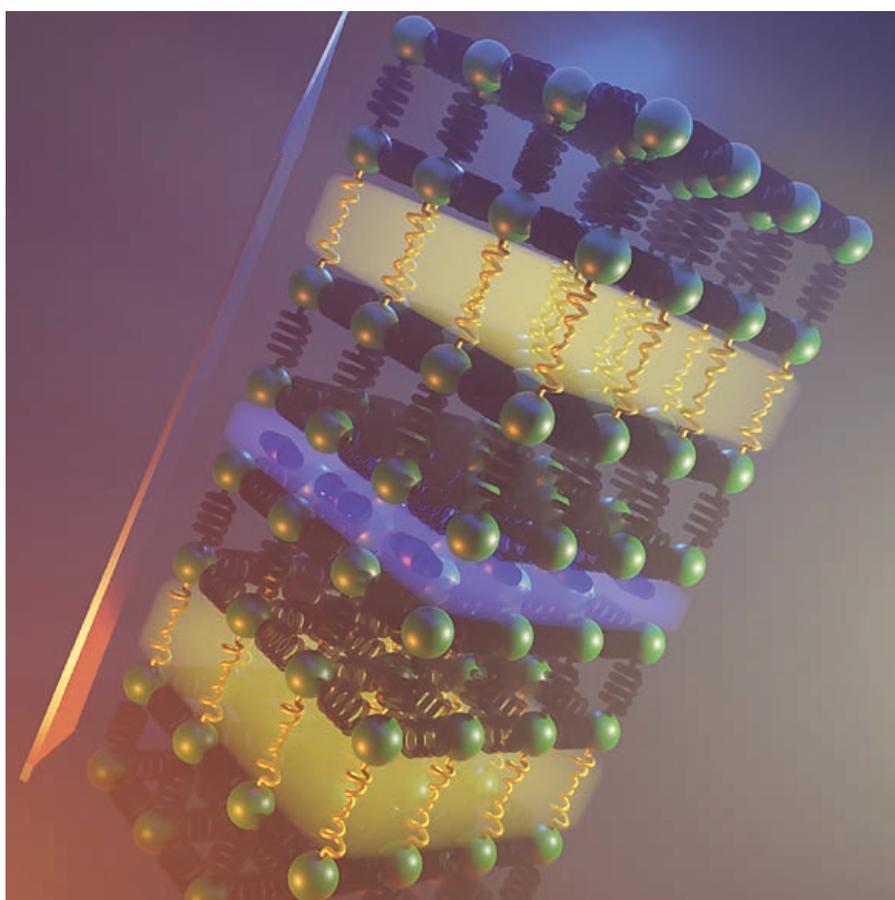
# Science Highlights



## Merlin

# Keeping it cool: an inorganic material with lowest thermal conductivity ever reported

A collaborative research team has discovered a new inorganic material with the lowest thermal conductivity ever reported for a bulk inorganic material. The discovery, reported in the journal *Science*, represents a breakthrough in the control of heat flow at the atomic scale, achieved by materials design. The new understanding will accelerate the development of new materials for converting waste heat to power and for the efficient use of fuels.



The research team designed and synthesised the new material so that it combined two different arrangements of atoms that were each found to slow down the speed at which heat moves through the structure of a solid. They identified the mechanisms responsible for the reduced heat transport in each of these two arrangements by measuring and modelling the thermal conductivities of two different structures, each of which contained one of the required arrangements.

*Two different atomic arrangements (yellow and blue slabs) that provide mechanisms to slow down the motion of heat through a solid.*

**Instrument:** Merlin

**Related publication:** Low thermal conductivity in a modular inorganic material with bonding anisotropy and mismatch, *Science*, 2021, 373, 6558, 1017-1022

**DOI:** 10.1126/science.abh1619

**Funding:** EPSRC, Royal Society

**Authors:** QD Gibson (University of Liverpool), T Zhao (University College London), LM Daniels (University of Liverpool), HC Walker (ISIS), R Daou, S Hébert (Normandie Université), M Zanella, MS Dyer, JB Claridge (University of Liverpool), B Slater (University College London), MW Gaultois (University of Liverpool), F Corà (University College London), J Alaria, MJ Rosseinsky (University of Liverpool)

## Chiplr

### Understanding neutron-caused errors in electronics

During his industrial placement, student Sebastian Blower used Chiplr's high-intensity neutron beam to showcase effective reliability improvements for the commercially available Artificial Intelligence (AI) accelerator, the NM500 neuromorphic neural network chip from General Vision.

The NM500 is an Edge AI accelerator, so it learns by saving information about an object in its category register. It then predicts whether any features of any objects resemble what it has learnt by comparing information that it is given with the information in its register. By processing data in the device rather than using cloud computing, Edge AI is quicker and therefore important for automotive applications. This study, published in IEEE Transactions on Nuclear Science, found that the errors that caused the device to fail were generated by neutron events in the NM500's category register.

Sebastian then investigated ways to avoid these errors causing device failure, adapting the triple mode redundancy technique for the NM500 by exploiting unused bits in the category register. At no extra cost or physical complexity, 96% of single event effects were corrected by the technique, a dramatic improvement of the device's reliability. This work serves as a promising proof-of-concept for further investigations into the reliability of AI accelerators.



NM500 neuromorphic neural network chip

**Instrument:** Chiplr

**Related publication:** Evaluating and Mitigating Neutrons Effects on COTS EdgeAI Accelerators, *IEEE Transactions on Nuclear Science*, 68, 8, 2021

**DOI:** 10.1109/TNS.2021.3086686

**Authors:** S Blower (ISIS), P Rech (Universidade Federal do Rio Grande do Sul), C Cazzaniga, M Kastriotou, CD Frost (ISIS)

## Engin-X

### Testing a cheaper, quicker method of making spacecraft components

Working with the companies TWI Ltd. and Airbus UK, researchers from the European Space Agency used the technique of Friction Stir Welding (FSW) to build the components of a prototype spacecraft propellant tank and came to ISIS to study the residual stress caused during manufacture. FSW would have lower costs and shorter lead times than conventional manufacturing techniques.

Previous research has looked at the residual stress inside flat FSW components, but this study, published in *CEAS Space Journal*, was the first to study curved components. Using X-ray and neutron diffraction alongside hole drilling, the collaborators were able to determine the magnitude of the residual stresses both at the surface and in the bulk of the material and evaluate these in the context of the requirements defined by the space industry.

They found that the residual stresses present at the joint were lower than for conventionally welded tanks, or for previously reported FSW examples. This confirms that using this new method for joining hemispherical and cylindrical structures was successful for manufacturing a propellant tank that meets the stringent acceptance criteria of the space industry with regards to residual stresses in the weld.

“

We had a new technology and were facing a challenging research problem with the structural integrity of these propellant tanks. The scientists and experts at Engin-X did an outstanding job and helped us design the experiment and evaluate the data. We are certainly hoping for future collaborations on similar topics.

Martina Meisnar from ESA

”



**Instrument:** Engin-X

**Related publication:** Advanced manufacturing of titanium propellant tanks for space applications part 2: a comparative study of residual stresses, *CEAS Space J* (2021)

**DOI:** 10.1007/s12567-021-00398-w

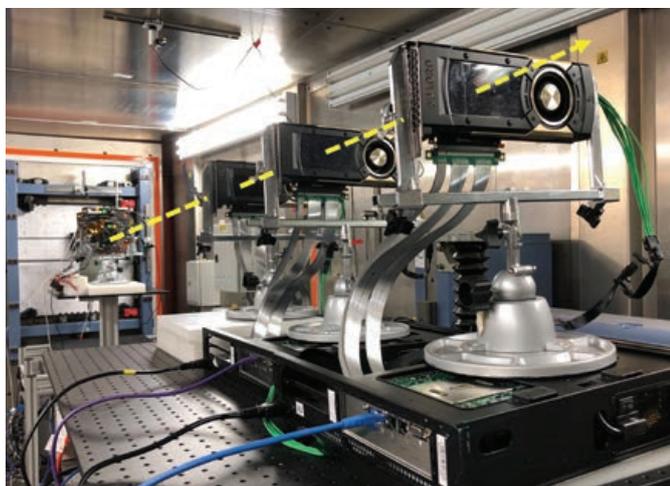
**Funding:** ESA, UKSA

**Authors:** M Meisnar (European Space Agency), JM Bennett (ISIS), D Andrews, S Dodds, R Freeman (TWI Ltd.), R Bellarosa (Airbus Defence and Space), J Kelleher (ISIS), A Graham, AF Norman, T Rohr, T Ghidini (European Space Agency)

## Chiplr

### NVIDIA uses Chiplr to reduce errors in GPU systems

Society is becoming increasingly reliant on computing systems such as data centres and we are on the cusp of having fully autonomous vehicles. These systems typically use advanced commercial ‘off-the-shelf’ hardware, such as Graphics Processor Units (GPUs), that contain error checking and correcting codes to increase the reliability of the hardware. The high computing capabilities of GPU acceleration in these systems is critical for their high performance and energy efficiency, making GPU resilience a priority for safety critical applications.



NVIDIA Quadro V100 GPUs in the Chiplr beamline, with a dashed line to show the direction of the neutron beam.

One cause of errors is neutron-induced single event effects from cosmic rays, known as soft errors, and NVIDIA brought sample GPU devices to Chiplr to test the effect of neutrons on GPU memories and applications. One main object of investigation was GPU DRAM, as this memory is the most area-consuming and sensitive part of the GPU.

During their experiments, the researchers discovered that the high-energy beam was causing unexpected intermittent errors in DRAM due to damage to the devices. They were able to isolate these errors from the soft errors. Once they had separated out the impact of soft errors, they could determine the DRAM logic structures that were most affected and design an error-correcting code that is able to correct soft errors more frequently, while simultaneously reducing the risk of silent data corruption.

“



The Chiplr beamline has been extremely valuable for our studies into the effects of soft errors on NVIDIA GPUs. The stability and strength of the beam and the well-thought-out infrastructure have made it possible to run more experiments in less time.

Mike Sullivan, NVIDIA

”

**Instrument:** Chiplr

**Related publication:** Characterizing and Mitigating Soft Errors in GPU DRAM, *MICRO '21: MICRO-54: 54th Annual IEEE/ACM International Symposium on Microarchitecture*, 2021, 641–653

**DOI:** 10.1145/3466752.3480111

**Funding:** US Department of Energy and NVIDIA

**Authors:** MB Sullivan, N Saxena, M O'Connor, D Lee, P Racunas, S Hukerikar, T Tsai, SKS Hari, SW Keckler (NVIDIA)

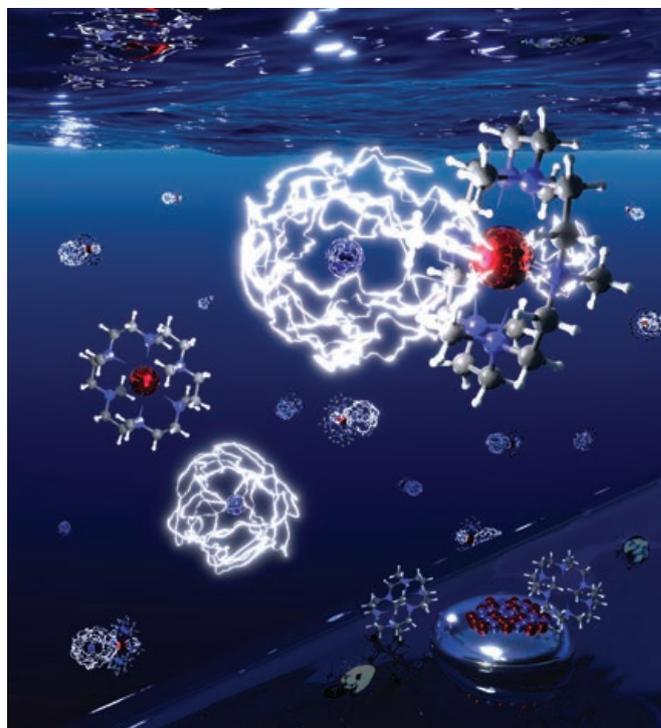
## Nimrod

### Discovering ion pairing in alkalide solutions

Alkalides are negatively charged condensed phases of the Group 1 metals such as sodium and potassium and are challenging to form due to the electropositive nature of these atoms. They have long been assumed to exhibit ‘gas-like’ behaviour, with very little interaction with their local environment. Neutron experiments on Nimrod have contributed significantly to calling this into question, providing strong evidence for ion association in solution.

In this comprehensive study, published in *Journal of the American Chemical Society*, the researchers show, for the first time, that alkalides do interact with their environment. This interaction occurs through the formation of species where the anion pairs with a large counterion, complexes of macrocycles and alkali cations termed ‘superalkalis’.

The observation of the interaction of alkalide metals in solution is an essential milestone in the development of alkalide applications. It indicates that, instead of the ‘gas-like’ model previously proposed, these systems could exhibit a subtle chemistry that could have applications in photo- or electro-chemistry.



Graphic showing the complex formed between a superalkali and an alkalide.

**Instrument:** Nimrod

**Related publication:** Superalkali-Alkalide Interactions and Ion Pairing in Low-Polarity Solvents, *J. Am. Chem. Soc.* 2021, 143, 10, 3934–3943

**DOI:** 10.1021/jacs.1c00115

**Funding:** European Regional Development Fund, GSK, Hofstra University

**Authors:** R Riedel (Imperial College London), AG Seel (University College London), D Malko (Imperial College London), DP Miller, BT Sperling (Hofstra University), H Choi (Cardiff University), TF Headen (ISIS), E Zurek (State University of New York at Buffalo), A Porch (Cardiff University), A Kucernak (Imperial College London), NC Pyper (University of Cambridge), PP Edwards (University of Oxford), AGM Barrett (Imperial College London)

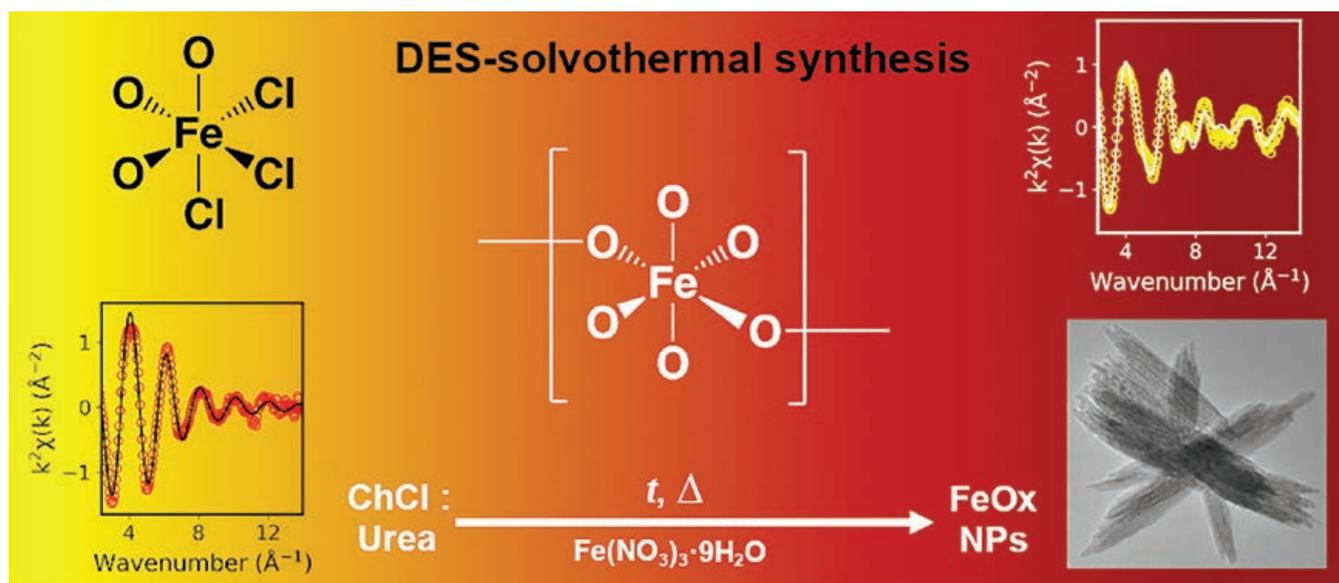
## Nimrod

# Developing environmentally-friendly solvents to make nanomaterials

Developing new solvents is a way to design new, more environmentally-friendly methods of synthesising functional nanomaterials. These, in turn, can then have an impact in a range of clean energy applications. For example, by making nanostructured thin films of the iron oxide known as hematite, its performance as an anode for splitting water into hydrogen using sunlight is enhanced. This study, published in *Nanoscale*, focuses on how using a deep eutectic solvent (DES) during synthesis influences the morphology of the hematite nanoparticles produced.

Using a multi-technique approach, including small angle neutron scattering and diffraction, the researchers were able to study the reaction *in situ*, the first time this type of study has been done in a DES. Their results show how the nanoparticle nucleation and growth is affected by

the presence of water in the DES. Understanding these solvents on the molecular level will enable scientists to develop new systems that are designed for creating specific nanomaterials in a more environmentally sustainable manner.



Neutron diffraction on Nimrod and *in situ* SANS and EXAFS were used to track a 'green' nanoparticle-forming reaction, and determine mechanistic differences caused by water.

**Instrument:** Nimrod

**Related publication:** Structural evolution of iron forming iron oxide in a deep eutectic-solvothermal reaction, *Nanoscale*, 2021,13, 1723-1737

**DOI:** 10.1039/D0NR08372K

**Authors:** OS Hammond, RS Atri (University of Bath), DT Bowron (ISIS), L de Campo (ANSTO), S Diaz-Moreno, LL Keenan (Diamond Light Source), J Douth (ISIS), S Eslava (Imperial College London) and KJ Edler (University of Bath).

## SANS2D

### Formulating engine lubricants for modern fuels and hardware

Inside an engine, acidic species form that can damage the engine. To prevent this damage, the oil used for lubrication contains detergents that are ‘overbased’ to neutralise these acids. In recent years, due to legislation to reduce sulfur content and increasing use of biofuels, the dominant acidic species has changed from inorganic acids to short-chain organic acids.

Understanding the effectiveness of conventional detergents in neutralising these organic acids is increasingly important, especially with the drive towards greener fuels. Researchers from Lubrizol used ISIS to learn more about the interactions between organic acids and lubricant additives.

Traditionally, the effectiveness of an overbased detergent in neutralising acidic species is described by its total base number (TBN). However, using small angle neutron scattering on SANS2D and infrared spectroscopy, the researchers found that the TBN alone was not an accurate predictor of how well an overbased detergent would neutralise an organic acid, but that the surface area of the detergent particle was important to its performance.



Engine Oil

“

Using SANS at ISIS has enabled brand new insights relating to the mechanisms involved in acid neutralisation, and therefore engine protection at a molecular level, and has advanced the industry understanding in this space.

David Growney, Lubrizol

”

**Instrument:** SANS2D

**Related publication:** Acid Neutralization Rates – Why Total Base Number Doesn’t Tell the Whole Story: Understanding the Neutralization of Organic Acid in Engine Oils, *SAE Int. J. Fuels Lubr.*, 14, 3, 297-309, 2021

**DOI:** 10.4271/04-14-03-0013

**Funding:** Lubrizol

**Authors:** D Growney, K Trickett, M Robin (The Lubrizol Corporation, USA), S Rogers (ISIS), D McDowall, E Moscrop (The Lubrizol Corporation, USA)

## Maps, Tosca

# Using catalysts to improve yield of light olefins from sustainable biomass

Using Tosca and Maps, researchers were able to study zeolite catalysts that alter reaction pathways to produce a higher yield of light olefins from compounds derived from a sustainable biomass source.

Light olefins, such as ethene, propene and butenes, are chemical compounds that are vital in the production of most consumer products sold today. Developing a more sustainable route to produce these chemicals from renewable resources is a vital task. One such method is to use biomass produced from agricultural waste to make methanol, which can then be converted into propene.

During this conversion, ethene is also created as a less-desired by-product. This study, published in *Nature Communications*, aimed to improve the ratio of propene to ethene produced during this process, using new tantalum-containing zeolites. These zeolites were found to exhibit a simultaneously high propene selectivity, propene to ethene ratio, and catalytic stability, which sets a new benchmark for methanol-to-olefin reactions.



Longfei Lin, Mengtain Fan and Lin Dong, University of Manchester, preparing a sample on the Tosca instrument.

**Instrument:** Maps, Tosca

**Related publication:** Control of zeolite microenvironment for propene synthesis from methanol, *Nat Commun* 12, 822 (2021)

**DOI:** 10.1038/s41467-021-21062-1

**Funding:** EPSRC, the Royal Society, National Natural Science Foundation of China and the University of Manchester

**Authors:** L Lin, M Fan, AM Sheveleva, X Han (University of Manchester), Z Tang (East China Normal University), JH Carter (University of Manchester, Diamond Light Source), I da Silva (ISIS), CMA Parlett (University of Manchester, Diamond Light Source), F Tuna, EJM McInnes (University of Manchester), G Sastre (UPV-CSIC Universidad Politecnica de Valencia), S Rudić, H Cavaye, SF Parker (ISIS), Y Cheng, LL Daemen, AJ Ramirez-Cuesta (Oak Ridge National Laboratory), MP Attfield (University of Manchester), Y Liu (East China Normal University), CC Tang (Diamond Light Source), B Han (Chinese Academy of Science), S Yang (University of Manchester)

## IMAT

# Quality control method for UK AEA's fusion component design

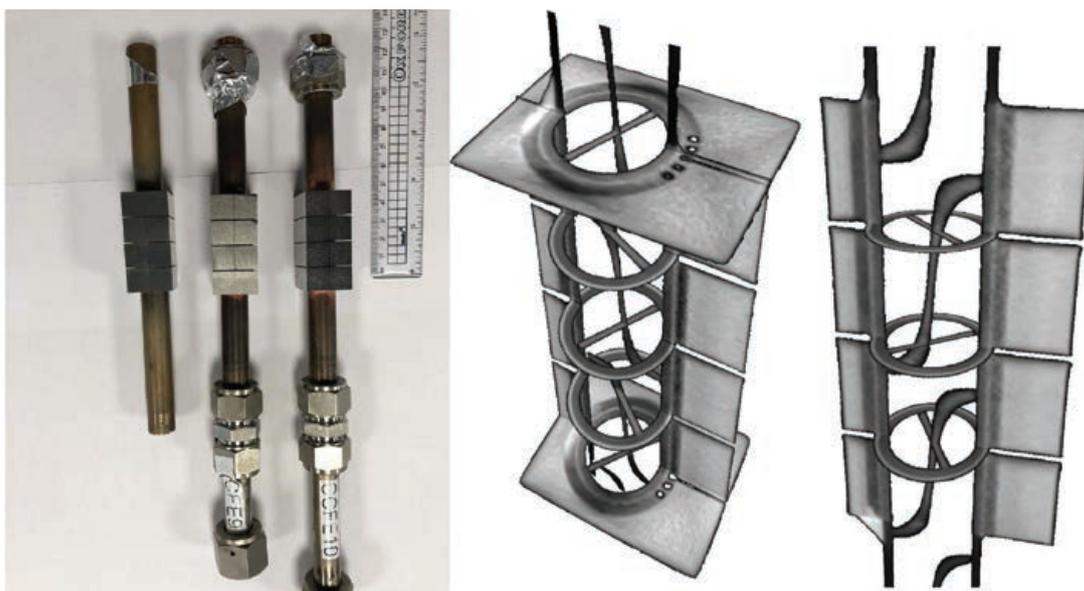
Using neutron tomography on the IMAT instrument, researchers have established that the technique could be used for testing prototypes of divertor target monoblocks before manufacturing hundreds of thousands of them for use in the DEMOnstration fusion power plant, DEMO.

The divertor target is one of the most delicate components in a fusion reactor and it is subject to extremely harsh conditions. The design being developed for DEMO is made of tungsten armour blocks threaded onto a CuCrZr cooling pipe separated by a copper interlayer.

The presence of these heavy metals makes it very difficult to examine using X-rays. However, neutrons are well suited for investigating defects within heavy metal structures.

This study, published in *Fusion Engineering and Design*, confirms that neutron tomography can be used to assess the structural integrity of divertor targets.

By measuring the divertor mock-up both before and after it had been through the equivalent of 100 fusion cycles, and seeing no defects develop, the group determined that their design was reliable under these conditions.



Photograph of the phase 2 thermal break mock-ups specimens for the DEMO divertor target (left). Ortho-view rendering of CCFE9 and CCFE10 DEMO divertor target mock-ups (right).

**Instrument:** IMAT

**Related publication:** Structural integrity of DEMO divertor target assessed by neutron tomography, *Fusion Engineering and Design*, 169, 2021, 112661

**DOI:** 10.1016/j.fusengdes.2021.112661

**Funding:** Euratom research and training programme, EPSRC

**Authors:** T Minniti, F Schoofs (UK AEA), LM Evans (Swansea University, UK AEA), W Kockelmann (ISIS), J You (Max Planck Institute for Plasma Physics), H Lewtas (UK AEA)

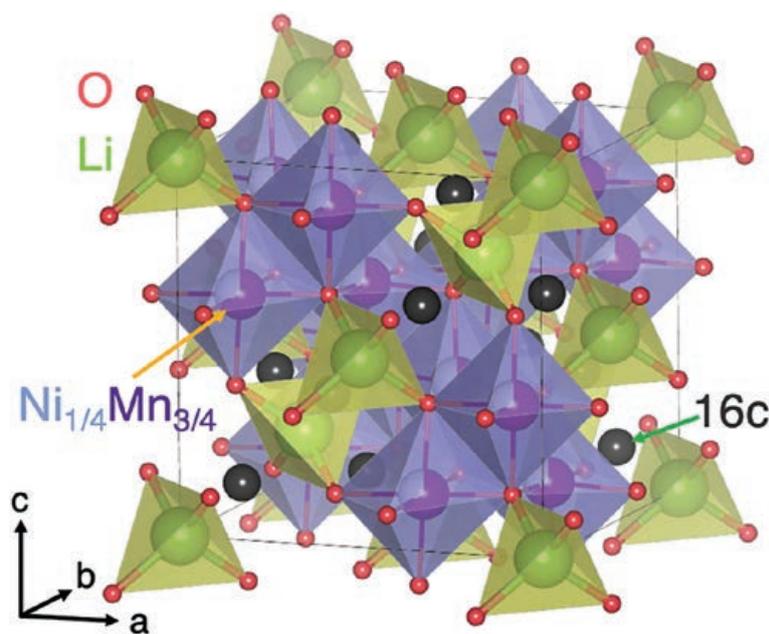
## Argus, Emu

# Negative muons used alongside positive muons to measure lithium diffusion in battery materials

Positive muon spin rotation and relaxation ( $\mu^+$ SR) is an excellent tool for studying lithium ion diffusion in battery materials. However, at higher temperatures, the  $\mu^+$  can itself diffuse through the material, leading to ambiguity when distinguishing between  $\text{Li}^+$  and  $\mu^+$  mobility. To confirm the diffusing species, it's possible to carry out the equivalent experiments using negative muons.

Using this combined technique, researchers can measure both the internal magnetic field at the atomic position in the lattice, from  $\mu^-$ SR experiments on Argus and at the interstitial sites with  $\mu^+$ SR on Emu. In 2020, the first study using  $\mu^{\pm}$ SR confirmed this approach is suitable for studying lithium ion diffusion in the olivine-type compound  $\text{LiMnPO}_4$ .

In this study, published in *Zeitschrift für Physikalische Chemie*, the focus was on the spinel-type battery material  $\text{Li}[\text{Ni}_{1/2}\text{Mn}_{3/2}]\text{O}_4$ . The research team found that lithium-ion diffusion could be measured using both  $\mu^+$ SR and  $\mu^-$ SR, confirming the suitability of this technique for studying battery materials.



The crystal structure of cubic spinel  $\text{Li}[\text{Ni}_{1/2}\text{Mn}_{3/2}]\text{O}_4$ .  $\text{Li}^+$  ions occupy the tetrahedral (8a) site, while Ni and Mn ions occupy the octahedral (16d) site.  $\text{O}^{2-}$  ions are located in each corner of the tetrahedron and octahedron. Dark grey spheres represent a vacant 16c site.

**Instrument:** Argus, Emu

**Related publication:** How Li diffusion in spinel  $\text{Li}[\text{Ni}_{1/2}\text{Mn}_{3/2}]\text{O}_4$  is seen with  $\mu^{\pm}$ SR, *Zeitschrift für Physikalische Chemie*, 2021, 000010151520213102

**DOI:** 10.1515/zpch-2021-3102

**Funding:** Swedish Research Council, Japan Society for the Promotion Science

**Authors:** J Sugiyama, K Ohishi (Comprehensive Research Organization for Science and Society), OK Forslund, M Månsson (KTH Royal Institute of Technology), SP Cottrell, AD Hillier (ISIS), K Ishida (RIKEN)

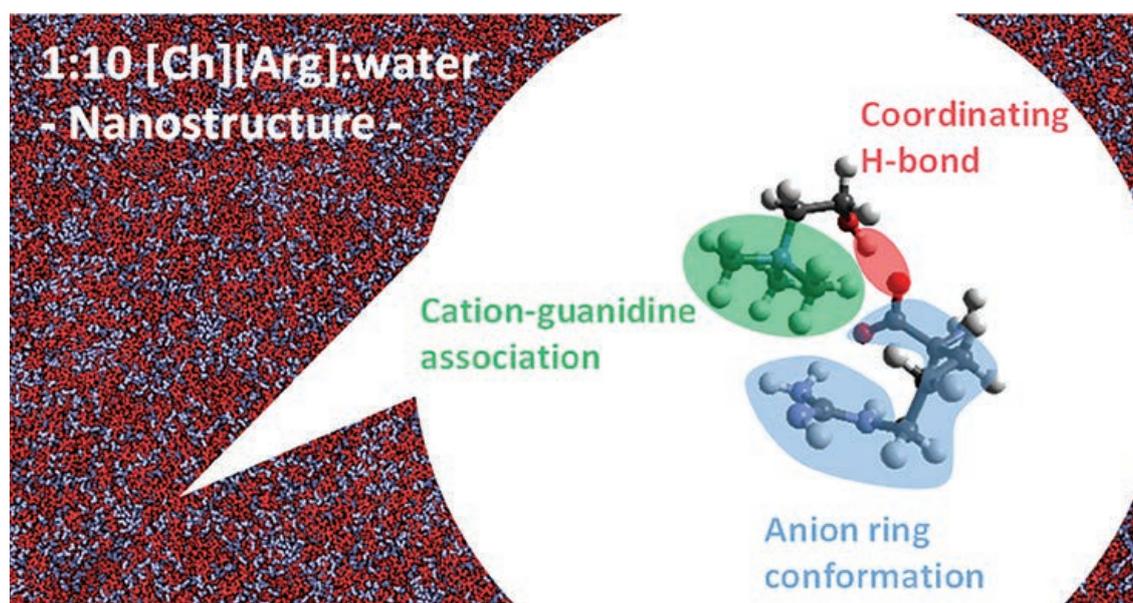
## Sandals

### Eco-friendly ionic liquids for biomass conversion

Ionic liquids have high thermal stability and good conductivity, as well as other properties that make them an attractive alternative to molecular solvents. One application where they have particular suitability is the extraction of specific compounds, such as lignin, from biomass. However, although they have been shown to help the biofuel conversion process, the ionic liquids themselves are expensive to produce and purify.

This study focusses on a potential solution to this problem: using ionic liquids made of naturally occurring biochemicals. The researchers studied the liquid nanostructure of one such ionic liquid at different concentrations and in the presence of a model lignin residue. Their results allowed them to understand how

the amount of water present influences the conformation adopted by molecules in solution. The relative positions of the molecules then determine what bonding is available for biomass breakdown and solvation, which influences the effectiveness of an ionic liquid for this application.



**Instrument:** Sandals

**Related publication:** Liquid Nanostructure of Cholinium Arginate Biomass Solvents, *ACS Sustainable Chem. Eng.* 2021, 9, 7, 2880–2890

**DOI:** 10.1021/acssuschemeng.0c08829

**Funding:** Australian Government Research Training Program, AINSE Limited, Australian research Council Discovery Project, US DOE Office of Science and Lawrence Berkeley National Laboratory.

**Authors:** M Brunner (The University of Western Australia), S Imberti (ISIS), BA Simmons (Joint BioEnergy Institute), GG Warr (University of Sydney), R Atkin (The University of Western Australia)

## Zoom

# Bigger is better for anions in water-in-salt electrolytes

Water-in-Salt (WiS) electrolytes could be a safer alternative to organic electrolytes for supercapacitors and battery applications. They show high lithium-ion mobility, crucial for use in batteries, but there is little understanding of the nanostructuring of the solutions and how this impacts the ionic movement. Two WiS systems were investigated in this study, published in *ACS Nano*, at varying salt concentrations and temperatures relevant to battery applications.

The researchers found that the system was made up of nanodomains of water inside the electrolyte. The shape of these domains depended on the concentration of the salt, but not temperature. As the nanodomains were confined

by an anion-rich matrix, the shape and size of the anion is key to the morphology. This finding suggests that using bulky anions could lead to a significant improvement in the performance of future lithium based WiS electrolytes.



*Eneli Härk and Sebastian Risse, Helmholtz-Zentrum, Berlin, looking at data from the Nimrod instrument during an experiment in 2018.*

**Instrument:** Zoom

**Related publication:** The Nanostructure of Water-in-Salt Electrolytes Revisited: Effect of the Anion Size, *ACS Nano* 2021, 15, 7, 11564–11572

**DOI:** 10.1021/acsnano.1c01737

**Funding:** CONICET

**Authors:** G Horwitz (Comisión Nacional de Energía Atómica), E Härk (Helmholtz-Zentrum Berlin), PY Steinberg (Comisión Nacional de Energía Atómica), LP Cavalcanti (ISIS), S Risse (Helmholtz-Zentrum Berlin), HR Corti (Comisión Nacional de Energía Atómica, CONICET-Universidad de Buenos Aires)

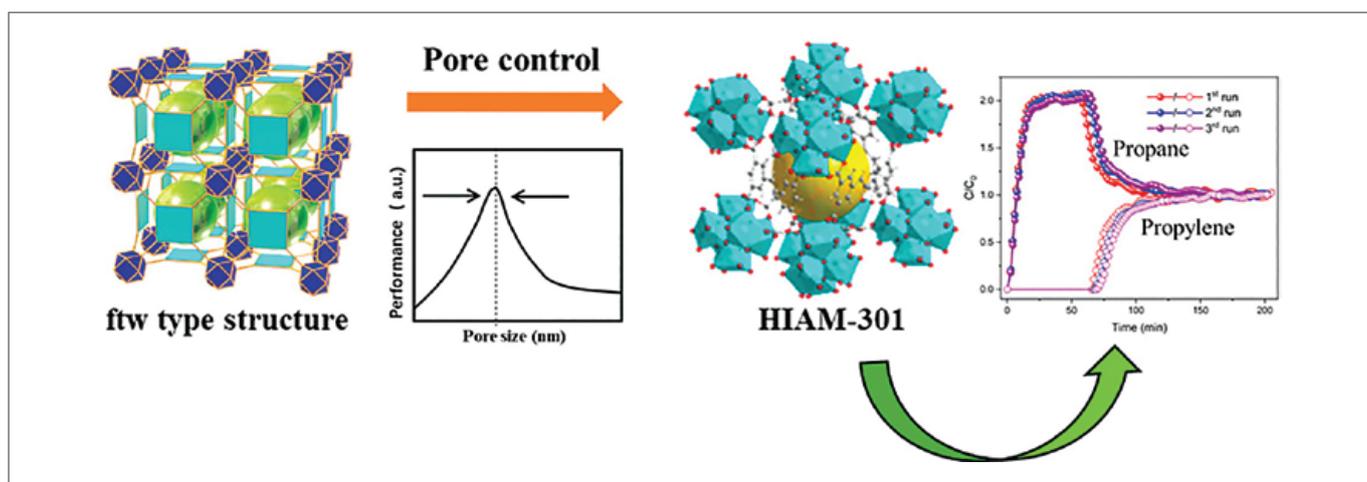
## Tosca, WISH

## Distorting pore shape to improve performance

In the petrochemical industry, the separation of propylene from propane is an important and challenging process because they have almost identical molecular sizes. The current process of cryogenic distillation is one of the most energy demanding processes in the whole refinery. An alternative would be using metal-organic frameworks, MOFs, which can be modified to have different functional groups and pore sizes. Balancing selectivity and adsorption capacity is challenging, with an improvement in one often hindering the other.

A group of researchers has designed a new MOF with a distorted pore structure, HIAM-301, which shows the highest adsorption capacity for propylene with the exclusion of propane. Their study used neutron diffraction and inelastic neutron scattering to study the binding

interactions of the propylene inside the pores. The results not only demonstrate the high performance of a new material, but also informs the design of future gas storage and separation candidates.



*Distortion of the pore structure in HIAM-301 has resulted in efficient separation of propane and propylene under dynamic flow conditions.*

**Instrument:** Tosca, WISH

**Related publication:** Pore Distortion in a Metal-Organic Framework for Regulated Separation of Propane and Propylene, *J. Am. Chem. Soc.* 2021, 143, 46, 19300–19305

**DOI:** 10.1021/jacs.1c10423

**Funding:** National Natural Science Foundation of China, the Guangdong Natural Science Foundation, Shenzhen Science and Technology Program and the U.S. Department of Energy

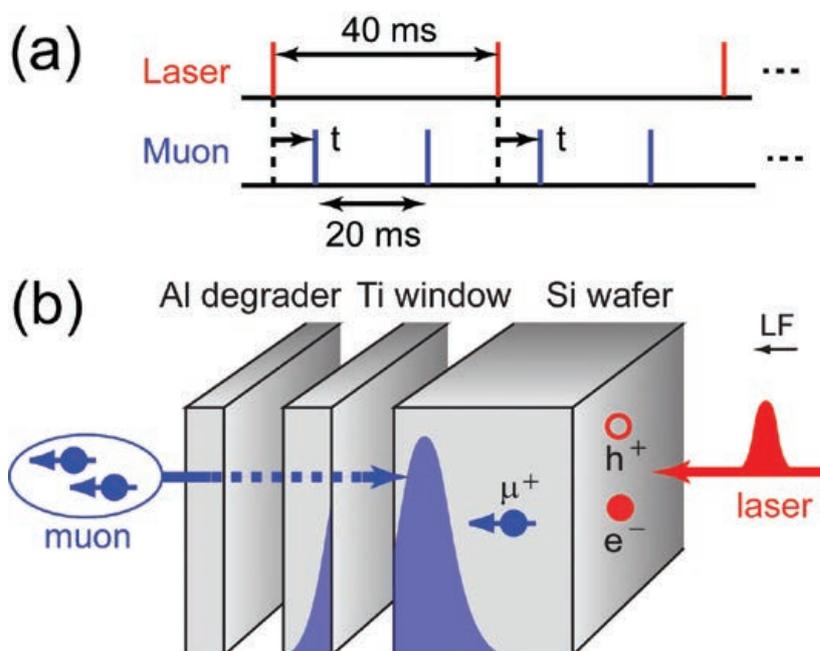
**Authors:** L Yu (South China University of Technology), X Han (University of Manchester), H Wang (Shenzhen Polytechnic), S Ullah (Wake Forest University), Q Xia (South China University of Technology), W Li (University of Manchester), J Li (Shenzhen Polytechnic, Rutgers University), I da Silva, P Manuel, S Rudić (ISIS), Y Cheng (Oak Ridge National Laboratory), S Yang (University of Manchester), T Thonhauser (Wake Forest University)

## HiFi

Photo- $\mu$ SR: a new method for studying photovoltaics

Charge carrier kinetics, especially their lifetime, ultimately determine the performance of silicon photovoltaic cells. With a thin layer of silicon, where carriers are generated by sunlight, it is important to control and understand their (unwanted) recombination not only in the bulk but also at the surface. However, decoupling these is challenging using laboratory characterisation techniques.

A new method of photoexcited muon spin relaxation (photo- $\mu$ SR) has been developed and, in this study, used to separate the bulk and surface recombination. Because the muons can be implanted at different depths within a Si wafer, the carrier lifetime spectrum can be measured at specific points. This enabled the researchers to use a simple model to separate the bulk and surface contributions. This technique could be extended to a range of other semiconductor systems, including power electronic devices.



(a) Carriers were injected optically using the HiFi Laser system. The laser pulses were synced with ISIS and timed to measure carrier lifetime spectra. (b) Putting more materials in the muon beam shifts its implantation depth. Interaction between muons and carriers appear in the  $\mu$ SR spectrum as a faster relaxation – this is used to quantify the carrier density.

**Instrument:** HiFi

**Related publication:** Decoupling bulk and surface recombination properties in silicon by depth-dependent carrier lifetime measurements, *Appl. Phys. Lett.*, 118, 252105 (2021)

**DOI:** 10.1063/5.0054291

**Funding:** ERC

**Authors:** K Yokoyama, JS Lord (ISIS), J Miao, P Murahari, and AJ Drew (Queen Mary, University of London)

## Engin-X

# How crumpling helmets protected Samurai warriors from bullets

Engin-X reveals microstructural details that show one type of Samurai helmet protected its wearer from firearms in the same way as a car crumple zone.

After the Portuguese introduced firearms to Japan in the 16th century, Samurai armour adapted to match the warfare style. This study, published in *Archaeological and Anthropological Sciences*, looked at the strain along an individual platelet of the helmet to see how the strain varied across the whole piece. This allowed the scientists to map out the helmet's mechanical properties.

The study revealed that the inward-facing part of the platelet is in a compressive state, which improves the helmet's performance because it is more resistant to deformation during an attack. Conversely, the outward area attenuates the blow by being prone to deformation, acting like a car crumple zone. When hit, the deformation causes redistribution of neighbouring plates to maintain the integrity of the helmet and protect the wearer.



A 17th century kabuto.

**Instrument:** Engin-X

**Related publication:** On the protective effect of the stress distribution on a lamellar Edo period Samurai helmet: a neutron diffraction study, *Archaeol Anthropol Sci* 13, 96 (2021)

**DOI:** 10.1007/s12520-021-01330-3

**Funding:** Consiglio Nazionale delle Ricerche

**Authors:** A Fedrigo (ISIS), J James (The Open University), SY Zhang (ISIS, Centre of Excellence for Advanced Materials), F Salvemini (ANSTO), F Grazzi (Consiglio Nazionale delle Ricerche)

## RIKEN-RAL

### Roman coin study reveals thriving empires

To understand the economic health of different periods of the Roman Empire, researchers brought three Roman gold coins to the RIKEN-RAL muon facility to see if they had been surface enriched or mixed with other metals. The coins analysed were issued during the reigns of three different Roman emperors: Tiberius (early 1st century AD), Hadrian (mid-2nd century AD) and Julian II (mid-4th century AD).

Previous surface-level analyses of these coins suggested that they were very high purity gold. However, these measurements were from the top few fractions of a millimetre of the coins. The Romans deliberately surfaced-enriched their silver coins to hide the fact there was a lot of copper in them, so it is plausible something similar happened to the gold.

By using muonic X-ray emission spectroscopy, the researchers were able to look below the surface at the very centre of the coins. Their results, published in *Journal of Archaeological Science*, showed that the high purity seen on the surface was representative of the whole of the coin, a testament to the economic health of the Roman Empire at the time.



Roman gold coin.

**Instrument:** RIKEN-RAL

**Related publication:** Understanding Roman Gold Coinage Inside Out, *Journal of Archaeological Science*, 134, (2021), 105470

**DOI:** 10.1016/j.jas.2021.105470

**Authors:** GA Green (University of Warwick, Ashmolean Museum, University of Oxford), K Ishida (RIKEN), BV Hampshire, K Butcher (University of Warwick), A Pollard (University of Oxford), AD Hillier (ISIS)

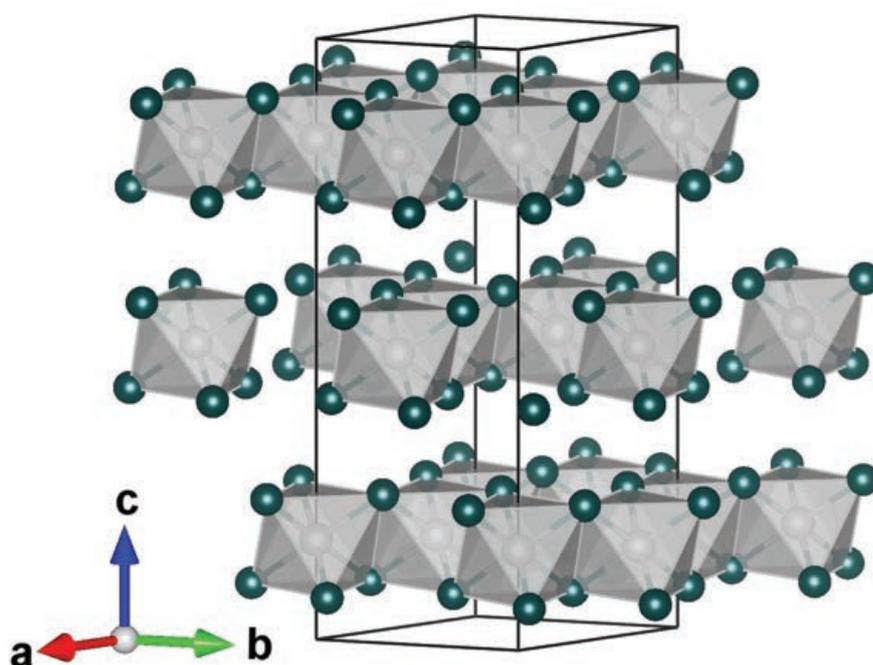
## Maps

### Looking between layers for long-range magnetic order

The material  $\text{VI}_3$  is of interest because of its unique magnetic properties: its layered structure offers the potential for long-range, two-dimensional magnetic order. This type of behaviour would be useful for application in future spintronic devices but is challenging to achieve due to the need to overcome thermal fluctuations.

To study the magnetic coupling and spin-orbital ground state, ISIS Facility Development student Harry Lane and his collaborators used neutron spectroscopy to probe the magnetic correlations at low temperatures. In their study, which was published in *Physical Review B*, they used novel data analysis methods to characterise the magnetic behaviour.

They found evidence for two distinct  $\text{V}^{3+}$  domains, caused by the distortion of the crystal structure to form two different environments. In combination with spin orbit coupling, this provides the basis for the desired long-range, two-dimensional magnetic order.



The crystal structure please of  $\text{VI}_3$ .

**Instrument:** Maps

**Related publication:** Two-dimensional ferromagnetic spin-orbital excitations in honeycomb  $\text{VI}_3$ . *Phys. Rev. B*, 104, L020411

**DOI:** 10.1103/PhysRevB.104.L020411

**Funding:** EPSRC, STFC

**Authors:** H Lane (University of Edinburgh and ISIS), E Pachoud (University of Edinburgh), JA Rodriguez-Rivera (National Institute of Standards and Technology and University of Maryland), M Songvilay (University of Edinburgh), G Xu, PM Gehring (National Institute of Standards and Technology), JP Attfield (University of Edinburgh), RA Ewings (ISIS), C Stock (University of Edinburgh)

## Merlin

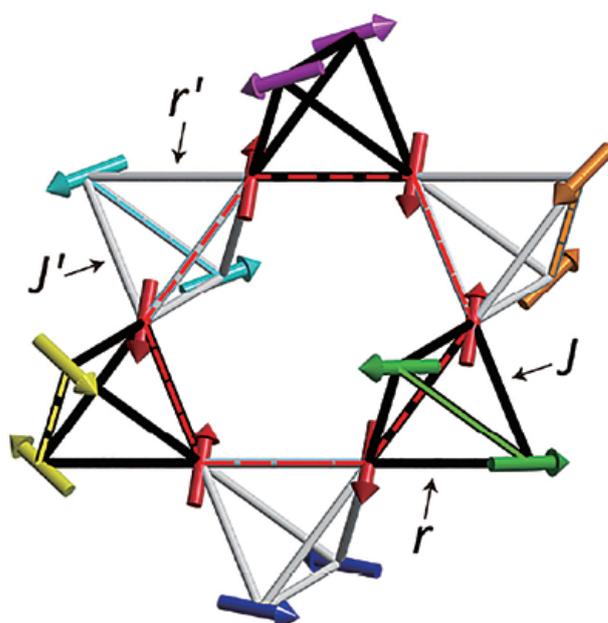
# Investigating exotic magnetism in a breathing pyrochlore lattice

Having spins on a triangular or tetragonal lattice causes geometric frustration, as the opposing interactions between neighbouring spins cannot be accommodated. This frustration can lead to the formation of ground states with exotic spin correlations and excitations. One example is the spinel oxide  $\text{LiGaCr}_4\text{O}_8$ , where the magnetic ions form alternating arrays of small and large tetrahedra, a structure known as a breathing pyrochlore lattice.

Using inelastic neutron scattering on Merlin, researchers were able to investigate the spin excitations in  $\text{LiGaCr}_4\text{O}_8$ . They found that both a dispersionless resonance mode and dispersive spin-wave excitations were present in the magnetically-ordered state. The origin of the resonance modes was found to be related to the Cr-Cr bond distance in the lattice.

By establishing the correct quantum spin model and determining the dominant magnetic interactions, this study provides the basis from which similar systems could also be understood.

*The sketch of a hexagonal spin loop on the lattice of  $\text{LiGaCr}_4\text{O}_8$ . The arrows marked by different colours stand for the spins belonging to different loops.*



**Instrument:** Merlin

**Related publication:** Neutron Scattering Studies of the Breathing Pyrochlore Antiferromagnet  $\text{LiGaCr}_4\text{O}_8$ , *Phys. Rev. Lett.* 127, 147205

**DOI:** 10.1103/PhysRevLett.127.147205

**Funding:** The National Key R&D Program of the MOST of China, the Innovation Program of Shanghai Municipal Education Commission, Shanghai Municipal Science and Technology Major Project and the National Natural Science Foundation of China

**Authors:** Z He (Fudan University), Y Gu, H Wo (Fudan University, Shanghai Qi Zhi Institute), Y Feng (Fudan University, Chinese Academy of Sciences, SNSSC), D Hu, Y Hao (Fudan University), HC Walker (ISIS), DT Adroja (ISIS and University of Johannesburg), J Zhao (Fudan University, Shanghai Qi Zhi Institute, Shanghai Research Center for Quantum Sciences, Collaborative Innovation Center of Advanced Microstructures)

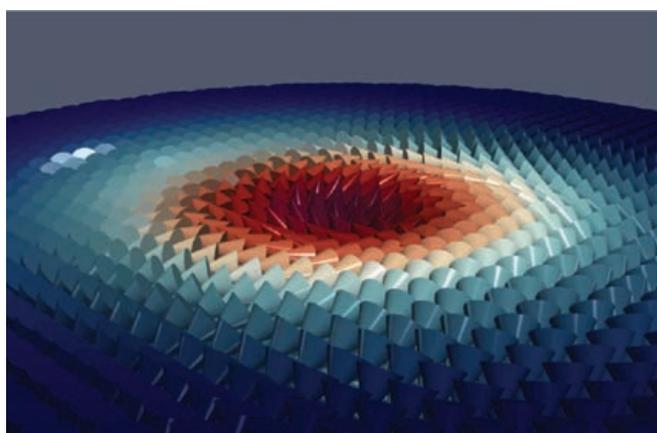
## Larmor

### Using SANS to study skyrmions

Magnetic skyrmions are nanoscale vortices of spins that may provide a number of interesting device applications ranging from high-density, low-power data storage to stochastic and neuromorphic computing. To form a hexagonal lattice of skyrmions requires the presence of competing interactions, namely the Dzyaloshinskii-Moriya interaction (DMI) and exchange interactions found in inversions of anti-symmetric materials.

One example is  $\text{Cu}_2\text{OSeO}_3$ , which has been found to contain a number of incommensurate magnetic textures, including skyrmions, cones and helices, at a range of temperatures. In this study, published in *Physical Review Research*, researchers used small angle neutron scattering to study and quantify the magnetic interactions present in  $(\text{Cu}_{0.98}\text{Zn}_{0.02})_2\text{OSeO}_3$  to elucidate the formation mechanisms of these magnetic states.

The authors found that they were able to investigate the anisotropic exchange interaction using the 3D vector-field magnet at the Larmor beamline, by orienting the conical states in the material along different directions and investigating the variations in the periodicity. Interestingly, the interaction changes sign on decreasing temperature, but without inducing a reorientation of the zero-field magnetic helix. This insight into the behaviour of this material is crucial for understanding how to create and stabilise these complex magnetic textures.



Magnetisation distribution of an isolated magnetic skyrmion, taken from *Nat Commun* 12, 2723 (2021), DOI: 10.1038/s41467-021-22857-y.

**Instrument:** Larmor

**Related publication:** Experimental evidence of a change of exchange anisotropy sign with temperature in Zn-substituted  $\text{Cu}_2\text{OSeO}_3$ , *Phys. Rev. Research*, 3, 043149

**DOI:** 10.1103/PhysRevResearch.3.043149

**Funding:** EPSRC, NSERC

**Authors:** SH Moody, P Nielsen, MN Wilson (Durham University), D Alba Venero (ISIS), A Štefančič, G Balakrishnan (University of Warwick), PD Hatton (Durham University)

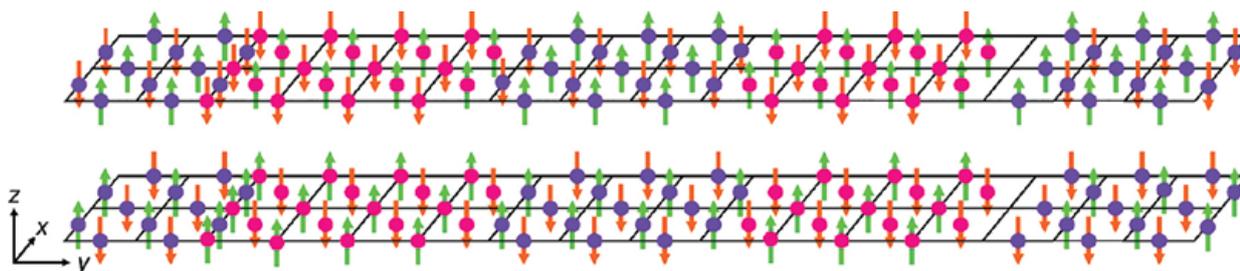
## HRPD, WISH

# Combining magnetoelectric and multiferroic properties in one material

Magnetoelectric multiferroic materials exhibit both magnetic and electrical spontaneous polarisations and could be used in a range of devices for the manipulation and storage of digital information. However, the properties that are required for ferroelectric and ferromagnetic behaviour are contradictory, making materials that exhibit both very difficult to design.

One method, explored in this study, is to introduce magnetic cations into a ferroelectric structure, which then leads to magnetoelectric coupling. In this example, the researchers performed low temperature cation-exchange reactions on  $\text{Li}_2\text{SrTa}_2\text{O}_7$  to form  $\text{MnSrTa}_2\text{O}_7$ . By using neutron diffraction, they were able to investigate

the magnetic ground state formed, finding that they had successfully formed a coupled magnetoelectric material. This technique could, in the future, be applied to other host phases, widening the pool of candidates of materials with this unique and sought-after property.



The refined magnetic structure of  $\text{MnSrTa}_2\text{O}_7$ . Pink and purple spheres represent Mn cations, green and orange arrows indicate the direction of the ordered magnetic moments.

**Instrument:** HRPD, WISH

**Related publication:** Directed synthesis of a hybrid improper magnetoelectric multiferroic material, *Nature Communications*, 12, 4945 (2021)

**DOI:** 10.1038/s41467-021-25098-1

**Funding:** Welch Foundation

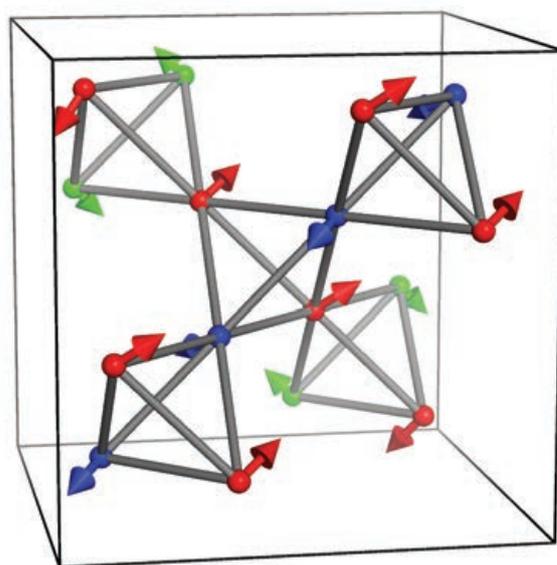
**Authors:** T Zhu (University of Oxford), F Orlandi, P Manuel, AS Gibbs (ISIS), W Zhang, PS Halasyamani (University of Houston), MA Hayward (University of Oxford)

## HRPD, WISH

# Neutrons enable the distinction between single- $k$ and multi- $k$ structures

The geometry of some crystal structures can cause geometric frustration, as neighbouring spins cannot form a configuration where their interactions are all favourable. This frustration can lead to exotic magnetic states, which can either be ordered or disordered. In some cases, both of these are present in one system. These partially-ordered systems could be useful in magnetic materials, such as magnetic skyrmions, but the nature of the magnetic structure is difficult to determine.

In particular, it is challenging to distinguish between magnetic structures that combine multiple periodicities, known as 2- $k$ , 3- $k$ , and 4- $k$  structures. In this study, published in *npj Quantum Materials*, researchers used neutron diffraction data measured at ISIS and ILL to investigate the partially ordered magnetic system  $Gd_2Ti_2O_7$ . These results, combined with a comprehensive symmetry analysis and inelastic neutron scattering data collected at NIST and ORNL, enabled them to characterise the low temperature magnetic state of  $Gd_2Ti_2O_7$  as 2- $k$ . Their work shows that it is possible to distinguish between single- $k$  and multi- $k$  structures without the need for single crystals or the application of external fields.



The 2- $k$  structure of  $Gd_2Ti_2O_7$

**Instrument:** HRPD, WISH

**Related publication:** Suppressed-moment 2- $k$  order in the canonical frustrated antiferromagnet  $Gd_2Ti_2O_7$ , *npj Quantum Materials*, 6, 99 (2021)

**DOI:** 10.1038/s41535-021-00391-w

**Funding:** Oak Ridge National Laboratory, Churchill College, University of Cambridge, STFC, EPSRC, ERC

**Authors:** JAM Paddison (Oak Ridge National Lab, University of Cambridge, University of Oxford, ISIS), G Ehlers (Oak Ridge National Lab), AB Cairns (University of Oxford and Imperial College London), JS Gardner (Oak Ridge National Lab), OA Petrenko (University of Warwick), NP Butch (National Institute of Standards and Technology), DD Khalyavin, P Manuel (ISIS), HE Fischer (ILL), H Zhou (University of Tennessee and Florida State University), AL Goodwin (University of Oxford), JR Stewart (ISIS)

## Polaris, WISH

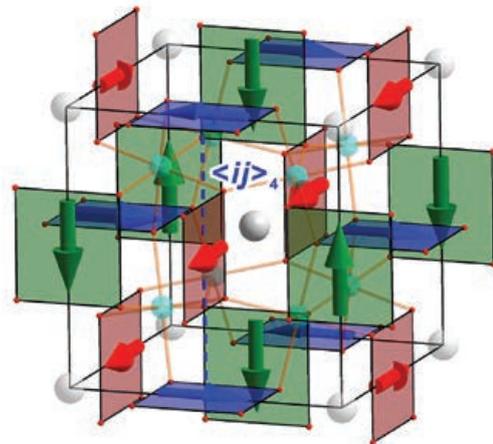
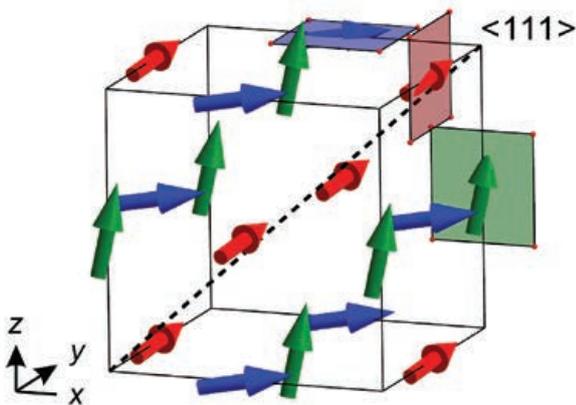
### A high-symmetry structure with unexpected magnetic behaviour

The material  $\text{CaFe}_3\text{Ti}_4\text{O}_{12}$  forms a high-symmetry structure where there would be expected to be conventional long-range magnetic order present. However, no order is observed, even down to 4.2 K. To understand what was happening at low temperatures, researchers came to ISIS to carry out magnetic neutron diffraction.

Their experiments, complemented by theoretical studies by Keeley-Rutherford Research Fellow, Attila Szabó, showed evidence of an unusual triple- $k$  ground state. This arises from three different antiferromagnetic sublattices within the cubic crystal symmetry interacting only among themselves, with near-neighbour interactions suppressed. On application of a magnetic field, the

magnetic  $\text{Fe}^{2+}$  sublattices switch from antiferromagnetic to ferromagnetic ordering and adopt a structure in which all spins are canted towards the  $\langle 111 \rangle$  body diagonal.

Their results provide important insights for understanding complex magnetism in structures where it would not be expected to be present.



Field-induced canted ferromagnetic structure ( $k = (0, 0, 0)$ ) (left), antiferromagnetic structure ( $k = (1/2, 1/2, 0)$ ) (right)

**Instrument:** Polaris, WISH

**Related publication:** Multi- $k$  spin ordering in  $\text{CaFe}_3\text{Ti}_4\text{O}_{12}$  stabilized by spin-orbit coupling and further-neighbor exchange, *Phys. Rev. Research* 3, 043208

**DOI:** 10.1103/PhysRevResearch.3.043208

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**Authors:** M Amano Patino, F Denis Romero, M Goto, T Saito (Kyoto University), F Orlandi, P Manuel (ISIS), A Szabó (ISIS and the University of Oxford), P Kayser, KH Hong, KN Alharbi, JP Attfield (The University of Edinburgh), Y Shimakawa (Kyoto University)

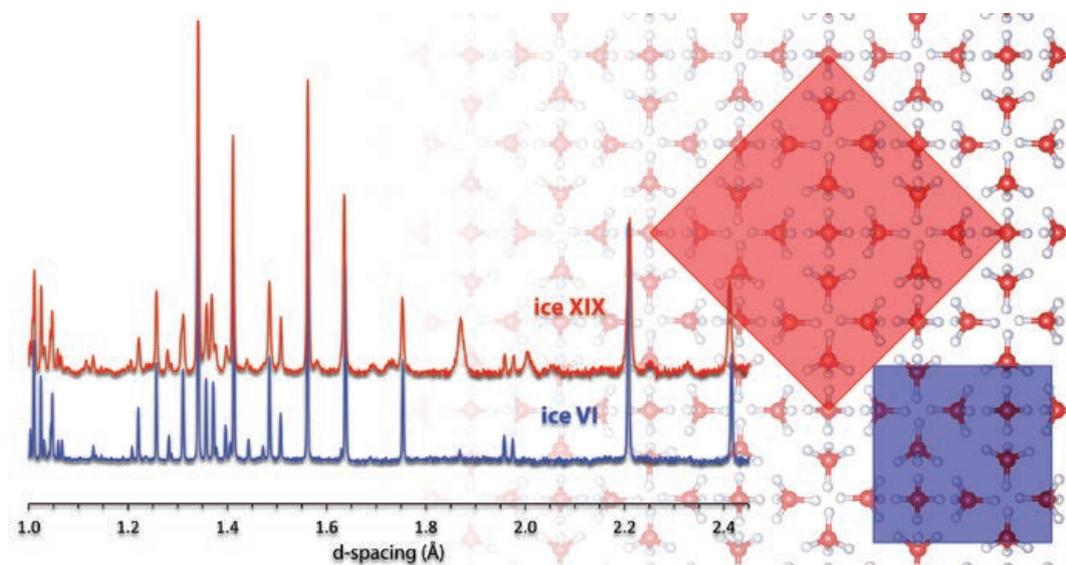
## HRPD

# Neutron experiments confirm the existence of new form of ice

Using diffraction experiments on HRPD, a team of Austrian researchers have confirmed the existence of an exotic form of ice: Ice XIX. While conventional ice and snow are abundant on Earth, no other forms are found on the surface of our planet - except in research laboratories and as inclusions in diamonds. However, many varieties of water ice are formed in space under special pressure and temperature conditions. They are found, for example, on celestial bodies such as Jupiter's moon Ganymede, which is covered by layers of different ice varieties.

In their recent study, published in *Nature Communications*, the researchers began with ice VI, which is formed at high pressure, such as in the Earth's mantle. They slowly cooled this further, increasing the pressure to around 20 kbar, causing the hydrogen atoms to arrange themselves in a unique way within the oxygen lattice, forming this new form: ice XIX.

To determine the crystal structure, the group needed to find a way to form ice XIX with deuterated water. They were then able to measure the neutron diffraction pattern on HRPD and solve the crystal structure.



The diffraction patterns and unit cells of ice XIX and ice VI.

**Instrument:** HRPD

**Related publication:** Structural characterization of ice XIX as the second polymorph related to ice VI, *Nature Commun*, 12, 1128 (2021)

**DOI:** 10.1038/s41467-021-21161-z

**Funding:** Austrian Science Fund (FWF)

**Authors:** TM Gasser, AV Thoeny (University of Innsbruck), AD Fortes (ISIS), T Loerting (University of Innsbruck)

## IMAT

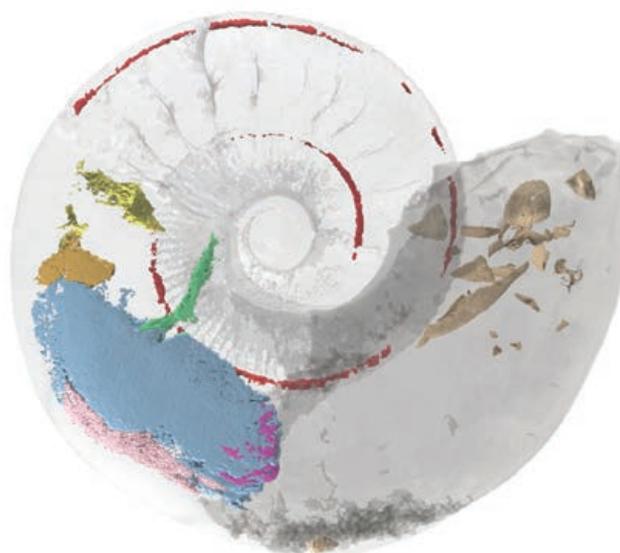
# Neutron imaging reveals never-before-seen 3D muscle structure in rare Jurassic ammonite fossil

For the first time, details of the soft tissues in an exceptionally preserved fossil have been revealed in three dimensions, throwing new light on creatures that thrived in the oceans 165 million years ago. The images, published in *Geology*, allowed the team to analyse the muscles and organs of an ammonite for the very first time, throwing new light on how the cephalopod mollusc was able to swim through the oceans and defend itself from predators.

Previous investigations using solely X-ray techniques were unable to see through the hard shell and determine the structure of the soft tissues. By combining these results with neutron imaging on the IMAT instrument at ISIS, the researchers were able to study the fossil in unprecedented detail and create a detailed 3D computer reconstruction of the muscles and organs inside the ammonite fossil.

The arrangement and relative strength of the muscles reveal that ammonites swam by jet propulsion through the funnel (hyponome), like modern squid and octopuses. This mechanism differs from the cephalopod *Nautilus*, which has previously been used as a body-plan for reconstructing ammonite biology.

Finding ammonites with the fossilised remains of soft parts is also virtually unknown in the fossil record. But this rare example, combined with the neutron imaging, has led to a major breakthrough in ammonite palaeobiology.



*The 3D model of the ammonite, showing the soft tissues.*

**Instrument:** IMAT

**Related publication:** Correlative tomography of an exceptionally preserved Jurassic ammonite implies hyponome-propelled swimming, *Geology* (2022) 50 (4): 397–401.

**DOI:** 10.1130/G49551.1

**Authors:** L Cherns (Cardiff University), ART Spencer (Imperial College London, Natural History Museum), IA Rahman (Natural History Museum, University of Oxford), RJ Garwood (Natural History Museum, University of Manchester), C Reedman (Cardiff University, Jurassic Coast Trust), G Burca (ISIS and the University of Manchester), MJ Turner (University of Manchester), NT Hollingworth (STFC), J Hilton (University of Birmingham)

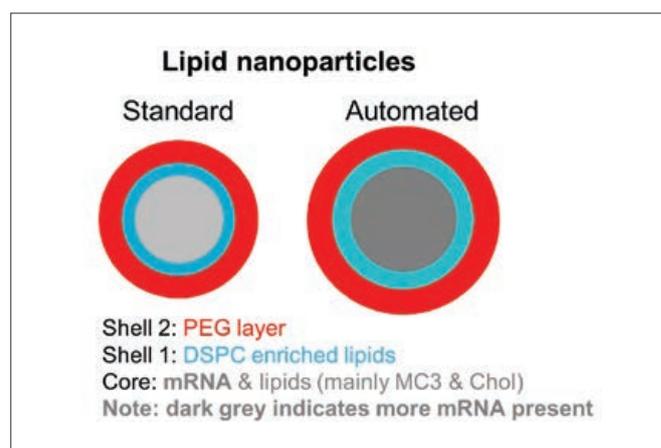
## SANS2D

# AstraZeneca uses SANS2D to understand potential new mRNA production method

Using lipid nanoparticles (LNPs) to deliver mRNA has many potential medical applications including vaccine delivery, cancer therapy and gene editing. Understanding how the structure of LNPs influences their ability to deliver drugs is key to the design and development of future medications. Researchers at the biopharmaceutical company AstraZeneca are developing a new platform to generate LNPs.

When evaluating the LNPs produced *in vitro*, they learnt that they were more successful at delivering mRNA than LNPs produced by a standard route. To understand what was causing this improvement, they compared LNPs produced by both methods using a series of characterisation techniques, including small-angle neutron and X-ray scattering (SANS and SAXS).

In their study, published in *Small*, they also tested the effectiveness of the LNPs at delivering mRNA *in vivo*, to see how effective they were at drug delivery. They found that the nanoparticles produced using their new automated system were larger, contained more mRNA, and ruptured more easily inside cells, making them 4.5 times more effective than LNPs made through a standard procedure.



A diagram of the model best described by the SANS and SAXS data: a polydisperse core with two shells.

“

We deeply appreciate the support from ISIS facility and scientists for the neutron beam time and the valuable knowledge which help us unveil the internal and surface properties of the mRNA LNP nanoparticles.

Lili Cui, from AstraZeneca

”

AstraZeneca 

**Instrument:** SANS2D

**Related publication:** Mechanistic Studies of an Automated Lipid Nanoparticle Reveal Critical Pharmaceutical Properties Associated with Enhanced mRNA Functional Delivery In Vitro and In Vivo, *Small*, 18, 9 2105832

**DOI:** 10.1002/smll.202105832

**Funding:** AstraZeneca

**Authors:** L Cui, MR Hunter, S Sonzini, S Pereira (AstraZeneca), SM Romanelli (University of Michigan Medical School), K Liu, W Li, L Liang, B Yang (AstraZeneca), N Mahmoudi (ISIS), AS Desai (AstraZeneca)

## Tosca

# Inelastic neutron scattering reveals the extent of active dissolution from Lucideon's iCRT platform technology

Lucideon, a leader in material technologies, used Tosca to explore and develop its drug delivery solutions and formulation development tools, benefitting a range of industry sectors.

Encapsulation, protection and controlled release of active ingredients are critical aspects of product function in industries including pharmaceuticals, consumer products and agriceuticals. Lucideon are developing a novel platform material, inorganic Controlled Release Technology (iCRT) which can bring unique functional properties, benefits and differentiation to products. To better understand and develop the iCRT platform technology, Lucideon used inelastic neutron scattering to help determine the amounts of the active ingredients bound within a series of active-loaded iCRT materials.

This collaboration enabled Lucideon's iCRT materials to be assessed in a new way and provided answers to questions that could not have been answered using standard methods. With more development of the experimental procedure and repetition on a broader number of samples with different active ingredients, the INS data may provide something which other methods cannot - confirmation that the active ingredient has been completely released from the iCRT particles. This will be a key piece of evidence to support the future development of the iCRT technology platform for pharmaceutical applications and, ultimately, increase the speed to market.

“

Access to the state-of-the-art facilities and associated expertise at ISIS Neutron and Muon Source really allowed us to evaluate our materials to a level that we would never normally have considered. It has provided us with a wealth of extra information and knowledge that no doubt will give a boost to the development and commercialisation of Lucideon's iCRT technology platform.”

Mark Cresswell, Lucideon Ltd

”

**LUCIDEON**  
Materials Development and  
Commercialization

**Instrument:** Tosca

**Research team:** G Gasparini (Lucideon), M Sarter, S Rudic, G Appleby, V Garcia Sakai (ISIS), Mark Cresswell (Lucideon)

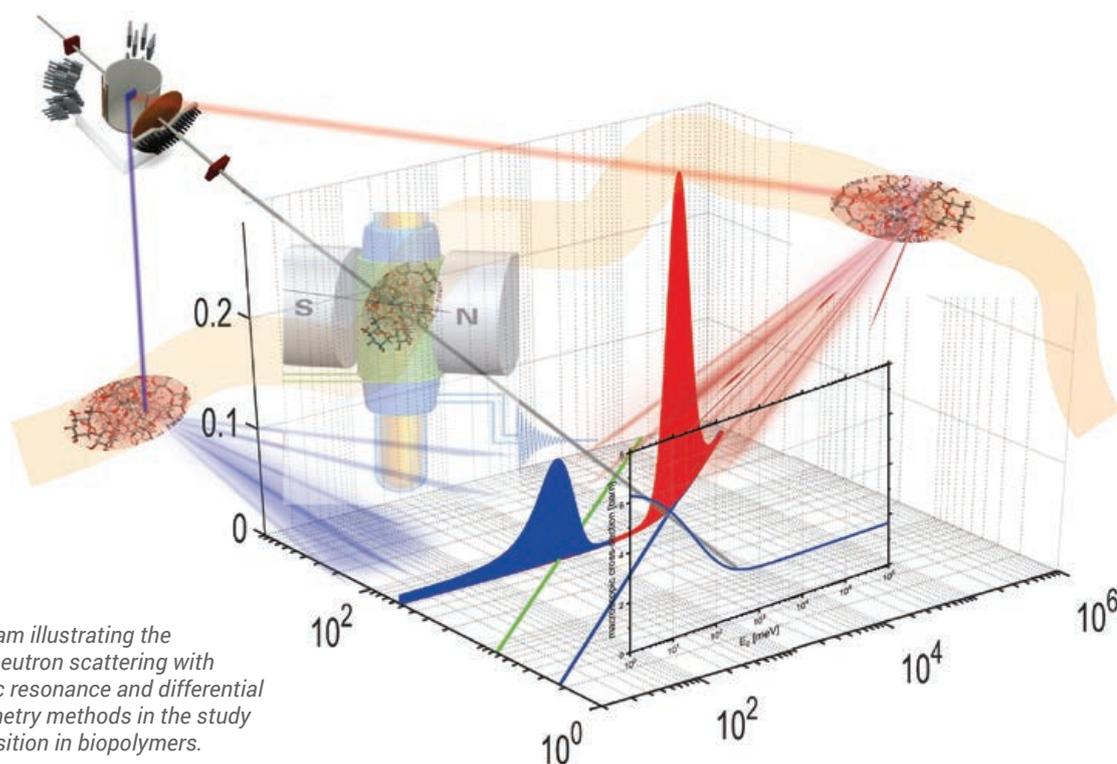
## Vesuvio

### Vesuvio enables comprehensive study of pasta properties

Glass transition measurements can be used to test the quality and stability of dried foods such as pasta. The behaviour of the material around its glass transition temperature, where it changes from being rubbery to glassy, is useful to understand as, either side of this boundary, other properties can also be different.

To unambiguously characterise the glass transition temperature of dry rice pasta, researchers used an unprecedented combination of experimental techniques. In their study, published in *Polymers*, they go beyond the standard techniques of NMR and DSC and use multiple techniques on ISIS's Vesuvio beamline.

With the addition of neutron transmission, diffraction and Compton scattering results, they were able to fully characterise the dry rice pasta across a range of temperatures, finding that it was almost entirely amorphous. At the glass transition temperature, the long-range order is partially lost, due to a change in the starch structure.



Schematic diagram illustrating the combination of neutron scattering with nuclear magnetic resonance and differential scanning calorimetry methods in the study of the glass transition in biopolymers.

**Instrument:** Vesuvio

**Related publication:** Glass Transition in Rice Pasta as Observed by Combined Neutron Scattering and Time-Domain NMR, *Polymers* 2021, 13(15), 2426

**DOI:** 10.3390/polym13152426

**Funding:** STFC

**Authors:** M Witek (University of Agriculture in Krakow), M Krzystyniak, G Romanelli (ISIS), T Witczak (University of Agriculture in Krakow)

## Professor Jacqui Cole

**Professor Jacqui Cole is Head of Molecular Engineering at Cambridge, BASF/ Royal Academy of Engineering Research Chair in Data-driven Molecular Engineering of Functional Materials and a joint appointment at ISIS, but she is not the traditional academic!**



Her highly interdisciplinary research combines artificial intelligence with data science, computational methods and experimental research to realise a 'design-to-device' pipeline for data-driven materials discovery. Accordingly, Jacqui holds two PhDs: one in Physics from the University of Cambridge and one in Chemistry from the University of Durham. But she's anything but the traditional academic.

Jacqui grew up a few miles from where the ISIS Neutron and Muon Source is located. After GCSEs, at the age of 16 she left school and got a job at a local warehousing and transportation company as a hand packer. "It was just what I thought people did," she says, "Leave school, get a job, work your way up." Then she got a phone call from school, asking if she was coming in to see her GCSE results. Slightly surprised, she did, and was asked if she would commit to doing A-levels. She studied Maths, Physics, Chemistry and History but, hedging her bets, didn't leave her packaging job.

Back at school, there was a visit from the Oxford Trust, a local organisation with a mission is to encourage the pursuit of science and enterprise, including engaging the next generation of scientists. It was a visit that changed Jacqui's life.

"I picked up a flier they left for a competition," she says, "You had to choose a local technical company, visit them and write a report on the company." The prize was an all-expenses paid trip to the British Science Association Festival of Science, that year hosted by Swansea University. She won, and it was an eye opener. "I just had no concept of university or what it was like," she says.

On returning to school, she decided to give university a go. Her A-level form tutor helped her navigate the application system and encouraged her to visit a variety of places to

get a feel for the different environments. Her first choice was Chemistry at Durham, liking the college approach and the small city. She enjoyed the course, but the highlight was a final year research project studying crystals. "I was really excited by the discovery side, seeing these structures for the first time, and the whole concept of being able to see atoms in place."

This made Jacqui determined to do a PhD but, initially, she didn't want to stay at Durham, feeling instead she'd like to experience life elsewhere. Then a professor at Durham came up with an idea: a PhD shared with the Institut Laue Langevin (ILL). As her PhD neared completion, she looked for more opportunities to develop, finding a post in Kent researching optical materials. "I was working with a lot of physicists and they had a much more mathematical approach. I felt it would be useful to up my game, so I started taking some Maths modules with the Open University."

This continued from her two-year PostDoc to her next post, a Junior Research Fellow at the University of Cambridge. She also started a PhD in Physics, expanding on the work she had done in her postdoc, on top of more Open University modules, which would lead to an Engineering degree, specialising in artificial intelligence (AI).

Jacqui's current research aims to provide a data-driven approach to materials discovery, finding ways to use molecular-level knowledge to address 21st century challenges. Jacqui says, "This is a unique opportunity to collaborate with STFC, industry and academia to discover new materials which can help us with today's grand challenges in engineering, using advanced data science methods."

# Source, Instruments and Technical Development



## ISIS running in 2021

2021 was an unusual year for ISIS operations due to both the Covid pandemic and the start of the long shut down. As a result, only two experiment cycles were run. The first of these was to both target stations but with users largely remote due to Covid. The second of these was with users back on site but was to the second target station only as the first target station refurbishment was in progress.

Statistics on the experiment cycles are given below.

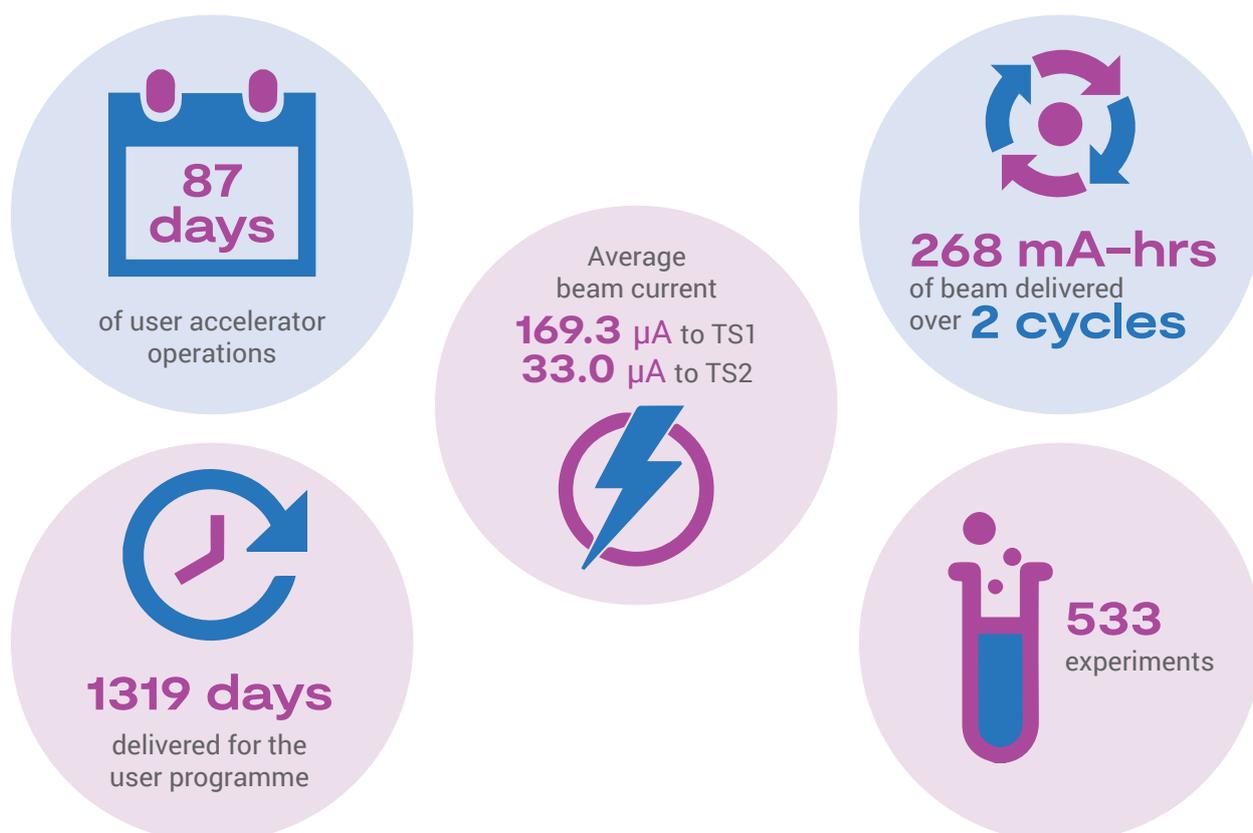


Table 1.1: Performance in 2021 Cycle by Cycle

Cycle	2021/1	2021/2
Beam on time (h)	1039.5	739.4
Availability (%)	87.1	81.2
Total Beam (mAh)	240.8	27.1
Mean current when beam on		
Synchrotron ( $\mu\text{A}$ )	231.6	36.6
TS1 ( $\mu\text{A}$ )	191.6	0
TS2 ( $\mu\text{A}$ )	40	36
Highest daily beam total (mAh)	238.4	38.4

# Sustainability

ISIS aims to embed sustainability across the facility, in how we operate, the science we deliver and in our day-to-day work. Over the past 12 months we have taken steps to reduce the environmental impact of our operations, developing a sustainability strategy that recognises our responsibility to minimise our own environmental impact whilst maximising the benefits of our research to addressing the challenges of environmental sustainability.

## Tackling global challenges

The research carried out at the facility makes a significant contribution to tackling global challenges, including supporting the UK government's plans for a carbon-neutral economy by 2050, reducing emissions, developing cleaner sources of energy and energy storage, and greener transport solutions.

The United Nations have outlined a set of 17 Sustainable Development Goals (SDGs), adopted in 2015 as part of the 2030 agenda for sustainable development, considered of critical importance for humanity. In 2021, publications from ISIS contributed to at least seven of these SDGs. We also contribute to the areas the UK

Government has prioritised in their ten-point plan for a green industrial revolution and their hydrogen economy and Carbon Net Zero strategies.

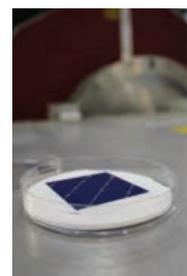
We are currently starting an evaluation of the impact of our research on the global challenge of sustainability, which will take place in 2023 / 24. The aim is to develop a methodology to assess quantitatively and qualitatively the environmental impacts from scientific research resulting from the facility, including our contributions to the Carbon Net Zero agenda and the UN Sustainable Development Goals.

UN Goal



We have installed PV panels on ISIS buildings

We have developed the ISIS Sustainability Strategy and are setting up an ISIS Sustainability Network group to discuss how we can embed sustainability in all that we do. This includes all aspects of the next ISIS large scale programme, Endeavour, as well as across our science, engineering, and computing divisions. We have created a cloud computing Environmental Sustainability Working Group to understand and reduce the environmental footprint of computing within ISIS and to use computing to improve the efficiency of ISIS operation. In November, we are piloting a sustainable design training package for our engineers.



Solar panels installed at ISIS, and being investigated using the HiFi muon instrument.

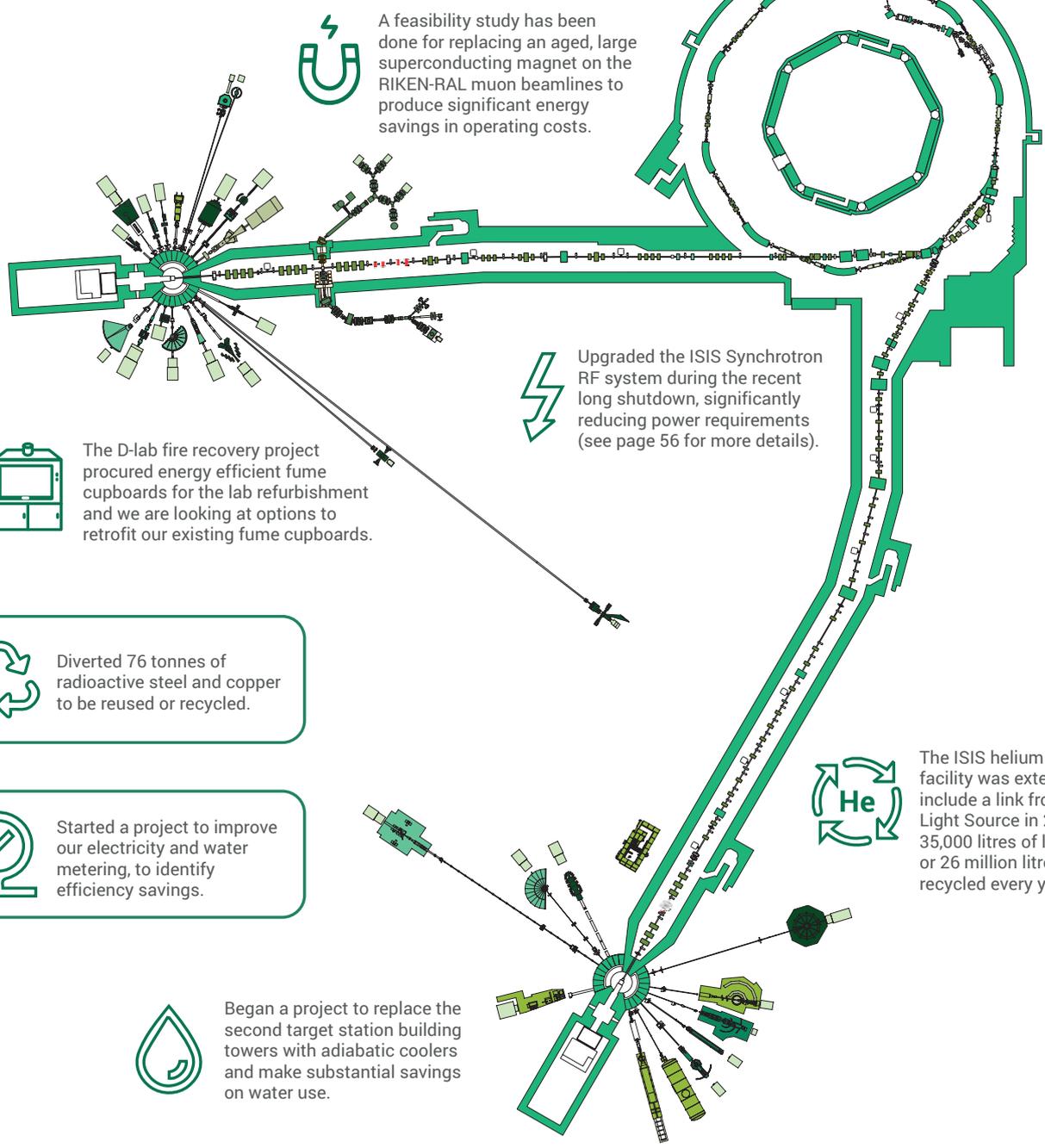
## Sustainability in operations



Started a Water Plant Carbon Reduction Project, to better understand the energy and water usage of the major ISIS plant systems and identify potential savings.



Completed a water systems project which deployed the latest, most efficient technology, combined with an intelligent control system, resulting in greatly reduced electricity consumption




A feasibility study has been done for replacing an aged, large superconducting magnet on the RIKEN-RAL muon beamlines to produce significant energy savings in operating costs.



Upgraded the ISIS Synchrotron RF system during the recent long shutdown, significantly reducing power requirements (see page 56 for more details).



The D-lab fire recovery project procured energy efficient fume cupboards for the lab refurbishment and we are looking at options to retrofit our existing fume cupboards.



Diverted 76 tonnes of radioactive steel and copper to be reused or recycled.



Started a project to improve our electricity and water metering, to identify efficiency savings.



The ISIS helium recovery facility was extended to include a link from Diamond Light Source in 2021. Over 35,000 litres of liquid helium, or 26 million litres of gas, is recycled every year.



Began a project to replace the second target station building towers with adiabatic coolers and make substantial savings on water use.

# Major Projects

Major upgrade and development projects at ISIS ensure the facility is able to operate well into the future, install new components that increase reliability and energy efficiency, and develop the instrument suite to deliver the best capabilities for science. This section details some of the major projects that have been ongoing over the past year. These projects have been in the planning and design phases for many years and have been brought to completion during the ISIS long shutdown: an 8 month off-period for the second target station (TS2) and 16 month off-period for the first target station (TS1). The projects include a complete refurbishment of the TS1 target, reflector, moderator and all associated services in order to ensure operation for decades to come; replacement of one of the accelerating tanks in the linear accelerator; replacement of a collimator in the proton beam leading to TS1, and complete refurbishment of the RIKEN-RAL muon beamlines. In addition, ISIS has also continued to construct two instruments for the European Spallation Source being built at Lund in Sweden.



## Installation of the new linac tank IV

A major project for the ISIS long shutdown was replacement of one of the tanks in the linear accelerator. After the old linac tank IV was removed in July 2021, the new tank was installed in six sections. The tank was then vacuum tested and aligned, followed by several days of RF conditioning, gradually raising the power and pulse rate to operational level. After a journey of almost 10

years from initial design work, through manufacture and testing and ultimately installation onto ISIS, the team was elated to see the tank successfully accelerate a beam. Not only did it accelerate – they were rewarded with a 94% transmission efficiency on the first attempt! The tank has now been operational for the first user cycles of 2022.



*The old tank being removed.*



*The team with the old tank.*

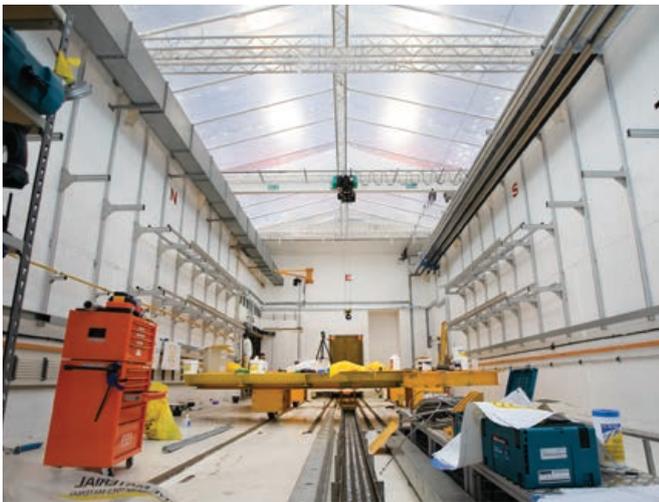
## First Target Station (TS1) Project

One of the major projects taking place during the ISIS 2021/22 long shutdown, the TS1 Project involves the replacement of the target, reflectors and moderators (TRaM) assembly and a refit of the target services area (TSA). It is part of ISIS's commitment to invest in its facilities and improve the operations of the target station that has been running for nearly 40 years.

During the autumn of 2021, the focus of the work was continuing to remove the old equipment from both the TSA and the remote handling cell (RHC). Pipework, frames and old equipment, along with kilometres of old cabling, some of which had been in use since the first days of ISIS, were removed and sent for further characterisation before either being stored, disposed of, or recycled.

Radiologically shielded flasks were designed in-house for these specific applications. This meant that even items that had been exposed to the proton beam (and neutrons) for almost 40 years could be safely removed from TS1 with minimal external doses.

In the remote handling cell, the team removed all the old TRaM equipment, including the largest item never to have been previously removed or replaced: the cantilever support frame that the old TRaM sat on. At nearly 2.4m long, it needed to be cut inside the RHC before it could be put in its flask. This is something that was trialled a lot outside of the area and it was a relief when it was finally in two sections.



*The empty target services area.*



*The target services area with the new equipment installed.*



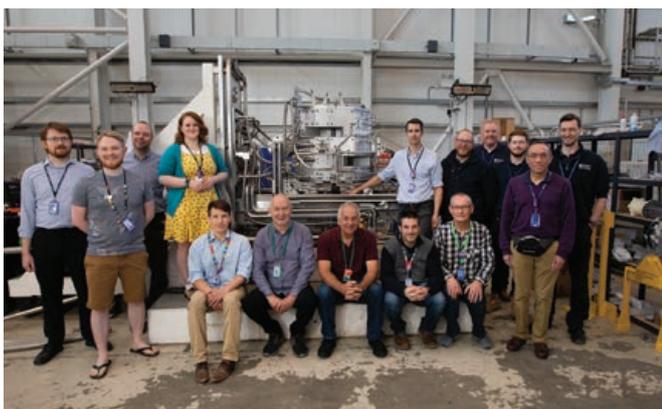
*The old target being removed.*

To enable easier and quicker removal of the TSA roof sections, a set of translucent roof sections was designed and constructed.



*The roof of the TSA being removed to enable easier access.*

A great deal of work has also gone on outside of the Target Station building, including the final assembly, testing, alignment and measurement of the new TRaM assembly. This work involved teams from many parts of ISIS, such as mechanical designers, target controls engineers, instrumentation physicists and technicians, electrical technicians, members of the plant section, the survey & alignment team, target operations technicians, external welders and crane operatives. It is a great example of the collaboration that happens at ISIS on a regular basis.



*Some of the TS1 team with the new TRaM.*

The New Year saw the start of the installation process, with the new service modules and ATEX room, which had already been built and tested, brought down and installed. These were then connected up with their associated pipework and cables.



*The installation of the water cooling trolley.*



*The ATEX room is lowered down in position.*



*Electrical cables being installed.*

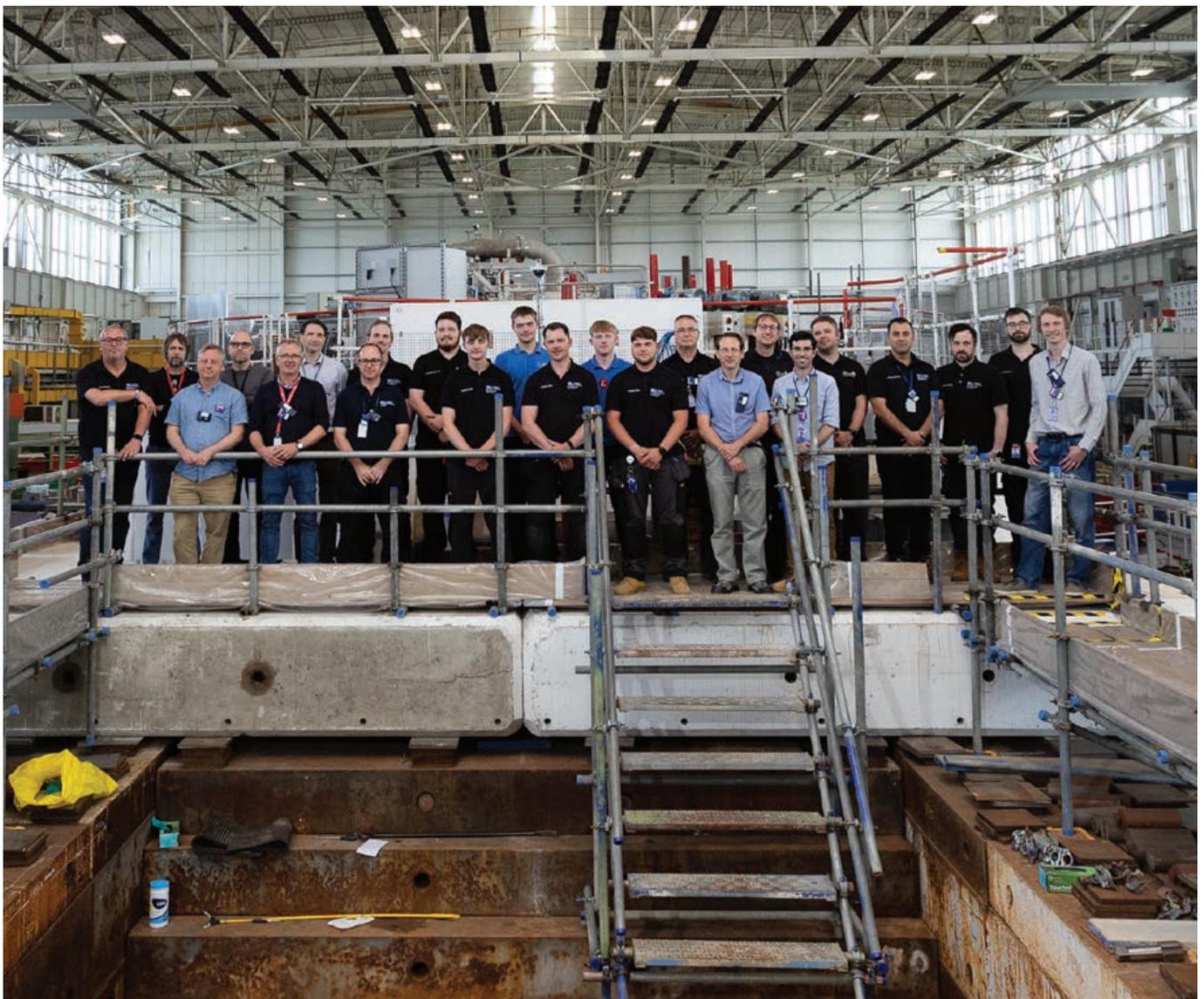
The installation is progressing in both the TSA and the RHC. Commissioning of the newly installed systems will begin in summer 2022 and wrap up in time to take beam to target in the autumn. However, before it is ready to take beam, there is a considerable amount of commissioning of the new systems to be done to ensure that it all works as planned.

## Extracted Proton Beam (EPB) 1 muon collimator repair

The muon collimator is installed downstream of the muon production target. It prevents scatter of the proton beam from making other downstream beamline components too radioactive. The muon collimator developed a water leak during a user run, and so needed to be replaced. The leak happened in a highly-radioactive area downstream of the muon target. Due to the elevated levels of radiation, the old collimator assembly was winched into a shielded container which was in turn placed into a secondary flask to further reduce radiation levels before removal from the building. The new muon collimator was lifted into place in May 2022 and the team moved on to vacuum testing before continuing with the installation of the remaining components.



*The new collimator assembly being lowered into EPB1.*



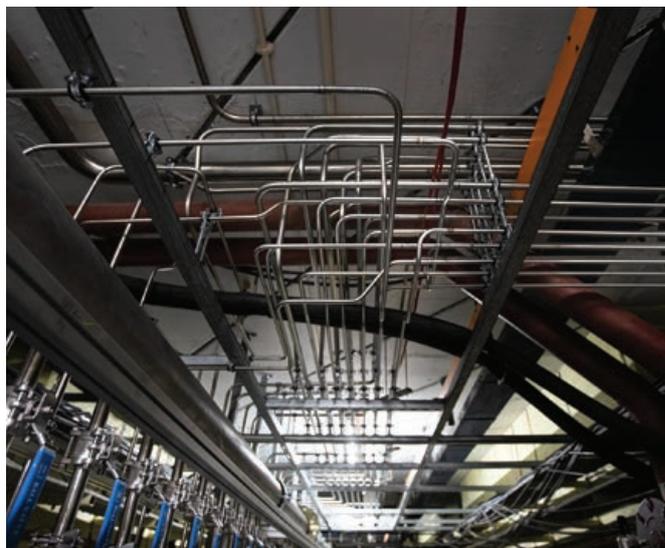
*The group working on the muon collimator replacement on top of the EPB before the roof was replaced.*

## Refurbishing the RIKEN-RAL beamlines

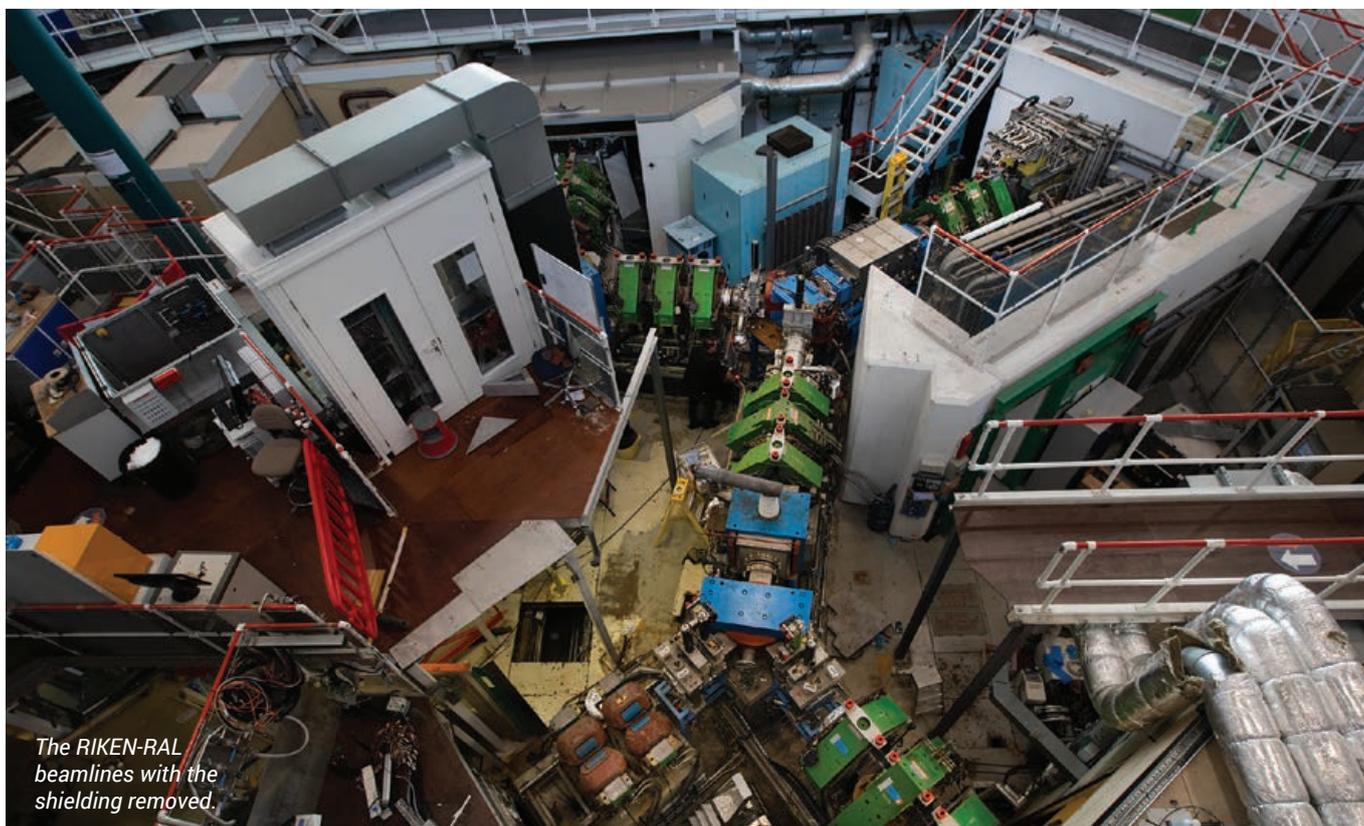
The RIKEN-RAL muon beamlines were built in the early 1990s through a collaboration with Japan. As part of the ISIS long shutdown, a large project has been underway to completely refurbish them.

This work has included the installation of 35 new power supplies which will run more efficiently and have higher stability than the previous ones. The magnets that focus the muon beams, some of which were second-hand when they were installed, have been refurbished to fix water leaks that were spotted before and during the shutdown work. Over 100 km of cabling has been replaced, as well as miles of copper pipes that have been changed to stainless steel to meet higher safety standards. A new vacuum system has been installed, as well as a new controls system. On top of all this, the three 200 keV particle separators are being taken apart and refurbished. Although the team hope that it will be another 30 years before major maintenance is needed, new shielding has been designed which is easier to remove in sections, improving access.

Over thirty people have been involved in the project throughout its different stages, making the most of the varied in-house expertise of ISIS staff.



*Some of the new pipework installed as part of the refurbishment.*



*The RIKEN-RAL beamlines with the shielding removed.*

## ISIS and the ESS

The United Kingdom is a partner in the European Spallation Source (ESS) which is currently under construction in Lund, Sweden. Recognising the ISIS facility's expertise in neutron instrumentation at spallation sources, the UK is delivering two instruments to the ESS suite: Loki and Freia. Both instruments reflect the strength of the UK research community in life and materials science at the nanoscale, and have strong industrial relevance. These instruments form part of a wider UK engagement programme, ranging from preparation laboratories, detector readouts through to data reduction.



*ESS and ISIS staff on Larmor for detector testing.*

Loki is a versatile broadband small angle neutron scattering (SANS) instrument which will provide enhanced capabilities to study complex materials that are structured on the sub-micron length-scale.



*The Loki detector vessel installed at ESS.*

This will have a broad application across the physical and life sciences but with an emphasis on soft matter, biosciences and the material science community. Loki is currently undergoing an intense period of installation at ESS. The installation activities are both in the experimental hall and at the front end, in-bunker section. The schedule and progress of Loki are such that it will be in the first tranche of instruments ready to take beam.

Freia is a high-flux liquid surface reflectometer that is designed to study interfacial phenomena. Such phenomena drive a wide range of behaviour of direct societal relevance, from understanding the mechanism of disease through to developing efficient, low-cost photovoltaics and sensors. Freia will have transformative

performance that will enable high-throughput parametric studies and allow access to the kinetic domain for complex materials. Freia is currently undergoing detailed design with a number of components already successfully procured, and is scheduled for completion in 2025/26.

The ISIS Support Laboratories team, led by Marek Jura, have been supporting the ESS team with the design and installation of their labs since work started in 2016. This support has included sharing ideas and experience, and the long-term loan of some key pieces of equipment.

With the labs now built and beginning operations, the ISIS and ESS team held a joint symposium in the new building at the ESS to celebrate the occasion and to act as an opportunity to discuss how to continue the collaboration. The group hopes to repeat the symposium at ISIS in 2023.



*The group outside the ESS target station.*

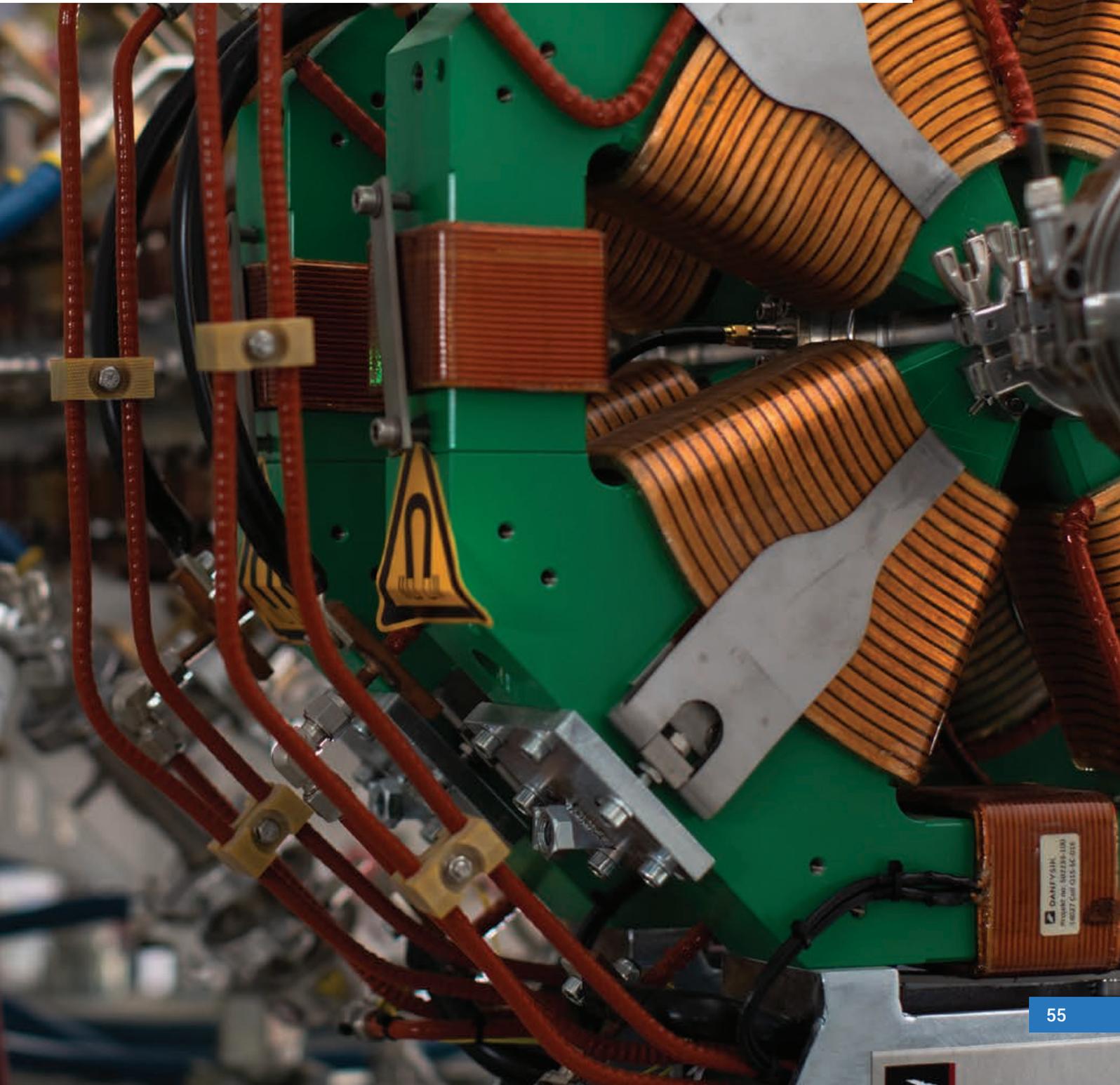


*Bryan Jones showing the group the ESS linear accelerator tanks.*

*Right: The new Front End Test Stand being tested by the Low Energy Beams group.*

# Accelerator Developments

The ISIS accelerator is an amazing machine that operates 50 times every second, accelerating protons to 800MeV from the ion source through the linear accelerator, into the synchrotron and on to the target stations. It is a very complex machine, with many thousands of components being continually monitored to ensure it is operating correctly. Regular maintenance work is required; but alongside this, ISIS accelerator physicists and engineers are constantly looking to upgrade components to improve reliability, deal with obsolescence, ensure we're using the latest technology and to decrease energy usage. ISIS staff also contribute to designs of future facilities. A variety of accelerator development projects is described in this section.



## Reducing ISIS's energy consumption by upgrading the synchrotron radio frequency systems

During the long shutdown, the ISIS synchrotron RF section replaced all six of the fundamental RF systems that drive the synchrotron acceleration. About 9% of the proton beam energy needed for producing neutrons and muons comes from the ion source and linear accelerator, but the rest is supplied by the six fundamental radio frequency (RF) systems in the synchrotron.

These systems were installed when ISIS was first built. At their core are valves known as tetrodes. During the 2021 long shutdown, the RF section upgraded the valves in all six RF systems. An upgrade of this scale required over a decade of planning but has brought huge efficiency savings: the fundamental RF systems require about 60% of the power they did before the change.

The team have also been working on the low power RF system: they have been able to set it up in a way that makes it able to run more intelligently, including adapting when the synchrotron is supplying only one target station. This is very timely, as the last two ISIS cycles have been TS2 only. Running the synchrotron in this way during a TS2-only cycle will save about 1.2 MW, which will have a huge impact on ISIS's overall electricity demand. The team's next step will be to do a similar upgrade for the second harmonic RF systems, continuing to reduce ISIS's energy consumption.



*Andy Seville, Dave Allen, Rob Mathieson, Neil Farthing, Dave Gibbs, Ryan Allinson (Left to Right) in front of the new control racks.*

## EHB3 magnet coil replacement

Due to a coil water flow blockage, the Extraction Horizontal Bending Magnet 3 required new coils to be fitted. Once the magnet had been removed from the accelerating ring, the two halves of the magnet body had to be surveyed before separating. With the old coils removed and new ones fitted, the beam pipe was reinstated. The next stage was to upgrade the insulating manifolds and add Swagelok fittings to the cooling circuit to ensure ease of serviceability and compatibility with current supplies before the magnet was reinstalled.



*EHB3 being craned out from synchrotron ring for repair.*



*EHB3 magnet yokes being assembled with new coils fitted.*

## Using light curtains to develop a new synchrotron search routine

A new interlocks system has been installed in the ISIS inner synchrotron that allows the crew to reduce the number of people needed for safety checks from four to two. The previous search process required four competent personnel to follow a precise route through the inner synchrotron and catacombs, visiting defined search points in the process.

The RF Group interlock section and main control room crew have developed a new interlock system that uses 14 'light curtains' and more search points to enable the area to be searched with just two staff members. The light curtains have been installed across the tops of all the catacomb entrances and at other points in the inner synchrotron. If any of the light curtains are triggered out of the set sequence, the search is cancelled and must be started again.



*Light curtains in the inner synchrotron: between computing racks (above) and at one of the catacomb entrances (above right).*



*Darren, Mark and Elliot next to the new electronics rack that controls the light curtains.*

## CERN ALPHA

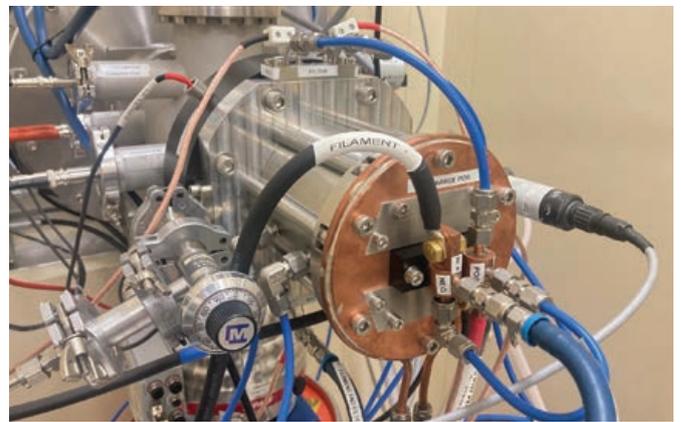
Physicists and engineers at CERN, The European Organization for Nuclear Research, use the world's largest and most complex scientific instruments to study the basic constituents of matter. ISIS staff, in collaboration with others from the Rutherford Appleton Laboratory (RAL), work closely with CERN on a number of projects.

The CERN ALPHA experiment makes precision measurements of antihydrogen atoms. ALPHA has now embarked on an ambitious upgrade programme aimed at directly comparing hydrogen and antihydrogen within their existing atom trap. One aspect of this upgrade is the development of a low-energy hydrogen ion source that produces both negative and positive ions and is compatible with ALPHA's existing beamlines. The ISIS Low Energy Beams Group (LEBG) has collaborated with

the University of Jyväskylä (Finland) and University of Castilla-La Mancha (Spain) to develop an  $H^-/H^+$  ion source and low energy beam transport that meet the beam current, emittance and vacuum requirements of ALPHA. The ion source was successfully tested by the ISIS LEBG and will be delivered to CERN in 2022 for integration to the ALPHA experiment. Three copies of the ion source were built by the RAL mechanical workshop, as ISIS will later use the high-brightness  $H^-$  source for injection studies into a fixed-field alternating gradient accelerator prototype at the recently commissioned Front End Test Stand (FETS).



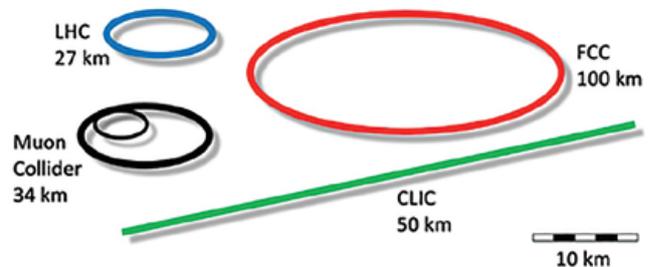
The ISIS Low Energy Beam Group delivering the  $H^-/H^+$  'PELLIS' ion source to CERN. From left: Chris Cahill, Trevor Wood, Dan Faircloth, John Macgregor, Olli Tarvainen, Scott Lawrie and Rob Abel.



The 'PELLIS' ion source and its low energy beam transport / differential pumping vacuum chamber at ISIS LEBG VESPA laboratory ready for the delivery to CERN ALPHA.

## Muon collider

Accelerator Division scientists have been sharing their expertise with CERN as it develops an R&D plan for the next big particle physics experiment, following on from the Large Hadron Collider (LHC), which is expected to finish operation towards the end of the 2030s. To be ready for construction at that time, development of the next facility must begin now. Options considered include an electron-positron synchrotron with a circumference around 100 km and an electron positron linear accelerator over 10 km long. ISIS has been instrumental in developing key technologies for another option: the muon collider, which would collide a form of matter that has never been used in an accelerator. In turn, the technologies required for a muon collider, such as high efficiency accelerating cavities and very rapid particle acceleration, may be of great benefit for a future upgrade of ISIS.



Comparison of the footprint of the muon collider complex, the Future Circular Collider (FCC) electron-positron synchrotron and the final stage of CLIC, an electron-positron linac. The LHC is shown for comparison. Credit: CERN.

## Haroon Rafique

Haroon tells us of his journey from University to CERN and to ISIS where he works as an Accelerator Physicist.

“ At ISIS there’s far more of an opportunity for you to overcome problems and learn a lot more on the job: this really excites me.

”



Haroon started his academic journey into the world of physics when he went to the University of Manchester to study a masters there in 2007. After completing his masters he then declined an offer to stay at Manchester and do a PhD, instead opting to continue his studies by pursuing a PhD in beam collimation at the University of Huddersfield as he felt that at Manchester he would just be working in an office all day.

His PhD at Huddersfield involved frequent collaboration with, and trips to, CERN, where he started to build up a network of contacts. After his PhD he returned to the University of Manchester as a post-doctoral research associate, where he helped contribute to the design of the proposed high energy Future Circular Collider (FCC). He wanted to move away from the topic of his PhD to expand his scientific horizons and knowledge base.

It was after this that he became a Senior Fellow at CERN, working on the Proton Synchrotron injector producing protons that would ultimately end up in the LHC. One of his main tasks was to solve the problem caused by the fact that the beam of particles would grow in size when travelling between accelerators. He designed and ran simulations to solve this and became the second largest user of CPU at CERN with over a thousand years of CPU time used!

Now working at ISIS as an accelerator physicist, Haroon says, “CERN was the perfect preparation for my role at ISIS.” Speaking about the differences in the two institutions, he notes, “At CERN everyone was a specialist so when you had a problem or a task you could go to someone who was a world leader in that field, whereas here at ISIS there’s far

more of an opportunity for you to overcome problems and learn a lot more on the job: this really excites me.”

Outside of the world of physics Haroon has spent a considerable amount of time as a basketball coach. His coaching career started aged 15 at his school, and continued into university. When he left Manchester to do his PhD in Huddersfield he continued by coaching the University of Huddersfield women’s basketball first team, as well as being an assistant coach for the men’s first and second team, taking them to four promotions in four consecutive seasons, with the fourth season also being an undefeated one. After leaving Manchester and joining CERN as a fellow he took on the role of being the head coach of the CERN men’s basketball team.

Alongside his basketball coaching Haroon has been heavily involved in scientific outreach programmes throughout his career. “Growing up I was always on the gifted and talented programmes put on at school. I feel like it is my duty as a scientist to give it back.” During his PhD Haroon gave talks to school children and sixth form students in colleges, and he used this time to develop and hone his presentations to be properly tailored for the correct audiences. “I want to use the outreach work to inspire the next generation of scientists. We have never needed more scientists; it is the responsibility of science to defend science.”

He has worked with the Tactile Collider project which aims to bring the science behind particle accelerators to the visually impaired. It uses interactive workshops that employ the mediums of touch and sound to communicate knowledge using “specially developed tactile objects and fascinating soundscapes”.

## Enabling technologies and facilities

A very wide variety of capabilities is needed to support the ISIS user programme and ensure ISIS instruments are able to get the best from the neutrons and muons delivered to them. The ISIS computing team develops software for data reduction, visualisation and analysis, looks after computing hardware, and creates the systems for users to submit proposals, book accommodation, etc. The ISIS support laboratories are a critical part of the science programme, enabling samples to be prepared and characterised on site before neutron or muon experiments. The ISIS Detector team maintains this key element of the ISIS instrument suite and develops new capabilities to improve neutron and muon instrumentation.



## Software and computing developments

### Scientific software

Mantid is ISIS's core framework for reduction, visualisation and analysis of ISIS data, and is a partnership with SNS in the US together with ESS and other European facilities. This year the collaboration governance was reviewed and opened to include other international facilities such as ANSTO and CSNS. ISIS Scientific groups have been developing their long-term scientific software strategies, as part of the overall ISIS strategy for this area. A variety of ongoing software projects have been supported as part of this, often in collaboration with the STFC Scientific Computing Department (SCD) and the Ada Lovelace Centre. Examples include the PACE project for Excitations Group instruments and DFT-based methods for modelling muon experiments. Machine learning applications are also being explored for a number of scientific (and accelerator) areas, again in collaboration with SCD. A new Research Software Engineering team has been formed within ISIS to make scientific software sustainable for the benefit of ISIS and its community for the future, including ensuring software is supported by several developers.



*Radu Coldea and Ryutaro Okuma (Oxford University) analysing data from WISH.*

### User programme software

This area covers all the systems used to support the user programme, including the proposal system, peer review panel management systems, instrument scheduling system, visits booking system and other key tools. The most significant new project that started this year is to replace the proposal submission system – the new system is due to be rolled out in Autumn 2022.



*ISIS Computing Division members in discussions.*

### Computing infrastructure

This programme covers more broad computing infrastructure to support operations and research, including new hardware (network, storage etc). Within this area, work has continued to develop the Data Analysis as a Service platform to allow external access to, and analysis of, ISIS data (and which proved essential to support experiments during Covid when users couldn't visit site).

## Detector systems group update

This year saw the merger of the former Neutron Detector and ISIS Electronics Support and DAE groups into the Detector Systems Group. The new group will provide a more integrated approach to detectors systems development.

### Neutron detector systems

After a period of research, design, simulation, prototyping and testing, several new large-scale neutron detector systems are being manufactured and rolled out for both ISIS and the ESS instruments.

The IMAT and Inter detector suites use scintillators with light collection via fluorescent wavelength shifting fibres, albeit with two drastically different geometries and requirements. Both detector suites are now being manufactured. Installation of these systems in 2023 will improve and expand the scientific capabilities of both instruments. Furthermore, the team has proven that these types of detectors can be produced in a cost-effective way with up to 75% thermal neutron detection efficiency and enhanced neutron position resolution.

Assembly of the boron-coated straw (BCS) tube detectors for the LoKi instrument at the ESS is complete. A crucial milestone this year was thorough testing of the BCS detectors on Larmor to verify their performance, demonstrate the SANS capability of this type of detector and successfully transfer data to Copenhagen for real-time event reconstruction. Final tests are underway before the detectors are packed and shipped to the ESS for installation.

DAE3 continues to be rolled out throughout much of ISIS, with installation on more than two-thirds of neutron instruments. The electronics team has also been developing the next generation of data acquisition systems containing streaming capabilities. In 2023, Maps and PolRef will be the first instruments to trial data streaming in a paradigm shift for ISIS.



*Internal view of the first production module for the IMAT diffraction detectors.*



*John Dreyer and Stefan Howarth assembling boron coated straw tubes for the LoKi instrument at the ESS.*

## Detectors for SuperMuSR

Critical developments of the new SuperMuSR muon instrument detector, data collection and analysis systems were achieved this year. For the first time, Si-photomultipliers are intended to be used on an ISIS instrument with an advanced event identification

system. This unique system is capable of counting positrons at significantly higher rates, greatly improving measurements of the muon decay asymmetry. The team is now working with Technology partners to improve manufacturability of these positron detectors.

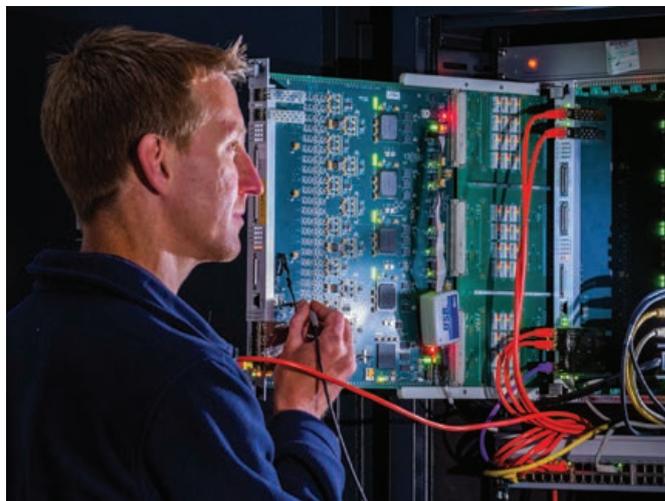
## Faster neutron detectors with nanoparticles and machine learning

Despite the excellent attributes of state of the art ZnS:Ag scintillators, detectors made with these scintillators are count-rate limited. In order to overcome these limitations, the ISIS scintillator team synthesised innovative nanoparticle ZnS:Ag. In the first ever investigation of its kind, these nanoparticles were found to have much faster scintillation than the current standard ZnS:Ag. Work is now underway to increase their brightness and make the nanoparticle scintillator neutron sensitive.

The ability to differentiate neutrons from unwanted gamma radiation is also critically important and classical methods begin to fail at high neutron rates. To solve this, the scintillation team, in collaboration with Technology and Scientific Computing Departments, developed novel methods based on machine learning to distinguish between neutron and gamma signals occurring within as little as 40 ns of each other. These machine learning methods can also improve data quality for detectors based on a much wider range of scintillators than currently available.



*Sarah Mann, a University of Bristol PhD student in the detector systems group, synthesising ZnS:Ag nanoparticles in the ISIS chemistry labs.*



*Dave Templeman testing one of the new streaming boards for ISIS data acquisition.*

## ISIS deuteration facility fire recovery update

On 13 May 2021 the deuteration facility lab (D-lab) suffered a major fire, that destroyed the lab infrastructure and much of the equipment. The source of the fire has been assigned to an electrical fault on lab equipment. Thankfully no one was hurt, and the majority of the d-materials were recovered.



*The Deuteration laboratory before the fire.*

Over the last year the D-lab team have focused their efforts on the recovery of the lab and setting up temporary operations within one of the prep labs in TS1. The team have been working on synthetic projects and, even with reduced capability of equipment and infrastructure, they have still managed to support a number of user experiments.

A great deal of progress has been made on the strip out of the damaged lab, and exciting new plans have been drawn up for a new lab design. The work on the fit out of the new lab starts in September 2022, and is due to complete by January 2023.



*The lab after the fire.*

# Instrument Developments

ISIS has 35 neutron and muon instruments. They are continually evolving in order to meet the needs of contemporary science and respond to new challenges and new science areas. Some of the current medium-sized instrument development projects are described here, with larger projects described in the next section.



## NMIDG – Neutron and Muon Instrument Development Group

NMIDG is a relatively new group at ISIS focused on the development of new muon and neutron instrumentation. The group has been very busy for the last two years with Endeavour (see pages 73-74), a massive instrumentation programme aimed at delivering four new instruments and five major instrument upgrades. NMIDG advises the science groups on best practice when designing instruments and performing instrument simulations.

In addition, NMIDG organises internal and external reviews of the proposed technical design. Utilising both internal and external instrumentation expertise ensures that the final design is fully optimised, cost effective and not unnecessarily complex, thus lowering project risk. The aim is to finish all reviews for Endeavour projects this year, so the projects are in good shape to go ahead next year when funds become available.

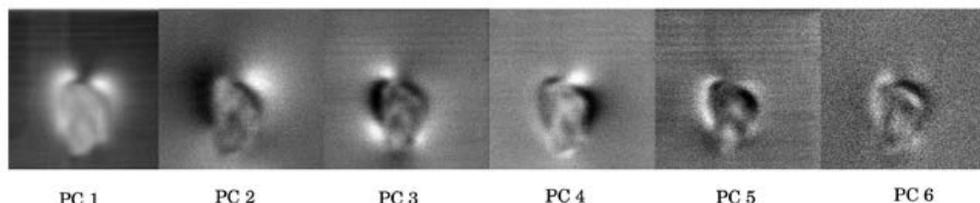
## Polarisation

One of the unique strengths of neutron scattering is the ability to do experiments with polarised beams, in which the spins of the neutrons are aligned. These not only allow us to separate the components of the sample scattering, but also to improve the experimental resolution in time and space, and to directly image magnetic fields. This power comes at a price, however: polarised experiments have traditionally been associated with a large reduction in flux, and hence long measurement times. Recent technical developments have mitigated many of these losses, and polarised neutron techniques are now flourishing at facilities worldwide.

In the last year, the Polarised Neutrons Section in the Neutron and Muon Instrument Development Group

has helped to add polarised capabilities to two new instruments at ISIS, bringing the total up to six (Zoom, IMAT, LET, PolRef, Offspec, and Larmor). July saw the first successful demonstration of polarised time-of-flight imaging on the IMAT instrument. An international team including researchers from Helmholtz-Zentrum Berlin and Institut Laue-Langevin imaged the magnetic fields generated by a coil and by a piece of magnetic material (see image below).

Alongside these new advances, the section continues to support experiments on the Larmor and LET instruments, and to develop new polarised neutron technology and devices. These will soon grant the power of polarised neutrons to even more instruments at ISIS.



## Chiplr

One of the commercial areas where Chiplr is making an impact is in the reliability testing of high-voltage (and high-power) devices to ground-level cosmic-ray neutrons. Chiplr has recently installed a new high voltage safety system that makes the use of high-voltage on the beamline easier and much more efficient, benefiting both users and ISIS staff.

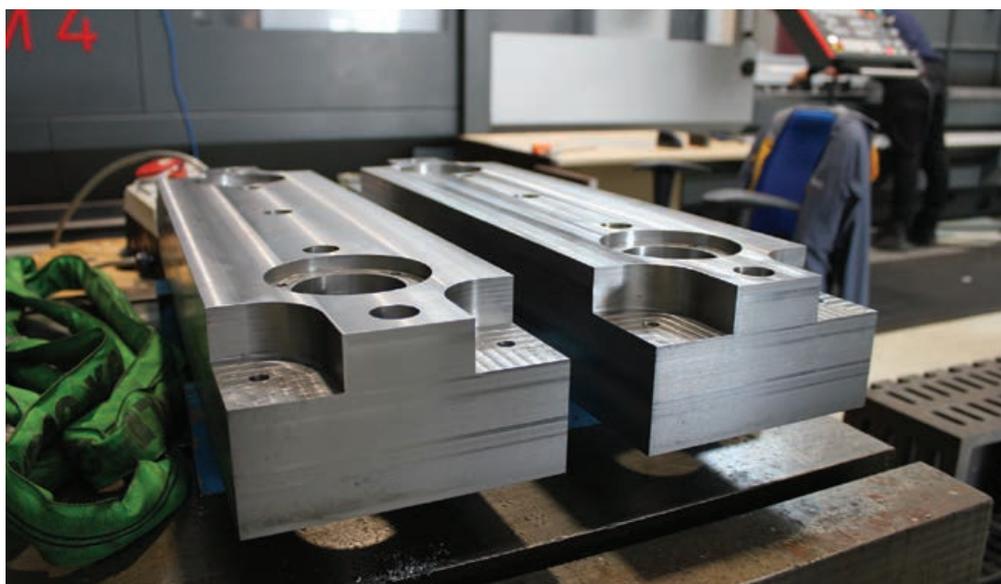
During the long shutdown, work was done to further optimise the beam profiles by shifting the final beam-size-defining collimation to provide a more homogenous beam when the beamline is operating with larger beams.

For system-level measurements, the high flux delivered by Chiplr occasionally needs to be attenuated to ensure the induced error rate does not overwhelm the tests. A fully automated, user controlled, 10x attenuator on the beamline has been installed to achieve this. It also acts as a 'secondary' shutter to lower further the background radiation levels at the very front of the beamline. The steel components of this shutter (below left) were machined by ISIS staff from recycled parts of previously decommissioned instruments.

A commercial air based cryo-cooler has also been installed to allow measurements of radiation tolerance at temperatures ranging from  $-40^{\circ}$  to  $80^{\circ}\text{C}$ : the demand for testing on Chiplr is now hotting up by cooling down!



*Maria Kastriotou loads a sample into the new cryo-cooler on Chiplr.*



*The new machined components for the Chiplr secondary shutter.*

## IMAT diffraction detectors

In the last six years there has been a great collaborative effort between many groups from ISIS to complete the design and construction of the Imat instrument with diffraction capabilities. The first diffraction spectra were collected on IMAT in July 2016 during tests of a prototype diffraction detector that had been built in-house. This pushed forward the development and construction of the diffraction detectors, taking advantage of the latest achievements in the field of photosensors and signal readout. The most notable accomplishment of 2021, despite the Covid pandemic, was the completion of the IMAT collimators by JJ X-Ray, Denmark, and the handover of all collimators to ISIS. The equipment will be installed on Imat next year once the diffraction detectors are ready.

The IMAT diffraction project was funded by the Swedish Vetenskapsrådet Research Council (Chalmers University of Technology) with additional financial contributions from STFC / ISIS.

“The complementarity between neutron tomography and neutron diffraction will be exploited on IMAT through the tomography-driven diffraction technique for different samples drawn from the engineering, archaeology and geology. This approach will allow neutron-imaging investigations of samples followed by a detailed diffraction analysis of the regions of interest by selecting any point within the 2D or 3D sample,” explains Genoveva Burca, the scientist leading the IMAT diffraction project.



(Left) Dr Jeff Sykora (ISIS Detector Group) and (Right) Dr Genoveva Burca (IMAT scientist) collecting first IMAT diffraction spectra on 20th July 2016.



First collimators delivered on IMAT (August 2021).

## SANS2D

The front end of SANS2D comprises five large blocks, each containing a collimation and guide section that can be moved in and out of the beam. This allows the beamline to match 'L1' (distance from the source to the sample) to 'L2' (distance from the sample to the detector) to achieve optimised resolution and flux for the Q-range of interest.

The long-standing reliability and obsolescence issues with the SANS2D front end set up have been addressed with a complete upgrade of the motors and drive system.

During the long shutdown all five blocks have had their aging and faltering motors and drive systems upgraded. The five encoders have also been replaced with absolute encoders. The full installation was completed at the end of February 2022 which allowed for a week of offline testing before successful commissioning with neutrons at the start of cycle 2021/2.

Not only does this work address the obsolescence and reliability issues being faced but also greatly improves the understanding of the system. Thanks to all those involved.



*The SANS2D blocks being returned into position.*



*The new drive systems for SANS2D.*



*The new motors in place in the beamline.*

## SEMSANS

Spin-Echo Modulated Small Angle Neutron Scattering combined with SANS (SEMSANS-SANS) measurements have been performed on Larmor in close collaboration with the group of Dr Roger Pynn (University of Indiana) in recent years. Using a unique piece of equipment, the superconducting Wollaston prism, the experiments enable the extension of the length scales that can be probed with SANS by producing an oscillating pattern in the position of the SANS beamstop. The ISIS detector group has developed a high count rate, linear, scintillator detector to measure the SEMSANS signal that is compact enough to allow small angle scattering measurements over a  $q$  range of about  $0.008\text{--}0.5\text{\AA}^{-1}$ . SEMSANS allows length scales of up to a few microns to be measured, so the combined

methods allow length scales of a few nanometres to a few microns to be measured simultaneously. It is anticipated that this range of length scales will be particularly useful for the study of multiphase systems such as those found in food science and additive manufacturing.

ISIS is currently in the process of designing and manufacturing its own Wollaston prism in close collaboration with the University of Indiana. This will provide routine access to SEMSANS-SANS measurements in the next 2-3 years. During this time, further developments in the detector technology and neutron polarisation analyser will improve the reliability and applicability of technique.

## Vesuvio+

Work is underway on the Vesuvio+ project. The first work package concerns the upgrade of the Vesuvio backscattering detectors. The detectors will be installed closer to the sample position to increase the count rate without compromising the resolution.

Within the second work package of the Vesuvio+ project, the optimisation of the Vesuvio beam stop is planned. The beam stop will be re-designed to minimise the parasitic gamma background and thus optimise the working conditions of the Vesuvio forward scattering detector banks. The work on the new beam stop is planned to start at the end of the long shutdown.



*Giovanni Romanelli, ISIS, and Fu Song, Queen Mary, University of London, loading a sample onto the Vesuvio beamline.*

## Sandals

The 2021/22 long shutdown has enabled ISIS to undertake the first part of a staged upgrade of its liquids and amorphous materials diffractometer, Sandals. The key elements of this phase of the project were the optimisation of the instrument's view of the new Target Station 1 methane moderator, the installation of a frame-overlap chopper, an upgrade of the primary neutron flight-line collimation, and an upgrade of the instrument's motorised beam defining jaws. The changes in moderator view and to the neutron beam collimating elements increase the flux of neutrons that can reach the sample position, whilst the frame-overlap chopper reduces

long-wavelength neutron background contributions that otherwise degrade the quality of the experimental data.

The successful completion of this primary flight-line upgrade has thus laid the foundation for the more ambitious Sandals-II project that is currently being developed as part of the ISIS Endeavour programme. When complete, Sandals-II will deliver an instrument that performs at least five times better than pre-Target Station 1 refurbishment capability, and that will enable higher throughput measurements, as well as deliver enhanced *in-situ* and *operando* experiment capability within the facility's Disordered Materials science programme.

## Gemma Draper

Gemma is the first chemist to join the Pressure and Furnace Team. Her scientific background helps the team prepare for an increasing number of complex experiments.



“ ISIS is like a living organism and it’s mind blowing how much goes on behind the scenes to keep it operational. ”

Gemma studied Chemistry at the University of Manchester and, with a preference for physical chemistry, began a PhD working at Manchester’s Dalton Cumbrian Facility (DCF) near Sellafield. She was studying coolants in pressurised water reactors, enjoying the process of research and developing instrumentation.

However, two years into the four-year programme, one of her supervisors retired, taking with them the direction for the project. Deciding that continuing with the PhD would not be the right thing to do, Gemma started looking for other options and came across a role in the Pressure and Furnace Team at ISIS.

“I thought I knew what a user facility was like, having been at the DCF, but when I came to ISIS for interview I was shocked at the scale of the facility. ISIS is like a living organism and it’s mind blowing how much goes on behind the scenes to keep it operational.”

Gemma was offered the job, which was also part of the STFC graduate scheme, and started in 2019. The rest of the section come from previous training in mechanical engineering, so her chemistry background enables Gemma to offer a unique perspective. With experience working in high pressure chemistry, she is ideally placed to offer guidance on the chemistry taking place in complex *in situ* experiments, and how this might impact the choice of equipment.

“I have to ask for help from those with an engineering background for particular tasks, but the rest of the section will also come to me for their queries in my area. I feel like I’ve really found a niche within the team.”

Her role involves acting as beamline support, speaking to users before their experiment and understanding what equipment they need, then setting it up for them and training them to use it safely. “I love the variety that comes with working with different groups of people,” she says. “It is a very different environment to working in an academic lab. Every day is different; I can’t imagine getting bored in this job.”

As part of the graduate scheme, Gemma has had the opportunity to take part in a variety of different types of training, and this has continued since she finished the formal scheme in 2021. As well as supporting users, she has also been able to work with other ISIS teams, including radiation chemistry studies for the moderators, and building a database that details the compatibility between chemical species and the materials used in the sample environments. She adds; “It’s been really rewarding to have created something that is useful for others.”



# Future Projects

ISIS aims to lead the way in the innovative development and exploitation of neutron and muon sources, science, instrumentation and technology. ISIS has a ten-year plan for major instrument developments, including significant upgrades to existing instruments as well as entirely new instruments – the Endeavour Programme. Endeavour is a package of large instrument projects which we anticipate will move to implementation next financial year. But ISIS instrument ambitions don't stop there – beyond this, further instrument projects are being created to ensure that ISIS remains a world-class neutron and muon facility, and some of these are described in the Beyond Endeavour section below. Further into the future, in order to maintain and develop the UK's neutron and muon capacity and capability, a new facility will be needed to replace ISIS. Work to consider a replacement facility – the ISIS-II project – has been ongoing for several years as specifications are considered and feasibility options for the accelerator worked out. Current progress with ISIS-II is also described below.



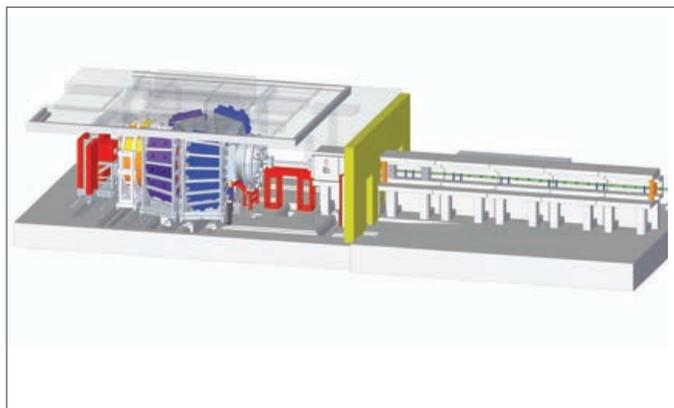
## Endeavour

Endeavour is the programme of new instruments and significant instrument upgrades that ISIS is aiming to carry out over the next ten years. Nine projects are included, with a total programme cost of around £90M.

Funding for Endeavour has been agreed by the UKRI Infrastructure Fund but can't be released until the Endeavour business case has been through its review and assurance processes. The outline business case passed all its stages, including UK Treasury approval, in June 2022. The full business case is now in preparation, and we hope it will complete its reviews by early 2023 ready for release of funds near the start of the 23/24 financial year.

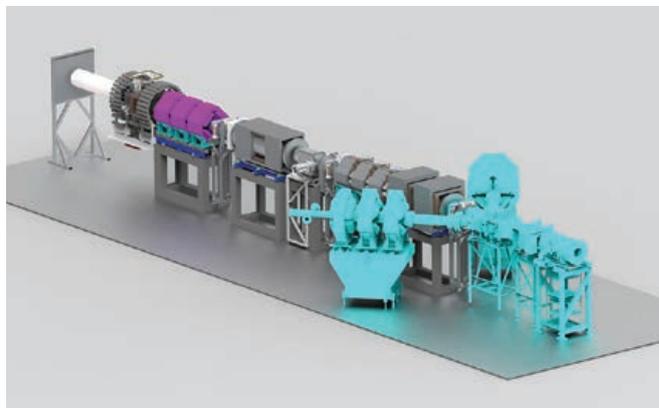
### HRPD-X

A high-resolution powder diffractometer for structural characterisation providing detailed information on materials such as MOFs and zeolites that are of considerable interest for gas separation, encapsulation and purification, for example for greenhouse gas management or the hydrogen economy. Complex *in operando* studies of battery and catalytic materials will become possible.



### SuperMuSR

The next generation of muon spectroscopy, providing significantly higher data rates and time resolution. The enhanced performance will give access to future energy systems such as nonconventional superconductors, functional materials and *in situ* battery research with industrial partners.



### LMX

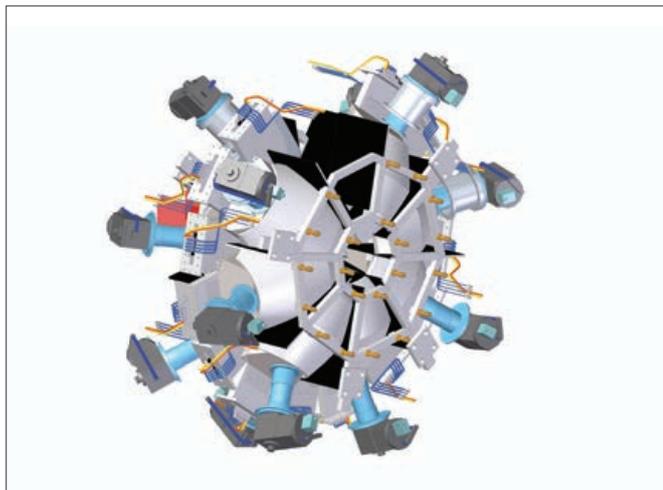
A large molecule diffractometer providing world-class capability for single crystal studies. LMX will enable advanced studies in supramolecular chemistry, functional materials, molecular magnets, energy harvesting materials and biomolecular science, including studies of the interaction of drug molecules in the active sites of virus proteins.

### e-map

Enhanced engineering capability and capacity through construction of a new instrument, e-map, offering a step-change in our ability to study real-world engineering components to meet the demands of industry.

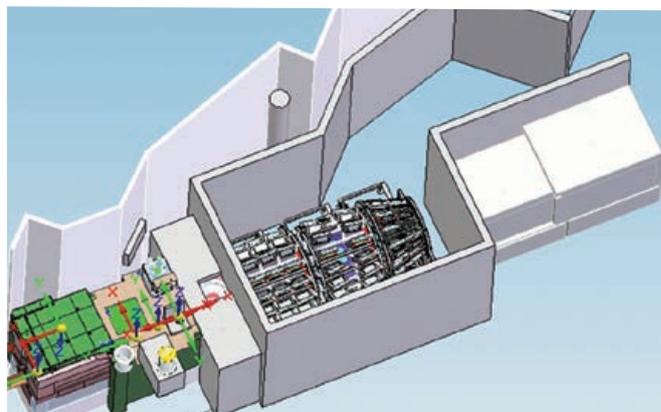
## Tosca+

A next-generation neutron vibrational spectroscopy instrument created through upgrading the existing Tosca spectrometer will provide new capabilities for catalysis and energy materials studies, providing advanced possibilities for industry and the UK Catalysis Hub.



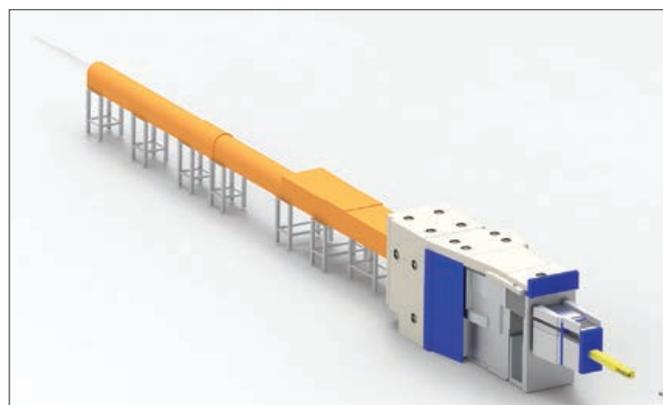
## Sandals-2

A diffractometer for chemical engineering in amorphous and liquid samples providing structural information on complex systems. This upgrade to the Sandals instrument will enable studies of multi-component samples as used in catalysis, drug release, hydrogen storage, oil industry systems, optically activated compounds and polymers.



## Osiris+

Osiris is a high-resolution spectrometer and diffractometer enabling studies of atomic and molecular-level motions across a broad range of applied systems. This upgrade will provide significantly increased neutron flux, advancing studies in areas such as catalysis and energy materials.



## Mushroom

An entirely novel concept with an enhanced flux that is potentially transformative for inelastic neutron scattering studies of materials. Mushroom will enable the use of much smaller samples, or more detailed parametric studies, or new types of sample environment and *in situ* equipment, in areas such as thin magnetic films, thermoelectrics, magneto-resistive materials, ionic conductors, superconductors and battery materials.

## WISH-2

The project is twofold: building a new single crystal and thin film cold neutron diffractometer, WISH-2, with a large continuous detector coverage (approx.  $2.5\pi$ ) and an upgrade to the existing WISH beamline to implement polarised neutron measurement capability.

## Beyond Endeavour

The Endeavour Programme captures our next major instrument projects. But instrument development plans continue well beyond those within Endeavour. New instrument concepts – to replace aging instruments, deliver new science capabilities using the latest instrument technologies, and to ensure the ISIS instrument suite remains world-class – continue to be developed. Further instrument concepts – in addition to those within the Endeavour Programme – are described in this section.

### Sherpa

Sherpa (Spectrometer with High-Energy Resolution and Polarisation Analysis) is a proposed quasielastic neutron spectrometer for development at ISIS. It would use polarisation analysis with backscattering geometry to fill in the high-flux “polarisation gap” in Q,E space between spin-echo, triple-axis and direct geometry spectrometers. Polarisation analysis allows clean separation of the coherent and incoherent scattering contributions. This will be revolutionary in the measurement of diffusion in heterogeneous materials from biology to magnetics and in background removal for confined materials. The preliminary McStas model that views the hydrogen moderator in the Iris position suggests 300 times the current Iris flux (unpolarised) at the detector can be achieved with only slightly reduced resolution. Siting the instrument on the poisoned methane TS2 moderator is also being investigated. This would offer larger energy coverage and higher resolution at the expense of some of the flux increase, although simulations are still preliminary.

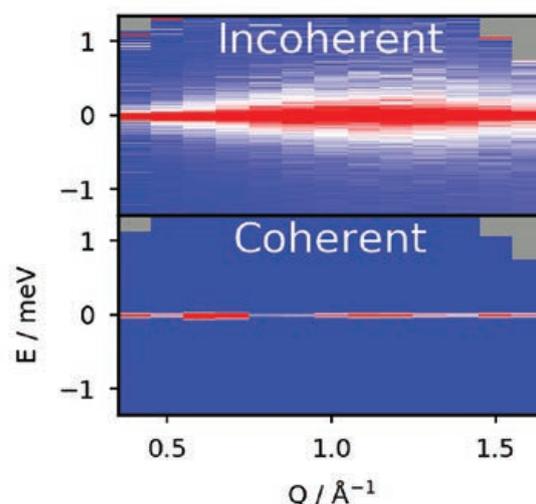
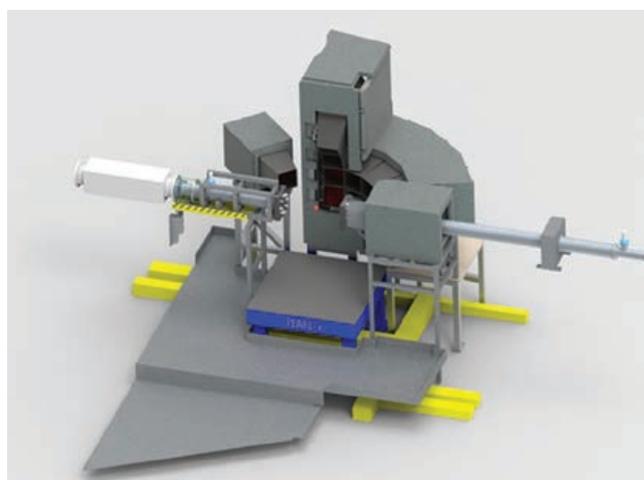


Figure shows excellent separation of coherent Bragg peaks from a zeolite host and incoherent scattering from mobile hydrocarbons using polarisation on LET. Initial calculations show Sherpa producing 130-fold increase in intensity over LET with improved resolution at higher energy transfer.

### Pearl-x

Pearl-x has been designed as a secondary sample-position for the Pearl diffractometer on TS1, taking advantage of the currently unused space in the existing blockhouse, extending ISIS's dedicated high-pressure capabilities. The key advantages of Pearl-x are the modular nature of the sample position itself and the ability to mount equipment from the base rather than from a flange in the instrument. Based on a large optical-table, Pearl-x will be able to accommodate new, larger pieces of sample environment, whilst also enabling the installation of precision alignment stages for more delicate equipment, such as diamond-anvil pressure cells. The detector coverage has been altered, compared with Pearl, to enable multiple different scattering orientations and provide access to higher resolution diffraction data. In addition, the new detectors will be pixelated to improve spatial resolution, enabling

new data correction techniques and providing the future opportunity for basic single-crystal studies at high-pressure.

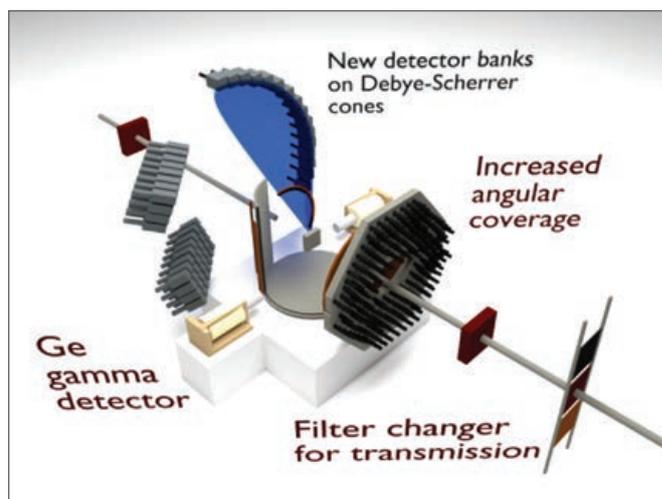


## ETNA – Epithermal and Thermal Neutron Analysis

Vesuvio uses a technique referred to as neutron Compton scattering (NCS), which employs electron-volt (eV) energy (epithermal) neutrons. NCS measures one atom at a time, thereby enabling the study of potentials of mean force and mean force constants of individual atomic species, quantities important in the assessment of local chemical dynamics of condensed matter and molecular systems. At present, detected flux is the main limitation in the technique. A next-generation eV neutron spectrometer ought to combine as many different techniques using thermal and epithermal neutrons as possible alongside NCS to increase the information content of measurements.

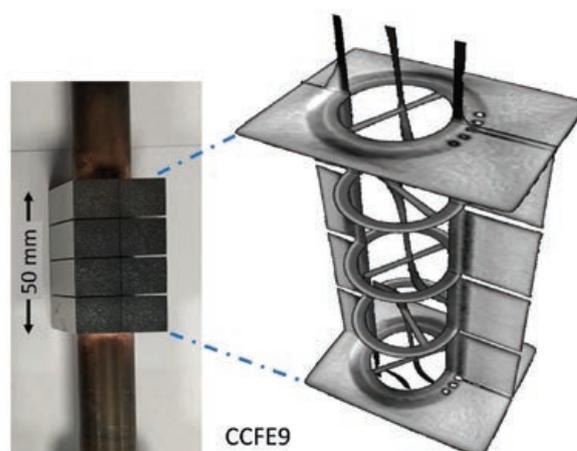
Experience on Vesuvio has led to the idea of a fully-fledged experimental station for Epithermal and Thermal Neutron Analysis, ETNA (see figure). ETNA would involve significant changes to the geometry and detector coverage of forward and backscattering banks compared with Vesuvio. Additionally, ETNA would use multiple resonant foils to simultaneously detect inelastic scattering events with multiple final neutron energies, thereby enhancing count rates further. Independently, energy selection of incident neutrons could be implemented to suppress the thermal region, to discriminate between purely elastic

and inelastic events, or to enhance mass selectivity and element specificity. Additional detector banks orthogonal to the neutron beam could also be employed for elemental analysis across the periodic table. Taking into account all of these factors, ETNA would provide a quantum leap in both capacity and capability compared with Vesuvio, transforming how epithermal neutrons from short-pulse spallation sources are exploited in the years to come.



## New thermal neutron imaging station for energy materials – Energ-I

Neutron imaging techniques are attracting a huge amount of interest in wide-ranging science areas including engineering, applied physics, chemistry, cultural heritage and life sciences. The IMAT imaging station at ISIS covers a number of these applications but favours those requiring cold neutrons. The recent push towards materials studies especially in areas of fusion and nuclear energy as well as battery research requires measuring to greater depths in highly-attenuating materials. Thermal neutrons are more penetrating than cold neutrons and better at providing good imaging contrast for large samples under such conditions. We are developing the concept for a new thermal imaging station at ISIS, Energ-I, which will go a long way to address this gap in the current ISIS imaging capabilities. Energ-I will be designed for white beam tomography with a large field of view and it will include energy-resolved imaging, i.e. capabilities that will be crucial to study energy materials including hydrogen containing materials and radioactive components.



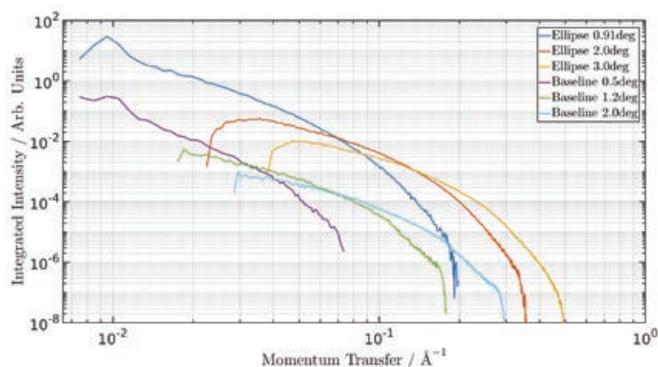
*Fusion energy thermal break component (left) and 3D neutron image of internal tungsten and copper parts (right) (UKAEA). T Minniti et al. Fusion Engineering and Design, Volume 169, 2021, 112661.*

## Future ISIS reflectometer upgrade options

By installing additional neutron optics and updated detector technology, the ISIS reflectometer suite has scope for significant performance increases at relatively low cost. With advances in detector technology, Inter and Surf will be upgraded soon, with up to an order of magnitude improvement in signal to noise anticipated on Inter.

PolRef and OffSpec would also benefit from similar upgrades, but more ambitious options are also being explored. Recent advances at the NIST Centre for Neutron Research with the commissioning of Candor and the future capabilities of the ESS and SNS Second Target Station mean that both instruments will require a significant boost in performance to remain internationally competitive. Simulations of the PolRef guide system have been undertaken to maximise performance for solid-state samples with a surface area of 10x10mm or smaller. By making use of divergent beams in the scattering plane and assuming specular reflection, the figure indicates that gain factors >50 could be possible over the existing

q range. This would also be combined with the capability to measure most of the existing q range at 1 instrument setting ( $\sim 0.91^\circ$ ) further increasing throughput by a factor of  $\sim 1.3$ -1.5.

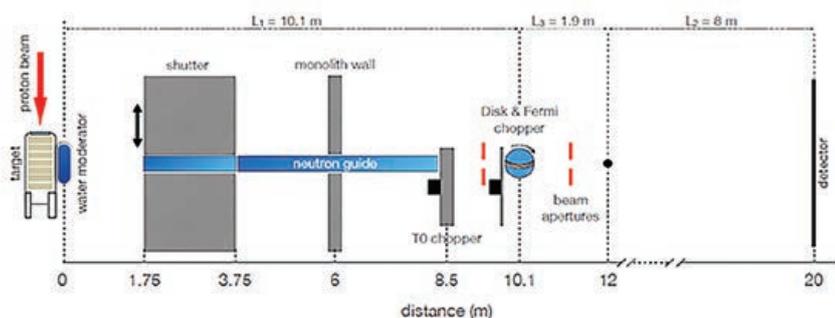


Comparison of the simulated existing (baseline) reflected intensity on PolRef from a 10x10mm silicon-air interface using 3 incident angles (0.5°, 1.2° and 2.0°) with divergent incident beam measurements (ellipse) at angles of 0.91°, 2.0° and 3.0°.

## Brill – a Brillouin neutron spectrometer for TS1

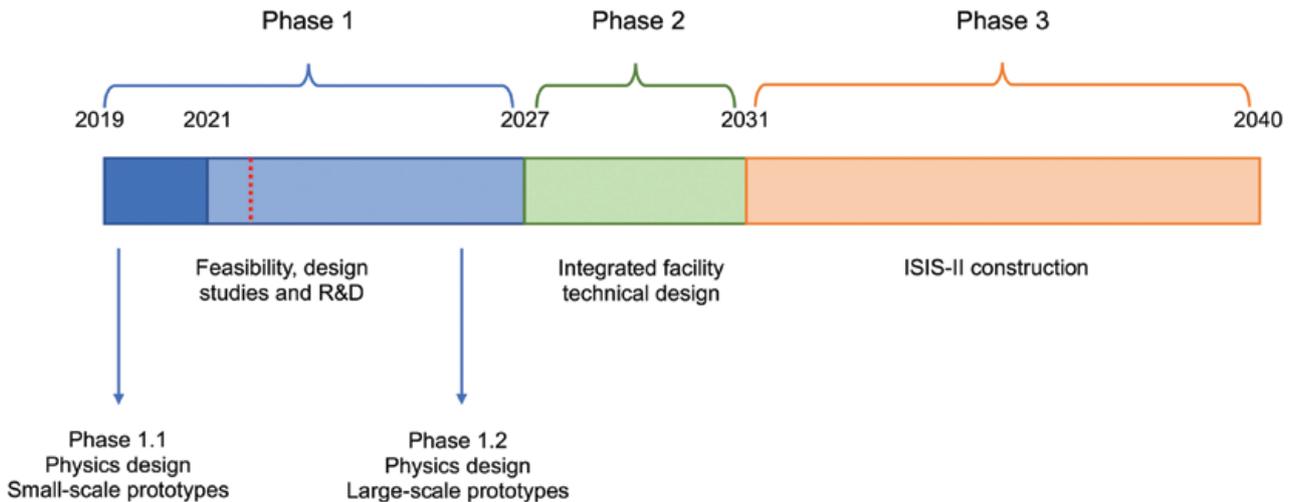
Advances over the last decade in computer simulations have made it possible to routinely calculate the collective excitations from disordered materials. These excitations govern key material parameters as well as giving information on the nature of intermolecular bonding networks. Examples include thermal conductivity, both in crystalline and amorphous materials; sound propagation in nanostructured materials – so-called phononic crystals by analogy to photonic crystals; and phase transitions in liquid crystals. Neutron spectroscopy operating in the

first Brillouin zone (Brillouin Neutron Scattering) can in principle access the relevant excitations and validate such calculations. Unfortunately, kinematic constraints and the low angle background on existing spectrometers around the world makes this impossible in practice without huge flux reductions. Brill is a proposal for a Brillouin spectrometer on TS1 which will address these technical constraints, opening up new science areas, while remaining competitive with the upgraded Maps spectrometer for the science currently covered there.



## ISIS-II

In response to the need for future neutron provision ISIS is developing options to build the UK's next generation neutron and muon facility which will provide a step-change in capability – 'ISIS-II'. Work on ISIS-II is currently being undertaken through the project titled "ISIS-II Feasibility, Design Studies and R&D" which is the first of three primary phases that will follow the schedule below.



The challenge of the initial phase is to optimise economic and science impact, risks, costs, sustainability and timescales over the remaining lifetime of ISIS and the full lifetime of the new facility to provide the conceptual design to be carried forward to Integrated facility technical design.

The project has completed Phase 1.1, which successfully progressed the initial designs for ISIS-II using a modest ISIS-internal budget. The initial stage of Phase 1.2 has now been granted £5.1M dedicated funding from the UKRI Infrastructure Fund for Preliminary Activities, and a further funding for the final stage of Phase 1.2 will need to be bid for in ~2025.

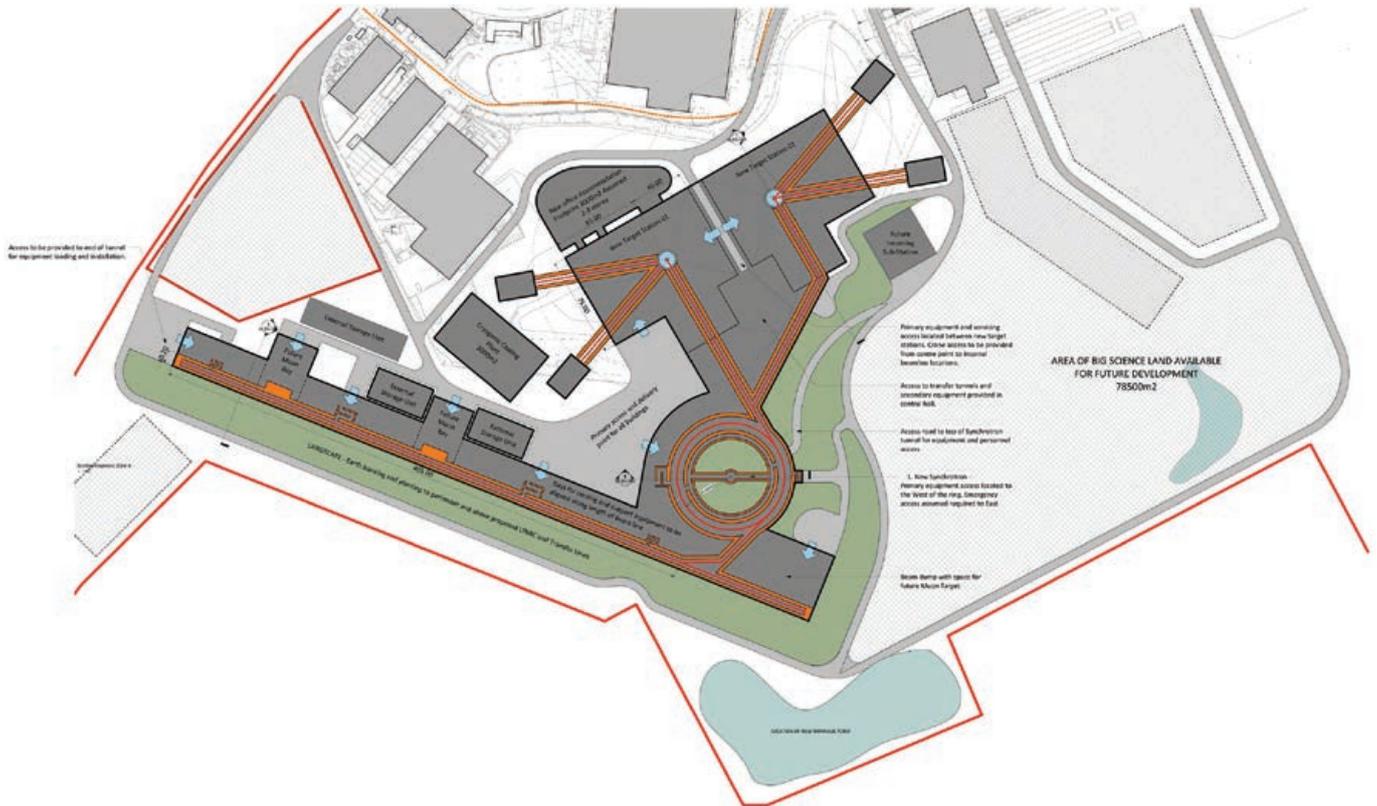
Accelerator and target designs are being progressed alongside facility-wide ISIS-II parameters discussions to establish the overall specification of the new facility.

The favoured option is a new, stand-alone facility, making use of large-science infrastructure already available at Harwell Campus. MW-class is expected, but dependent on target technology, with two target stations from day one.

Accelerator options under consideration are:

- Low energy linac with rapid cycling synchrotron to bunch compress and accelerate up to 1.2 GeV (similar to ISIS and J-PARC).
- Low energy linac with fixed-field alternating-gradient accelerator (FFA) to bunch compress and accelerate up to 1.2 GeV.
- Full energy linac with accumulator ring to bunch compress at 1.2 GeV (similar to SNS).

There has been significant engagement with Harwell Campus Joint Venture to reserve appropriate land for ISIS-II and with a team of architects to look at the footprint of the facility and ensure buildability. In 2040 ISIS may be host to a new facility that could look something like this...



# Partnerships



## National Partnerships

ISIS has an annual call for facility development studentships – joint PhD projects between ISIS scientists and university colleagues. Since 2014 ISIS has co-funded 86 studentships, each of which represents a partnership between ISIS and a university; 13 of these have also been funded jointly with the Diamond Light Source, 3 jointly with the Catalysis Hub based at RAL, and 3 with the Faraday Institution. ISIS also supports a number of

joint appointments with UK universities, including with Royal Holloway (posts in crystal growth and a part-secondment from ISIS to RHUL), Cambridge (molecular science and data engineering), UCL (condensed matter theory), Imperial (accelerator science) and, most recently, Manchester (materials engineering for fusion, in partnership with the Culham Centre for Fusion Energy).



*Facility development students at ISIS.*

## International Partnerships

ISIS is the UK's national neutron and muon source, but it has a very wide international usage, and world-wide collaborations and partnerships. ISIS aims to continually develop its international links, both to support international use of the facility and to provide additional resources for instrument or accelerator projects. In addition, ISIS has a wide variety of partnerships and collaborations within the UK – locally with other STFC facilities and departments, within the wider Harwell Campus and with universities and institutions across the UK.



### Italy

The partnership between ISIS and Italy is one of ISIS's longest standing collaborations. A new six-year agreement was signed between ISIS and the Italian National Research Council (CNR) in Autumn 2021, providing Italian scientists with access to the facility and contributing to instrument developments. The CNR President, Professor Maria Chiara Carrozza, visited ISIS with colleagues in February 2022.



### ILL

In addition to signing a new Memorandum of Understanding (MoU) for collaboration with the CSNS, ISIS also renewed its partnership agreement with the Institut Laue-Langevin (ILL) in Grenoble, France this year. ISIS and ILL collaborate across a range of scientific and technical areas, and the new MoU supports the further development this partnership.



### China Spallation Neutron Source (CSNS)

In June 2022, ISIS and the CSNS signed a new agreement for collaboration in neutron science and technology following an initial MoU signed in 2014. CSNS colleagues are applying for funding from the Chinese Ministry of Science and Technology to support joint working and collaboration with ISIS, and so we anticipate increased collaboration over coming years.



### Sweden

ISIS has a long-standing partnership with Sweden involving support for Swedish researchers to use ISIS, contributions to ISIS instruments, and the funding of collaborative projects between ISIS, Swedish researchers and the ESS. In addition, ISIS is contributing to the construction of the ESS in Sweden in a variety of ways – there are more details on p54.



## Portugal

Portuguese researchers use ISIS for a wide range of science including fundamental and applied magnetic systems, photovoltaics, semiconducting materials, cancer-related studies, framework materials such as zeolites and other investigations; and two recent ISIS Impact Awards have been won by Portuguese scientists. To further develop the use of ISIS by the Portuguese community, ISIS and Portuguese neutron and muon users are planning ways to support further joint working, including the possibility of an agreement with Portuguese science funders.



## India

The use of ISIS by researchers from India has grown significantly over recent years. This has been helped by UK Government Newton funding, and has led to a partnership agreement with the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) for a Dept of Science and Technology (DST) Nanomission project. This agreement supports Indian scientist use of ISIS and provides funds for instrument developments.



## Japan

The RIKEN-RAL Muon Facility at ISIS, constructed by RIKEN (Japan) in the early 1990's, has been the focus for a continuous partnership with Japan for over 30 years. The current agreement includes a continuing user programme for Japanese scientists together with a major refurbishment of the facility – there are more details of this on p53.



## Canada

Canada has a well-developed strategy for neutron scattering which includes partnering with international facilities to ensure its research community has access to the facilities they need. A group of Canadian universities is seeking funding for international partnerships, and ISIS hopes to enter a new agreement with Canadian colleagues over the next year or so to develop Canadian use of the facility together with supporting the Endeavour Programme.



## LENS

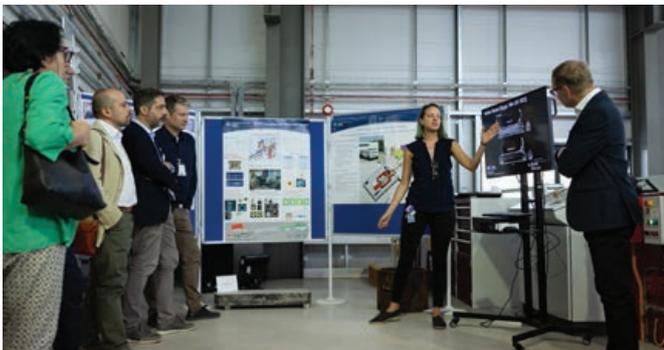
ISIS is a founding member of the League of advanced European Neutron Sources (LENS), and Robert McGreevy, former ISIS Director, is currently the Chair of LENS. As part of LENS, ISIS collaborates with neutron and muon facilities around Europe, including coordinating the LENS contributions to a large Horizon Europe grant which was awarded this year for studies of materials for the circular economy.

## Visitors to ISIS

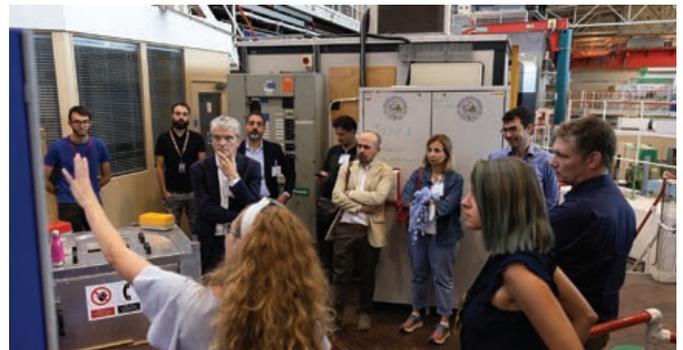
Throughout the year, we have welcomed visitors from government, academia and industry to the facility to meet our staff and discuss future collaborations.



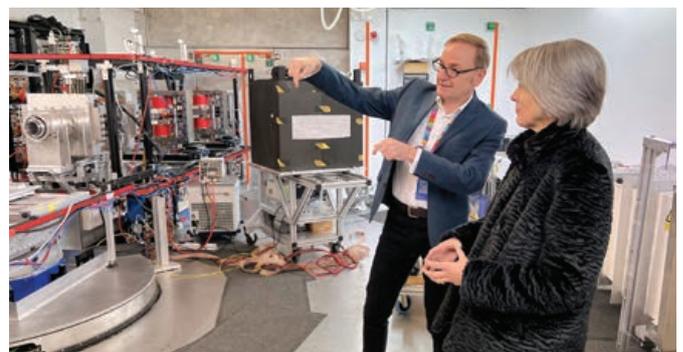
*The Science Minister, George Freeman MP visiting ISIS.*



*Italian Delegation visits ISIS in 2022.*



*David Johnston MP for Wantage with Dr Philip King, ISIS.*



*Dame Ottoline Leyser, CEO of UKRI, with Professor Sean Langridge from ISIS.*



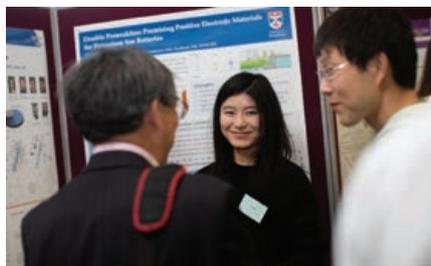
*Sir Andrew Mackenzie, UKRI Chair, with Professor Roger Eccleston in Chiplr (left) and with colleagues next to Zoom and SANS2D (right).*

## User Meetings

This year has seen a return to in-person user meetings, including the Disordered Materials and Theoretical & Experimental Magnetism Meetings.



*ISIS Student Meeting.*



*Neutron and Muon Science and User Meeting.*



*Attendees at the Neutron and Muon Science User Meeting.*

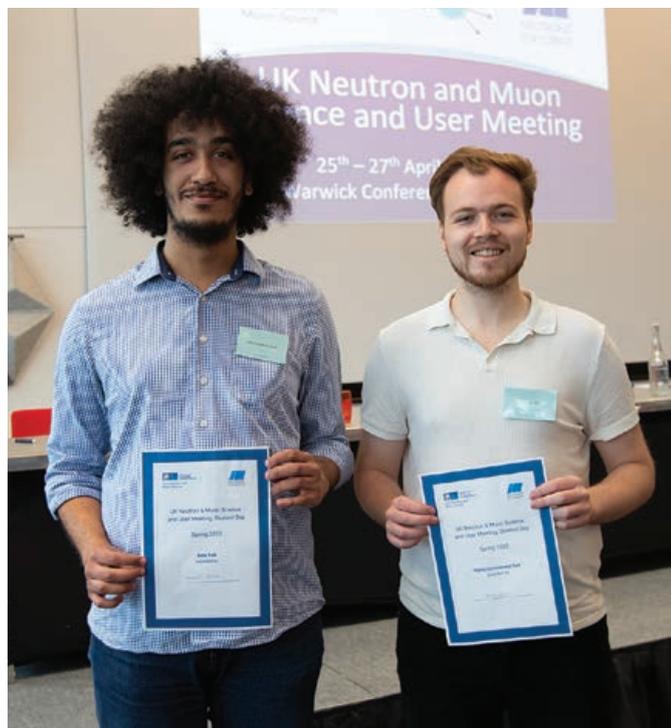


*TEMM2022 at Cosener's House.*



*Disordered Materials group at Cosener's House.*

## Neutron and Muon Science and User Meeting (NMSUM)



The UK Neutron & Muon Science and User Meeting (NMSUM) took place at Warwick University from 25-27 April 2022.

This meeting, jointly organised by the Institute of Physics and Royal Society of Chemistry's Neutron Scattering Group, ISIS and ILL, was a chance for UK users of neutrons and muons to hear about latest science using these techniques, together with facility updates and other news of interest to the community. It took place in the Warwick Conference Centre and attracted over 250 participants including over 90 for the student day.

*Student talk prize winner Mohamed Aoane (left) and Highly Commended speaker George Gill (right).*



*NMSUM attendees.*

## Student Conferences

Every year, ISIS holds two meetings for PhD students who use neutrons and muons in their research: one standalone conference and one as an extra day to the UK neutron and muon science user meeting (NMSUM). These meetings offer a chance for them to present their work in a relaxed environment, as well as meet each other and get new ideas about how to use the range of techniques available at ISIS.

In October, over 60 PhD students come to RAL for the annual ISIS student meeting. Because of the pandemic, the last in-person student meeting had been two years ago. This year we offered a live stream of the talks, as well as attendance at RAL. It was worth waiting for; the standard of the talks was extremely high, and the lively discussions around the posters were great to see.

The second day saw further talk and poster sessions followed by a careers panel featuring previous ISIS PhD students who are now working both inside and out of academia. The students asked lots of great questions.

“

Meeting was organised really well, interesting topics for talks and posters & lovely to see everyone so engaged and interested.

”

“

Great format and it was lovely that it was a student-based meeting, so it felt less intimidating. Also, the careers panel were great, and I'd love to see this continued in future.

”



*Attendees at the ISIS Student Meeting.*

# People



# 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 PhD students. Although in-person work experience placements were cancelled, we still hosted 14 ISIS students as part of the online RAL work experience programme.



**27**  
Graduates



**49**  
Co-sponsored  
PhD students



**2**  
Vacation  
students



**17**  
Apprentice  
placements



**32**  
Undergraduate  
sandwich students

ISIS frequently opens its doors to schools and the general public, receiving thousands of visitors from across the UK who come to explore our cutting-edge science and engineering, meet our staff and hear our stories. Despite the pause of in-person activities in 2021, this year ISIS has reached thousands of school students, teachers and members of the public through our Public Engagement programme. In combination with a return to on-site visits for other groups, ISIS has maintained a high level of engagement with a range of communities.

Total number  
of visitors

**3446**

**2668**

School students, teachers  
and public visitors

**603**

Business and  
government visitors

**175**

Higher  
education

## Robert McGreevy

In 2021, Robert McGreevy retired from his role as ISIS director and, in 2022, was recognised as a Member of the Order of the British Empire (MBE) for his outstanding service to science and his long-term significant impact in the field of neutron scattering.



Robert graduated and received his PhD from Oxford University and was a Royal Society research fellow and lecturer there until 1992. His 'neutron career' began in 1978 as a PhD student at Oxford University, carrying out experiments at the ILL, the Dido and Pluto reactors at Harwell in the UK, before becoming a postdoc and one of the first users of ISIS.

He says, regarding his MBE, "I am delighted to receive this honour, more as a recognition of the many people I have been fortunate enough to work with, rather than the work I have done, both at Harwell and ISIS and around the world."

During the 1980's he developed the Reverse Monte Carlo method for structural modelling, enabling the study of disordered in materials ranging from simple liquids to superconductors. In 1992, Robert moved from Oxford to Sweden, becoming Director of the Studsvik Neutron Research Laboratory between 1994 and 2002, when he moved back to the UK to become a Division Head at ISIS.

After a year at Oak Ridge National Laboratory in the US, he became Director of ISIS in 2012.

Professor Mark Thomson is Executive Chair of the Science and Technology Facilities Council, which funds ISIS. He says, "Congratulations to Robert on this honour recognising his contribution to science over many decades both for STFC and for the wider neutron science research community. Robert's most recent work at STFC, as Director until 2021 of the UK National ISIS Neutron and Muon Source, has helped put in place a legacy of development that will see us through the next decade and will enable many hundreds of research teams to benefit from this world leading facility."

Robert has been actively involved in European collaborations over many years, from being one of the earliest users to benefit from an EU Access programme, and now Chair of the League of advanced European Neutron Sources (LENS), launched in 2019.



Members of the ISIS leadership team with Robert in September 2021.

## Zoë Bowden

2022 saw the retirement of Zoë Bowden, Head of ISIS Operations and Deputy Director, after over forty years with the facility.



Joining the Rutherford Appleton Laboratory in 1979, before the construction of ISIS, Zoë was chosen to work in the fledgling Neutron Beams Research Unit on the equivalent of an apprenticeship scheme, developing instrumentation for the Harwell linear accelerator, which was the first accelerator-driven neutron source in the UK.

During the construction, she was part of the team that installed and commissioned the IRS spectrometer and the LAD diffractometer – both of which have been adapted over the years into instruments that operate today. Her work involved a range of equipment including detectors, choppers, sample environment and data reduction software.

“Because the staff numbers were much lower than they are today, everyone worked on everything,” says Zoë. “I gained a very wide grounding in neutron instrumentation, which has proved hugely beneficial throughout my career.”

As ISIS prepared to go into operation in 1984, Zoë worked on the build of the High Energy Transfer (HET) instrument and became one of the first instrument scientists. As the facility grew and Zoë’s career developed, she held various scientific and technical posts across neutron instrumentation and sample environment, taking on increased responsibilities and becoming group leader of the User Support Group, covering much of the experimental operation.

“I always thought it was really important to recognise the roles of engineers and technicians,” she says. “These groups are vital in enabling the research that the facility does and so, to do the best science, we need not only the best scientists but the best engineers, the best technicians, and the best software developers.”

In 2007, Zoë became Division Head of the newly formed Experimental Operations Division, championing improvements in operational health and safety as well as the expansion of the materials characterisation and deuteration laboratories. She became ISIS Facility Head of Operations and Deputy Director in 2014.

Zoë says, “I feel privileged to have had such a rewarding career at ISIS, being able to use my expertise across the whole of the facility, encouraging best practice, facilitating innovation and working on ways to improve the use of facility and its resources to maximise the science we deliver. I’ve seen a huge amount of change during my career at ISIS – we have constantly striven to maximize our impact and to keep the facility at the forefront of research.”



Zoe working on HET.

## International Women's Day Symposium

On 8-9 March 2022, ISIS celebrated International Women's Day with a symposium on the theme "Equality today for a sustainable future". The theme was inspired by UN Women's observance of the day which recognised that a sustainable future also requires an equal future. The symposium featured sustainability-focused science talks from members of the ISIS user community, including keynotes from Professors Serena Cussen (Sheffield) and Emma Kendrick (Birmingham), student flash presentations, an after-dinner speech from former ISIS Deputy Director Zoe Bowden, and a panel discussion featuring women at various stages of careers in and around neutron science.

For many attendees, it was their first post-Covid event and the atmosphere was one of considerable excitement! The panel discussion was a particular highlight, with lively conversation far outlasting the scheduled timeslot. The event closed with an inspiring talk from STFC's Head of Environmental Sustainability, Jo Colwell.

Organiser, Helen Playford, said; "Overall, I really enjoyed hearing about a wide variety of science and the event was a great opportunity for community building. Planning for next year's International Women's Day is already underway, and we have some exciting things planned... watch this space!"

## Student travel grant supports novel automotive steel study

During 2020 and 2021, the combination of pandemic-related closures and the ISIS long shutdown means that students may have experienced an unusually long time without being able to use ISIS for their research. Because of this, ISIS offered financial support for students travelling to other neutron or muon sources over this period. ISIS has supported over 20 student visits so far.

One recipient of the grant was Anastasia Vrettou, a student at the University of Birmingham. Anastasia's research aims to replicate the conditions experienced by steel components during car manufacture to develop a way to test the resilience of new materials. Current standard testing only applies a stress in one direction, which is very different to what happens in real applications. As part of her research project, Anastasia has designed a special rig that recreates industrial conditions. She takes samples of commercially available advanced steels and investigates their structure before and after they are put under stress.

As they were unable to use ISIS, the team applied for, and were awarded, beamtime on the POLDI instrument at SINQ, The Swiss Spallation Neutron Source based at

the Paul Scherrer Institut. They were able to use the ISIS student travel grant to support their trip. Her supervisor, Dr David Collins adds, "Anastasia started her PhD in 2019 and the first year was very disrupted by the pandemic. The ISIS student travel grant was very welcome, as it leaves funds available for her to present her work at a conference in the future."



*PhD students Anastasia Vrettou (left), Mohammed Said (middle), & James Ball (right) at the POLDI beamline.*

## Inspiring the next generation

Despite the pause of in-person activities in 2021, the development of virtual tours and interactive workshops has allowed ISIS to continue its Public Engagement programme with huge success, inspiring new and diverse audiences during a time of social distancing and remote learning. Our activities span a wide range of themes, to reflect the varied research and work undertaken at ISIS. Long-standing events, such as RAL Stargazing and Particle Physics Masterclass, have been adapted for online delivery, increasing our reach to more remote audiences. New activities linking to global events, such as the UN Climate Change Conference COP26, have inspired and captivated new audiences.

Engaging diverse and under-represented audiences is an important part of our Public Engagement programme and we have significantly increased our engagement with schools from areas of high deprivation. We have continued to create and deliver events highlighting diversity in STEM, linking into campaigns including Black History Month and International Women's Day.

ISIS continues to host work experience students from across the UK, offering unique insights into the facility and our science and engineering. Below is some student feedback on the ISIS work experience webinar. The facility also hosted virtual and in-person events as part of CPD training days for over 50 UK educators.

“

I loved the fact that the tour was 360 and so students can get a real feeling of what it is like to be in the lab.

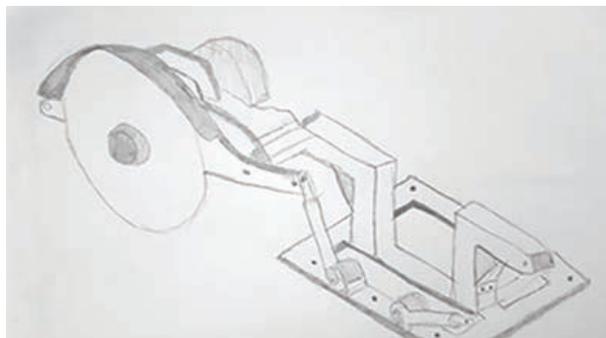
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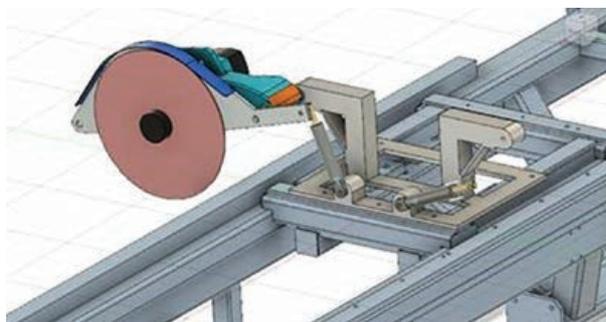
I found the examples of objects that were analysed very interesting, and I found it surprising how much could be interpreted from passing neutrons through an object.

”

This year, ISIS also led in the development of a new STFC initiative, the Engineering Experience Programme, where A-level students from local schools worked with STFC graduates to undertake a real engineering challenge over six months. Working with ISIS Graduates, students from Oxford Spire Academy were tasked with designing a device that could be used on the TS1 target, reflector and moderator assembly to cut up the cantilever beam. The students worked together to create a detailed CAD model and outlined a suitable testing procedure that could be used for the full-scale cutting rig to verify its success.



*Final design sketch.*



*CAD model and assembly of final design.*

We look forward to opening the doors of our experimental halls for in-person events, while continuing to capitalise on the benefits the online activities bring. We now have the opportunity to reshape our activities and programme so that we continue to reach new and diverse audiences, including those who are unable to visit ISIS in-person, to inspire the next generation of scientists and engineers.

## Institute of Physics Technician Team Award

The ISIS Cryogenics Team has earned the 2021 Technician Team Award for providing exceptional ultra-low temperature and high magnetic field technical support, contributing to more than 500 neutron and muon scattering experiments annually.

Team members Richard Down, Jeff Keeping, Chris Lawson, Dave Bunce, Paul Frodsham, Robert Major, Jon Timms, Dale Keeping, Matthew Baston, William Bradbury, Alexander Jones and Mark Devonport are responsible for developing, operating and maintaining the large inventory of cryogenic equipment used by our international community of more than 3,000 academic and industrial researchers. Working closely with researchers, they support more than 500 experiments annually, with over 100 at less than 1 Kelvin.

“

It is a great achievement for the team to be recognised by the Institute of Physics (IOP) with a Technician Team Award; especially when the Technician Commitment has become so prominent within STFC. The Cryogenics Team are extremely happy to have been proposed for this award, in acknowledgement of their valiant efforts over the past years, the visibility the award brings to all technicians in STEM roles can only lead to greater prospects for the future.

**Richard Down, Cryogenics Team Leader**

”



*The IOP technician team award.*

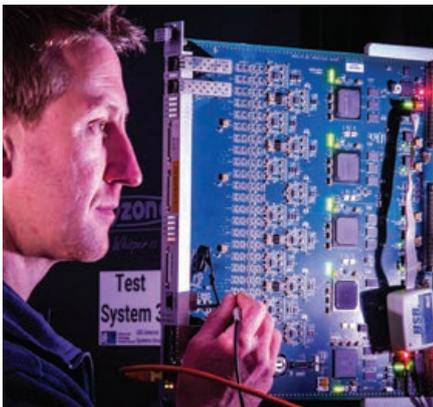
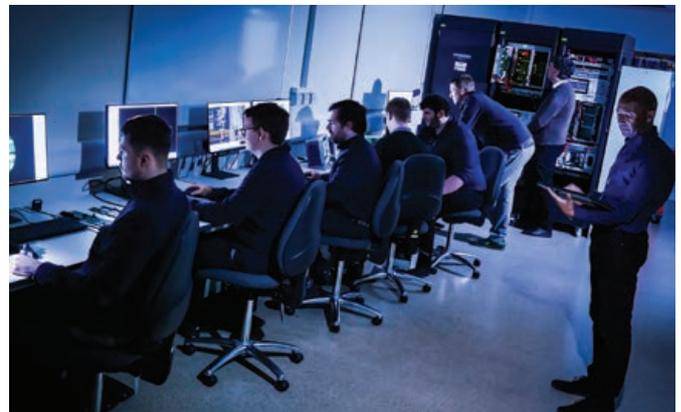
# Technicians Commitment, and committed technicians!

ISIS employs over 100 technicians, covering mechanical, electrical, computing, cryogenic, pressure, chemical, biological, mechatronic, operations and safety, without whom the facility would not be able to function!

Technicians play a key role in ensuring the facility is operating effectively, efficiently, safely and sustainably, but they also support the science directly, providing vital equipment for cutting edge research.

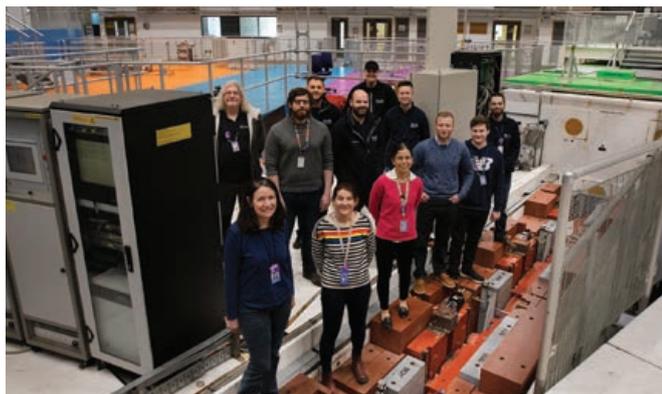
We actively support the Technician Commitment, a university and research institution initiative, which aims to ensure visibility, recognition, career development and sustainability for technicians working in higher education and research, across all disciplines.

Technician **Commitment**



## Developing careers

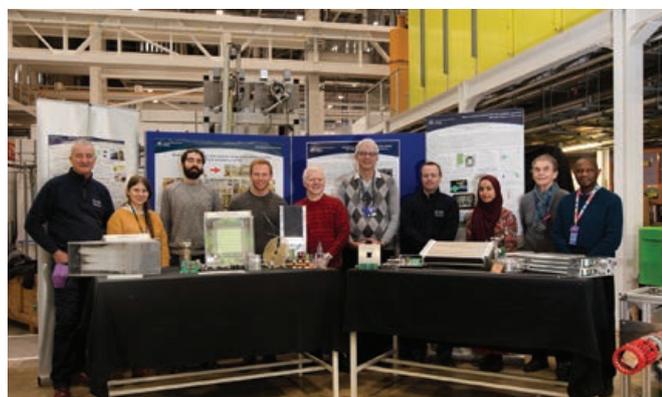
“Through training and coaching I’ve had the privilege of working in every role in the electronic support section over the last 10 years. We’re a close-knit group and we’ve got the responsibility of doing really important work supporting the experiments here at ISIS.” Jamie Nutter, Instrument & User Support Section Leader.



Jamie Nutter (back row, far right) as part of the team installing the new shutters for SANS2D.

## Underpinning innovative engineering

The remit of the ISIS Detector group is responsible for ensuring that our instruments are performing to the best of their ability and developing new detectors to meet the demand of a cutting edge facility. “Our technicians have a vital role in our team, providing expertise as well as a key role in assembling, installing and maintaining our detectors.” – Jeff Sykora, Detector Group.



The ISIS detector group.

## Supporting our science

Dr Mi Tian from the University of Exeter studies new materials for hydrogen storage in clean energy applications at ISIS. She says, “The whole technician team is so good – world class!”.

Valeska Ting, University of Bristol said, “The sample environment team that helped us with our pressure experiments and the cryogenics team with our low temperature experiments were amazing! They were so knowledgeable.”

## On the international stage

Technicians do not just support the work of ISIS. The UK is part of a collaboration working on the construction of the European Spallation Source in Lund, Sweden, and our technicians are applying their knowledge and expertise to make the project a success.



Katie Mordecai and Jacob Simms working on the LOKI instrument for the ESS.

Sarah Langham, ISIS Senior Lab technician, played a crucial role in the design of the ESS user labs. Her extensive experience and knowledge of user requirements helped ensure the in-kind project delivered excellent lab facilities for the future users of the ESS. Sarah is continuing to support the ESS Lab Group, through a series of staff exchanges and work-shadowing activities.



Sarah Langham in the lab at the ESS.

## Richard Waite

Richard joined ISIS's Scientific Computing division after finishing a PhD as part of the ISIS Facility Development Studentship scheme.



“

When I first came to ISIS as a PhD student, I felt very welcomed, despite working across two groups. I think ISIS has a great atmosphere of inclusivity.

”

After studying Physics at Durham University, Richard joined the Centre for Doctoral Training (CDT) in Condensed Matter Physics at the University of Bristol. During his first year, he did a 3-month project with ISIS's Toby Perring modelling the results of inelastic neutron scattering experiments. It was this, combined with work during his master's year on X-ray crystallography, that got him interested in large facilities.

At the end of the first year of the CDT programme, Richard applied for an ISIS facility development scheme project with Russell Ewings, which he began in 2016. His initial project aim was to develop a pressure cell for use during inelastic neutron scattering experiments.

“But things don't always go to plan!” Richard explains. “The cell was actually better suited to diffraction experiments, so I ended up working closely with the team on the WISH beamline. This meant I was able to get to know more people at ISIS, across a wider range of science areas. When I first came to ISIS as a PhD student, I felt very welcomed, despite working across two groups. I think ISIS has a great atmosphere of inclusivity. It was a lovely place to come and spend time.”

Although Richard was mostly based in Bristol, he made frequent trips to ISIS, and took part in the student conferences and user meetings, where he was able to present his work. The pressure cell that he developed is in use as part of a collaboration with ISIS's Fabio Orlandi, as well as attracting interest from external users. “I found the goal of producing some deliverable for the facility motivating and gave the project a good sense of direction,” he says.

“During one visit for beamtime, I saw a poster in the beamline hutch that said ‘Mantid needs you!’, advertising roles in the computing division at ISIS,” says Richard. “I spoke to Lamar, who leads the group, and he explained that they were looking to recruit scientists into the group without the need for them to have had specific programming experience.”

Having done some coding during the data analysis as part of his PhD and found it interesting, he applied for the role and started as a junior software scientist in 2019. “I hadn't finished writing my thesis when I started, and that's definitely not something I would recommend!”

Richard settled into the role and after completing an Open University course on Software Engineering was promoted to software scientist in 2020. He mainly works on the Mantid data analysis framework but has also recently started working on the SpinW software, which simulates experimental results for users to analyse their data.

Richard adds, “I feel like I can make a bigger contribution in this role instead of focusing on a narrow area in my own research, as I can write software that improves the work done by academics across a range of fields.”

But that's not to say his academic career is over. He has also done some experiments as a user since joining as a software scientist and has felt supported by his team to continue his own science programme.

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# Theses 2021

Alexander Armstrong. Adsorption of organic friction modifiers at static and sheared interfaces, University of Cambridge, 2021

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Joe Blake. Magnetic Properties from Density-Functional Theory Calculations, Royal Holloway University of London, 2021

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Kamil Domosud. First Principles Modelling of Half Heusler Alloys, Royal Holloway University of London, 2021

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Nicolás Flores-González. Mechanochemical synthesis of ternary lithium halides and their evaluation as solid-state electrolytes: insight into the structure-property relationship, University of Glasgow, 2021

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William Griggs. Disorder- and strain- mediated magnetic phase modifications in FeRh thin films, University of Manchester, 2021

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Alexander Paul Hawkins. The application of neutron scattering to investigate hydrocarbon conversion over zeolite catalysts, University of Glasgow, 2021

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Nitesh Raj Jaladurgam. Deformation mechanisms and load distribution in multi-phase engineering materials, Chalmers University of Technology, Sweden, 2021

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Harry Lane. From local degrees of freedom to correlated states in anisotropic 3d transition metal compounds, University of Edinburgh, 2022

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Emilio Macaluso. From Data Storage to Quantum Computing: a Combined Theoretical and Experimental Study of Molecular Nanomagnets for Information Technologies, University of Parma, 2021

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Alexandra Martin. Anionic Phospholipid Variety: A Physicochemical Study of Model Mammalian and Bacterial Cell Membranes, University of Birmingham, 2021

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Innes McClelland. Towards Operando Measurements of Li<sup>+</sup> Diffusion in Batteries Using Muon Spectroscopy, University of Sheffield, 2021

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Kerrie Morrison. Polymer stabilised phospholipid nanodiscs – Protein: polymer interactions, University of Bath, 2021

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Johannes Nicol. Effect of Prior Plastic Strain on the High Temperature Creep Deformation and Damage Response of Type 316H Stainless Steel, The Open University, 2022

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Yevhen Onykienko. Frustrated and Noncollinear Magnetism studied by Neutron Scattering Techniques, TU Dresden, 2021

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Riccardo Rossini. Multidisciplinary protocol in the study of meteorites:  $\gamma$ -ray spectroscopy and neutron techniques combined with  $\mu$ -Raman and SEM-EDS, University of Milano-Bicocca, 2021

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Zifan Wang. Influence of Processing Methods on Microstructure and Multiscale Functional Properties of Nitinol, University of Oxford, 2021

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Tatchamapan Yoskamtorn. Structural and dynamic studies of Zr-based metal-organic frameworks toward external stimuli, University of Oxford, 2021

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Andrea Zachariou. Diffusion, reactivity and structural change in microporous materials, University of Glasgow, 2021

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*Attendees at NMSUM 2022*





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