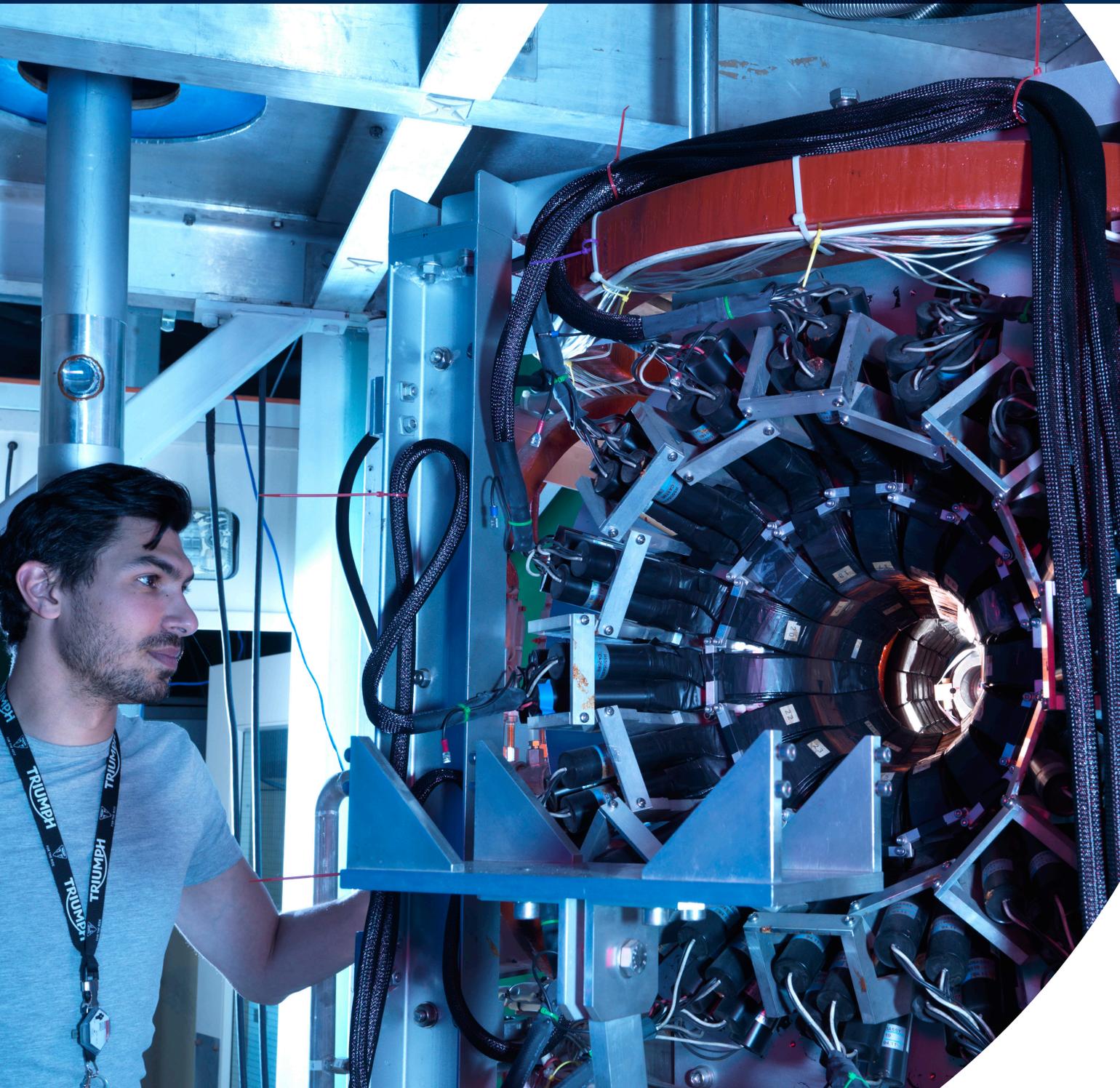




Science & Technology
Facilities Council

UK Research
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ISIS Neutron and Muon Source Annual Review 2018



ISIS Neutron and Muon Source Annual Review 2018 was produced for the ISIS Facility, STFC Rutherford Appleton Laboratory, Harwell Oxford, Didcot, Oxfordshire, OX11 0QX, UK

ISIS Director, Prof Robert McGreevy	01235 445599
User Office	01235 445592
ISIS Facility Web pages	http://www.isis.stfc.ac.uk

ISIS production team: Andrew Collins, Emma Cooper, Sara Fletcher, Poppy Holford, and Rachel Reeves

Design and layout: Andrew Collins and Poppy Holford

December 2018

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RAL-TR-2018-013

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Contents

Foreword	3
Overview	4
Inaugural Impact Awards	10
Science at ISIS	12
Industrial Science	14
Science Highlights	18
International Collaborations	42
Technology	44
Major Projects	46
Instrument Update	48
Accelerators and Targets	50
Computing	53
Skills	55
Inspiring the next generation	57
Developing the student community	59
Developing the neutron community	61
Developing our people	63
Publications	67
Theses	94

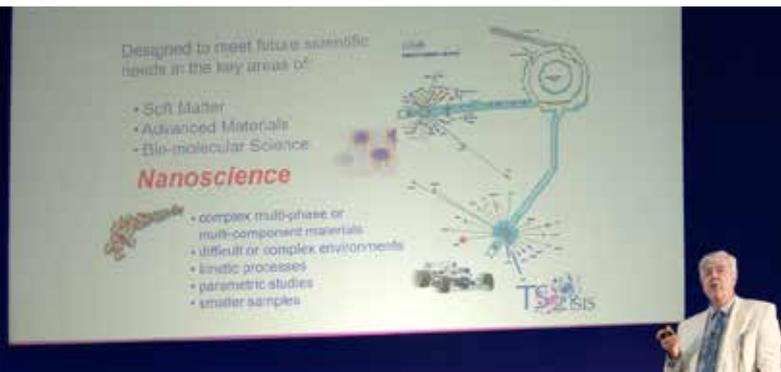


Professor Ashutosh Sharma, Secretary, Department of Science and Technology, DST, Government of India, visited ISIS on the 21st April 2018. Left to right: Professor Sean Langridge, Dr Andrew Taylor, Professor Ashutosh Sharma and Dr S K Varshney, High Commission of India, London, in front of the ZOOM instrument

“It’s fantastic to see the power of neutrons and muons working together for materials, engineering and a whole lot of other things for society. I am very happy to see participation of India’s scientific community in the facility of ZOOM in particular.” – Prof Sharma, 21 April 2018



A delegation from Sweden’s Council for Research Infrastructures visited ISIS on the 5th September 2018 to celebrate 30 years of collaboration with Sweden.



Dr Andrew Taylor was one of several ISIS presenters at an event celebrating the 10th anniversary of first neutrons for Target Station 2 on 18th May 2018

Foreword

Welcome to the ISIS Neutron and Muon Source Review for 2018!

By the time the foreword to the 2019 ISIS Annual Review is written we face the prospect of the UK no longer being part of the European Union, so it is almost impossible not to reflect on the major benefits that EU collaborations have brought us. ISIS has had long and successful bilateral partnerships with several European countries – for example, this year we celebrated 30 years since the first agreement with Sweden – and a long history of participation in EU projects.

The EU Framework Programmes (FPs) for Research and Technical Development, of which Horizon 2020 is the latest incarnation, have funded international projects since 1984. Construction of the muon beamlines, together with some user access and training, was supported by the EU in FP2 in the late 1980s, so it is sometimes still referred to as the European muon facility. In FP3 the first EU Access programme for ISIS neutrons started, and was then supplemented in FP4 by a new muon programme. In FP6 ISIS coordinated the first joint European neutron and muon programme – NMI3 – covering access, technical development and networking. We also coordinated the I3 Network that connected all of the research infrastructure collaborations. A third FP6 project actually provided a significant amount of funding to support the construction of instruments on TS2.

Although EU programmes can reasonably be criticised for being very bureaucratic they have provided an immensely valuable framework for collaboration where the gain has easily outweighed the pain. The very first EU access programme was a pilot project at the DR3 reactor in Denmark in FP2, so neutrons were one of the early adopters - and I was one of the very first beneficiaries! Over the next 20 years these programmes enormously broadened the European user community. The neutron Round Table, supporting inter-facility networking, started in FP3. It was shortly followed by the formation of the European Neutron Scattering Association and then the International Society for Muon Spectroscopy. In all of these activities European neutron and muon facilities and users, have been early initiators of collaborative opportunities. ISIS has fully played its part. I sincerely hope that the UK will retain the possibility of being part of EU science programmes after Brexit. ISIS will survive without our EU friends and collaborators, but it will be diminished.

Reflection over. The rest of this ISIS Annual Review is as usual packed with examples of excellent science and technology, and of course collaboration.

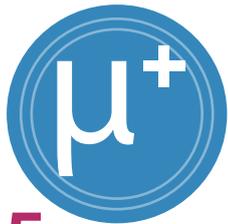
Robert McGreevy, Director of the ISIS Neutron and Muon Source



Members of the ISIS muon group. In 2017 an international review of the muon instruments at ISIS says the facility - comprised of 7 muon experimental areas - is the "most powerful pulsed muon source in the world."

ISIS hosted the Polarised Neutrons for Condensed Matter Investigations (PNCMI) conference, held at Milton Hill House in Oxfordshire from 3 - 6 July 2018

The ISIS Neutron and Muon Source



5 Muon instruments



27 Neutron instruments



588 PhD students visited as users



1085 proposals received from **32** countries

2512 user visits

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

We are part of the global research structure, providing tools for over 2,000 scientists a year to use our suite of 32 instruments.

Our science spans a wide range of disciplines, from magnetism to cultural heritage, engineering to food science, chemistry to environmental science.

We contribute to inspiring the next generation of scientists by welcoming over 1900 school pupils, teachers and general public to the facility as part of our public engagement programme.



500 Journal and conference papers



264 Xpress proposals



142 remote users



4011 Visitors including 1907 school pupils and public

31% new users



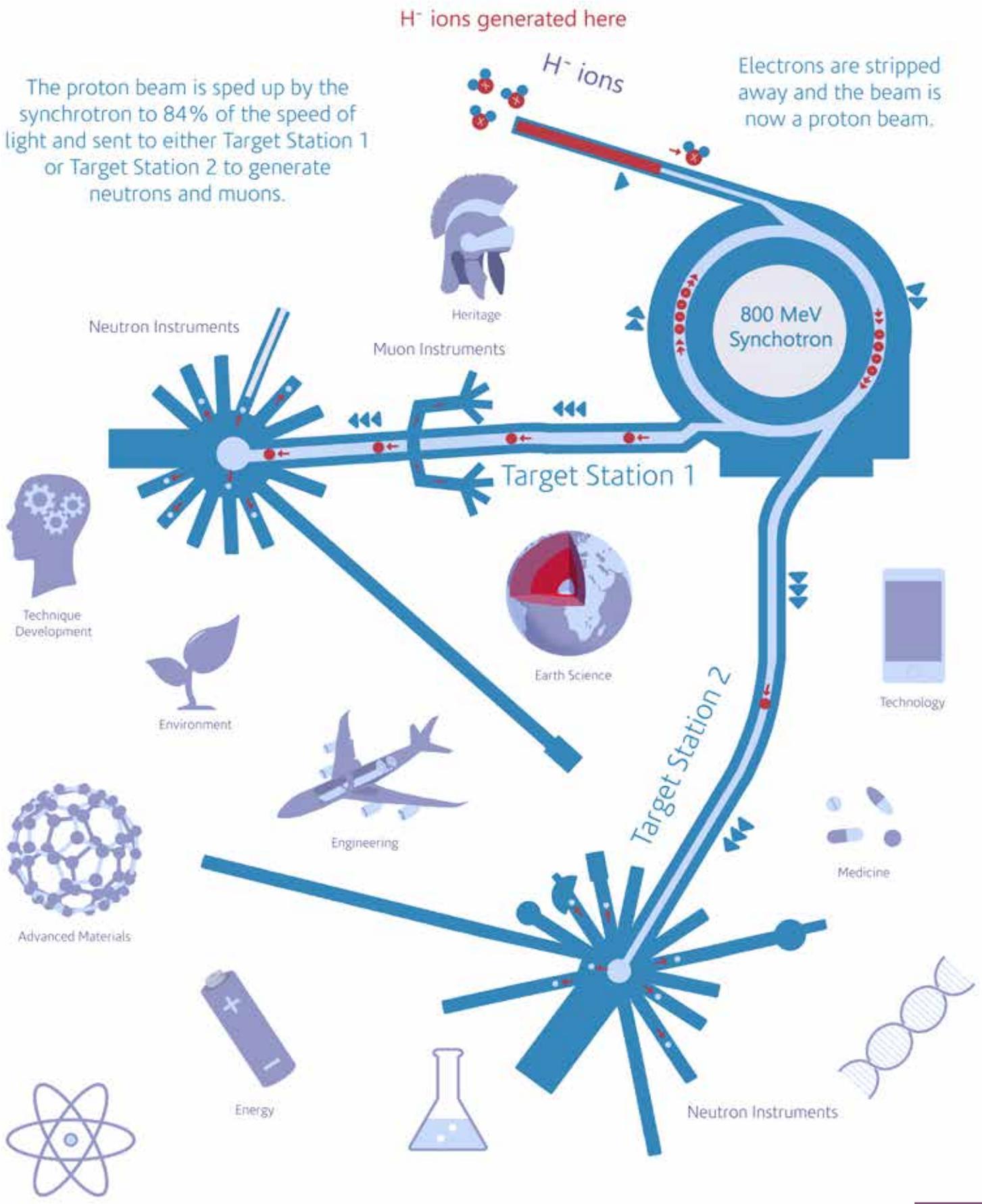
60 Companies

involved in experiments including healthcare, energy, automotive and chemical engineering

H⁻ ions generated here

The proton beam is sped up by the synchrotron to 84% of the speed of light and sent to either Target Station 1 or Target Station 2 to generate neutrons and muons.

Electrons are stripped away and the beam is now a proton beam.



Celebrating 10 years of TS2, solving

On the 3rd August 2018 ISIS celebrated ten years since the first neutrons were detected in the INTER beamline, the first instrument to be completed as part of the Second Target Station (TS2) project.

The decision that ISIS was to be expanded through the building of a Second Target Station was announced back in April 2003 by the then Science Minister, Lord Sainsbury. Starting with the commissioning of seven instruments, the second phase of the project has now increased the TS2 instrument number to eleven. Built with the intention of expanding research capabilities in the areas of soft matter, advanced materials and bio-science, TS2 instruments have been used to tackle some of the greatest challenges of the 21st century.

Advanced materials

Advanced materials capitalise on our knowledge of how the atomic scale structure of a material is linked to its properties on the macroscopic scale. This allows us to fine-tune existing materials to maximise performance and to design new materials with specific properties in novel applications.

- High temperature superconductors could dramatically improve efficiency in power transfer. However, conventional superconductors can currently only perform at temperatures below 30 K. Research on WISH has been used to study unconventional superconductors with the potential for much higher temperatures.
- NIMROD and SANDALS have been used to study Deep Eutectic Solvents (DEEs) to aid the synthesis of nanostructured ceria, a technologically-important material, used in catalysis, emissions control and solid oxide fuel cells.
- WISH and TOSCA have been used to study NOTT-300, a new type of porous material called a Metal Organic Framework, with potential to store CO₂, and take us a step closer to a low-carbon economy.



Target Station 2

21st century challenges!

Healthcare – tackling cancer and antibiotic resistance

One of the initial aims of TS2 was to allow new areas of research to flourish, particularly within the fields of soft matter and bioscience. Over the past ten years, scientists from all over the world have been coming to ISIS to study the structure and dynamics of complex biological systems for a multitude of healthcare applications.

- In 2015, researchers from ISIS and Newcastle University created the first working model of the outer membrane of the bacterium *Escherichia coli* (E.coli). The synthetic model was constructed at ISIS and studied using POLREF.
- This year the team used the same model to study Polymyxin B, a last resort antibiotic that interacts with the outer membrane of Gram-negative bacteria on INTER.
- Research completed using our SANS2D instrument studied whether selective kinds of drug-bearing nanotubes, like cyclic peptide-polymers, can be used in anti-cancer therapy.
- Scientists from Birbeck College, London used INTER to study how ozone attacks molecules in our lungs, exacerbating asthma symptoms.

Food security

One of the biggest challenges of the 21st century is ensuring that we have enough safe, nutritious food to feed seven billion people, in a sustainable way. As the world only has a limited number of resources, scientists are looking at new, inventive ways of increasing crop yields and improving the efficiency of agriculture.

- INTER has been used to investigate how the fine-tuning of pesticide formulations could further increase crop yields.
- In an initial proof-of-concept experiment, a team from the University of Greenwich used the SANS2D and LOQ to characterise a new oral vaccine delivery system for chickens, providing an alternative to conventional vaccination methods, which are often labour-intensive, costly and time-consuming.
- Combined data from INTER instrument and X-rays from Diamond Light Source have been used to gain a clearer picture of water and mineral distribution in soil and plants. These two imaging techniques can be applied to the study of all sorts of crops, from rice to maize to wheat.



Cleaner, greener energy

The need for sustainable green energy is a global problem. TS2 instruments are being used to test and develop new technologies that will help the world in its mission to go green.

- Using LARMOR, a team from Sheffield were able to provide important insights into how nanoscale solar cell films could be manufactured using high-volume printing, a much cheaper and simpler option than using current fabrication methods.
- Scientists from the Open University and EDF Energy used SANS2D to gain a greater understanding of how cracks propagate in the graphite shielding of their Advanced Gas Cooler Reactors to improve how welds are assessed in these safety critical systems and determine whether reactor lifetimes can be extended.
- Thermoelectric devices are currently used in space craft to produce power over decades without maintenance. Modest improvements to their efficiency would open up numerous applications on Earth, harvesting waste heat in car exhausts or power stations. Recent research used LET to investigate Cu₂Se, one of the best current thermoelectric materials, to see if it can live up to its promise.

Safe, sustainable transport

In 2011, ISIS launched the second phase of the TS2 expansion project (phase II) to increase the total instrument number from seven to eleven. As part of this second-phase instrument suite, CHIPIR was built to facilitate fast neutron testing for the semiconductor industry and has recently started its commercial testing programme.

- In 2018 scientists from Brazil, working with NVidia and other semiconductor companies, have been using CHIPIR to test whether off-the-shelf electronics meet the strict standards required for use in the automotive industry.
- One of the applications of such state-of-the-art technology is within the transport sector, most notably for the safe testing of aircraft and automobile electronics.
- Another instrument, OFFSPEC, has been used to study an extremely sensitive hydrogen detector capable of detecting gas leaks, helping ensure the quality and safety of hydrogen sensors, taking us one step closer towards a hydrogen economy

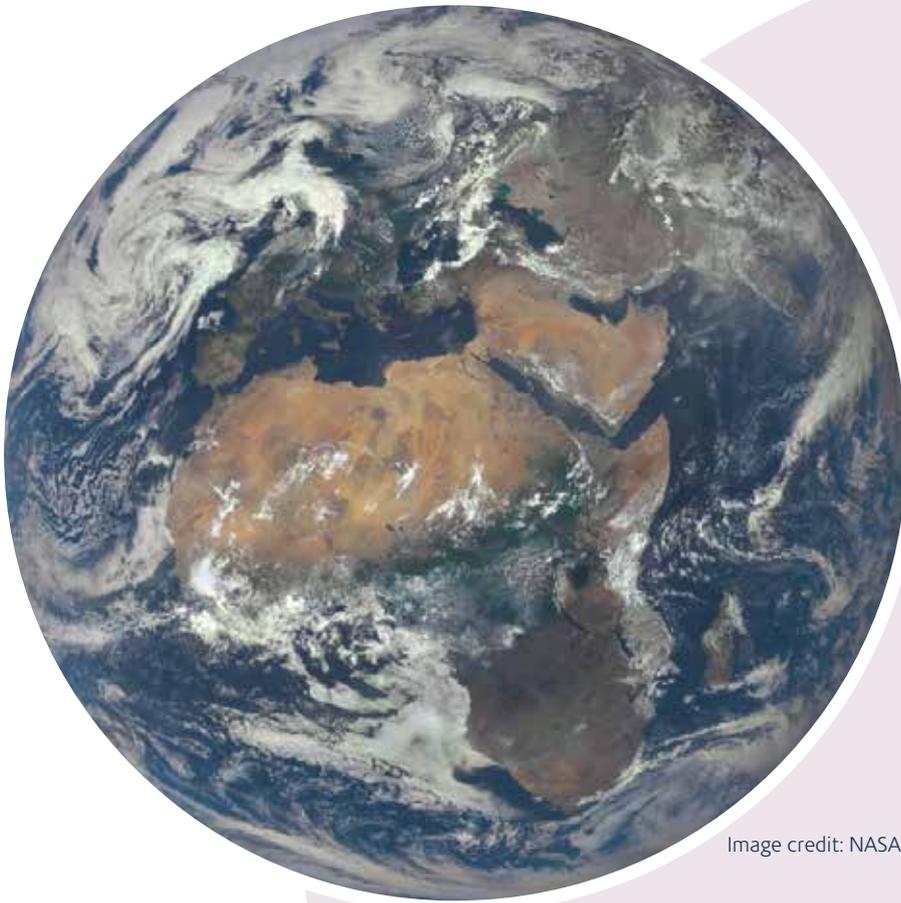


Image credit: NASA

Protecting our heritage

TS2 instruments at the ISIS Neutron and Muon Source have not just been used to look forward; they have also been used to uncover the secrets of our past. Over the last decade, TS2 has allowed scientists to use cutting-edge modern neutron techniques to study ancient artefacts.

- IMAT has been used to non-invasively investigate the content of two sealed from the 3000 year old tomb of 'Kha and Merit'. The team could determine the content of two sealed vases without having to break into them, providing details of the inner morphology, structure and elemental composition of both vases and helping shed light on the mystery of the Seven Sacred Oils of Ancient Egypt.
- Exploring how the millimetre thick wood was used to construct Amati violins, and how small details of the instrument's shape influence sound production.
- Closer to home, IMAT was recently used to study the iconic "Sheldonian heads" that surround Oxford's famous Sheldonian Theatre, to determine why the second generation of sculptures decayed much quicker than the first.



“By utilizing the unique capabilities of the new neutron imaging instrument IMAT and the consolidated capabilities of ENGIN-X we were able to non-invasively study these precious artefacts. The combined information from neutron imaging, diffraction and PGAA techniques have allowed us to shed light on the halo of mystery around the Seven Sacred Oils of Ancient Egypt.” – Dr Triestino Minniti, IMAT instrument scientist

The Inaugural ISIS Im

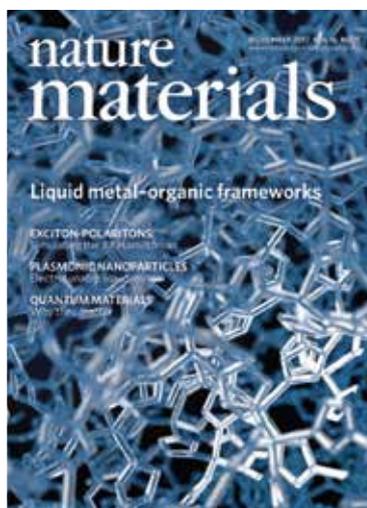
This year saw the introduction of the ISIS Impact awards for facility users, celebrating the scientific, society, and economic impact generated by the user community. These three separate awards recognised the diverse ways neutrons and muon research can advance knowledge, improve quality of life and impact on the economy. The three worthy winners received a trophy, an invitation to present at the Neutron and Muon Science and User Meeting and a detailed case study on their research.

Scientific Impact Award: Dr Thomas Bennett, University of Cambridge

Metal-organic frameworks (MOFs) are a highly topical class of nanoporous materials containing inorganic nodes linked by organic ligands. Over 60,000 crystalline structures exist to date, finding commercial uses in a diverse array of applications such as fruit packaging, harmful gas storage and in vehicular H₂ storage.

The major benefit of this research was the elucidation of a structure of a melt-quenched metal-organic framework glass – the first example of the new hybrid glass family. Room temperature neutron data were collected and combined with that from I15-1 (XPDF), to aid in producing an atomic configuration for the glass via reverse Monte Carlo modelling. This model was then used with high temperature synchrotron data to produce an atomic configuration for the MOF in the liquid state.

The work featured on the front cover of Nature Materials, and was highlighted in both the same journal and also in Nature Reviews Materials. It was number 1 in the ISIS Neutron and Muon Source's top 10 most-discussed journal articles of 2017, and also featured in C&EN and Chemistry World. The group's wider research programme on amorphous MOFs has led to over 40 publications from this group.



Reprinted by permission from Springer Nature: Cover, [Nature Materials, Liquid Metal Organic Framework, Romain Gaillac, Pluton Pullumbi, Kevin A. Beyer, Karena W. Chapman, David A. Keen et al.], (2017)



Impact Awards

Society Impact Award: Dr Alan Williams, the Wallace Collection

The winners of the ISIS Society Impact Award demonstrated the value of neutron techniques for the non-invasive study of irreplaceable historical objects; and some of the most important objects in English history may now be candidates for analysis at ISIS.

The Wallace Collection has the largest collection of princely European armour in London, and one of the finest collections of Indo-Persian armour outside the subcontinent. Researchers have undertaken a program of analysis of these arms and armour for a number of years, and have shown neutron techniques to be particularly valuable analytical methods for museum objects since they are entirely non-invasive.

In 2018 the Dean and Chapter of Canterbury Cathedral agreed to allow the helmet of the Black Prince (d 1376) to be taken down from where it hangs over his tomb in Canterbury Cathedral and brought to ISIS Neutron and Muon Source for examination. This is probably the oldest helmet in England with a known owner.

Researchers used neutron diffraction on the INES instrument to analyse the helm, and showed that its three plates are made of similar low-carbon steels, with traces of stress in the front plate. This is consistent with the helm being a local product rather than an import. The stress in the front plate evidently resulted from being struck, and subsequently straightened out, indicating that the helm was probably worn by the Black Prince in battle.

The outcomes of these studies will be vital importance in making decisions on the ethical conservation and restoration of the Arms & Armour collection at the Wallace Collection, and will influence future decisions about other historical collections in the UK and beyond.

David Edge from the Wallace Collection holding the helmet.

Economic Impact Award: Dr. Andrea Lazzarini from the University of Oslo

The winners of the ISIS Economic Impact Award used neutrons to gain a greater understanding of activated carbons that will inform future product developments for their industrial partner Chimet S.p.A.

Activated carbons are widely used in industrial catalysis, usually employed as a support for nanoparticle-based catalysts. Heterogeneous catalysts are manufactured by depositing a dispersed active phase (in the form of isolated ions or nanoparticles) on a high-surface-area support, which needs to be cheap, inert and stable.

Despite their widespread use, the way in which activated carbons interact with the active phase of the catalyst and/or with the molecules involved in the reaction is still far from understood. This is mainly due to the strong light-absorbing nature of activated carbons, which makes their investigation with traditional spectroscopic techniques extremely difficult.

Thanks to neutron spectroscopy and a multi-technique approach, researchers were able to discriminate the type and the behaviour of the different species present on the surface of the catalyst, and to describe how they influence the activity and selectivity of different hydrogenation processes. The use of inelastic neutron scattering was essential for investigating the state of the hydrogen-rich surface of the support, which interacts with the active phase and reaction's substrate.

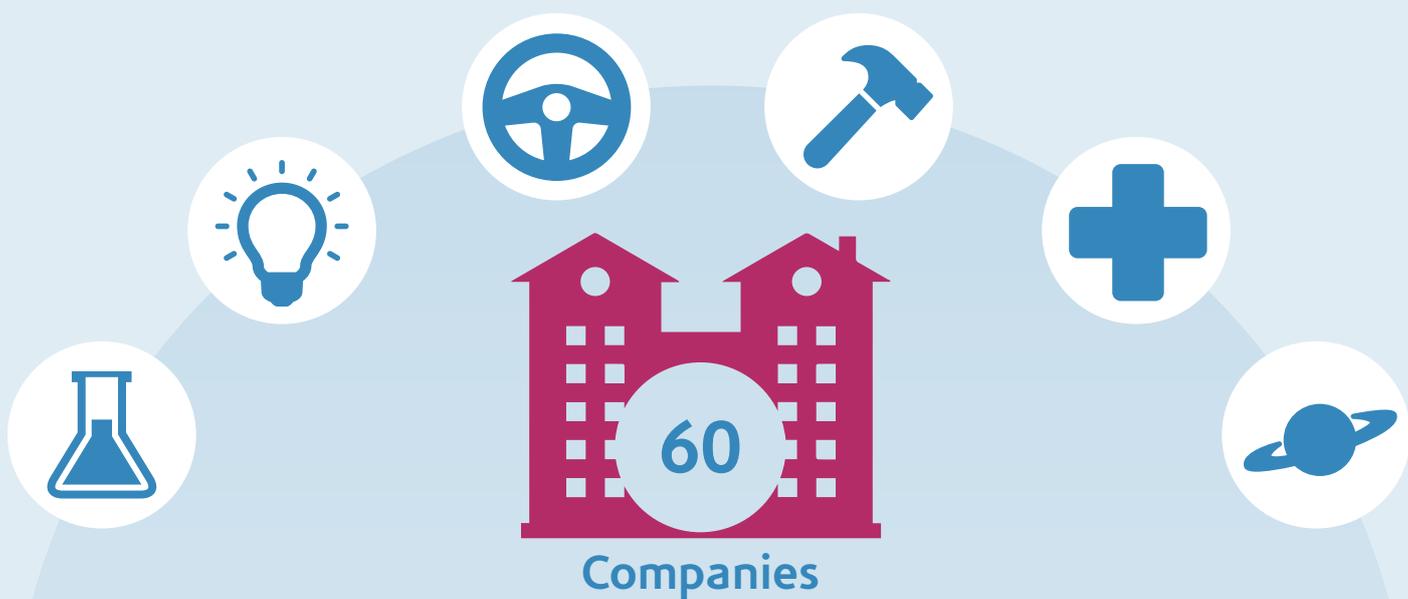
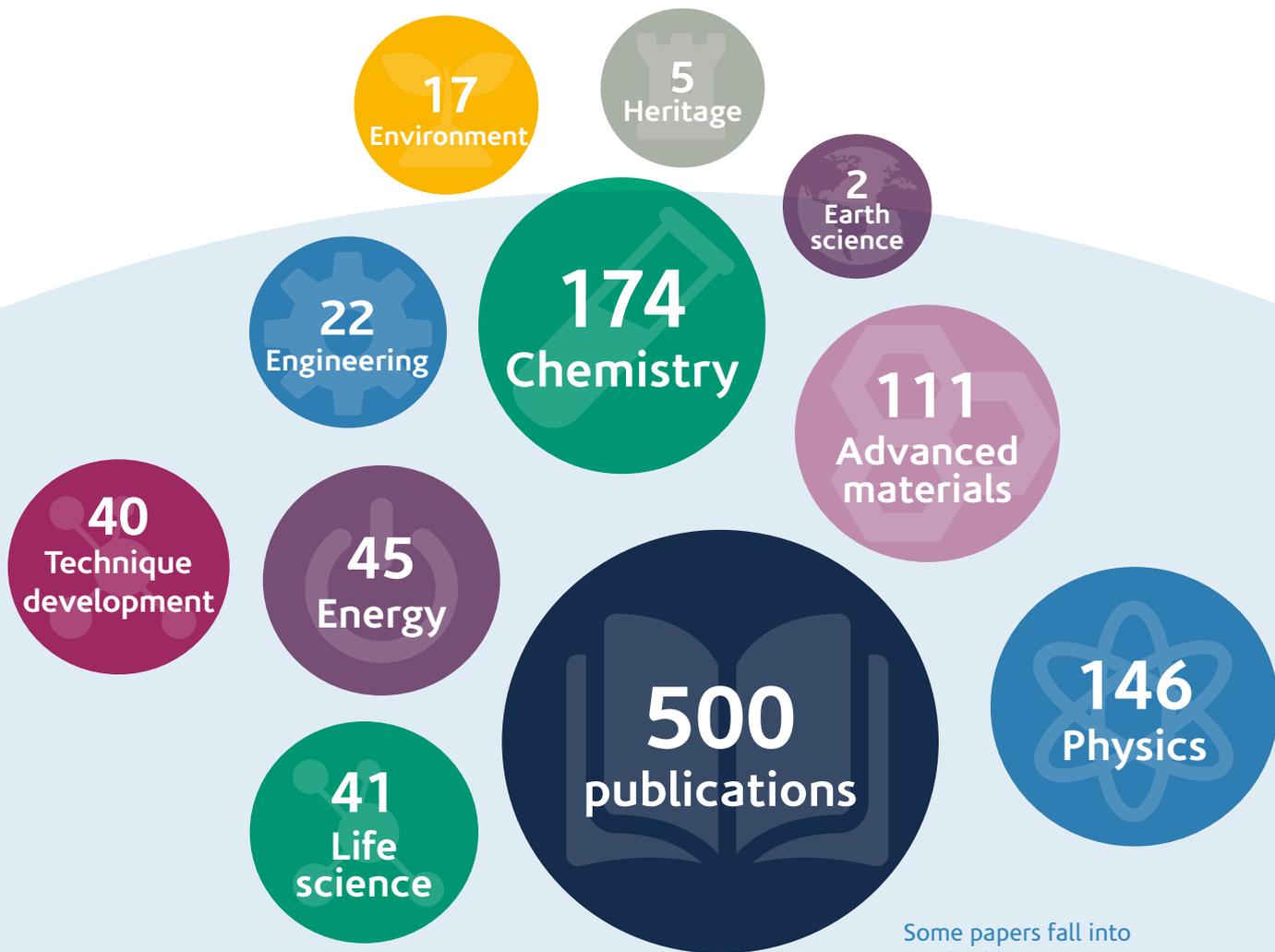
The industrial partner, Chimet S.p.A., provided both financial support and the samples to be investigated. The results increased their understanding of the catalyst, allowing Chimet the opportunity to develop more efficient and more durable catalysts in the future. In addition an exhaustive protocol was developed for the characterization of activated carbons for catalytic purposes and for carbon-based materials in general. The results shed light on the behaviour of the catalysts under reaction conditions and the influence that the support (the main target of the study) has during catalyst operation.

Science at ISIS



Science at ISIS

Science at ISIS spans a wide range of scientific disciplines, including pharmacology, cultural heritage, engineering, chemistry and fundamental research. The facility is used by over 2,000 scientists every year from both academia and industry. This section gives a snapshot of ISIS research over the past year.



Industrial Science



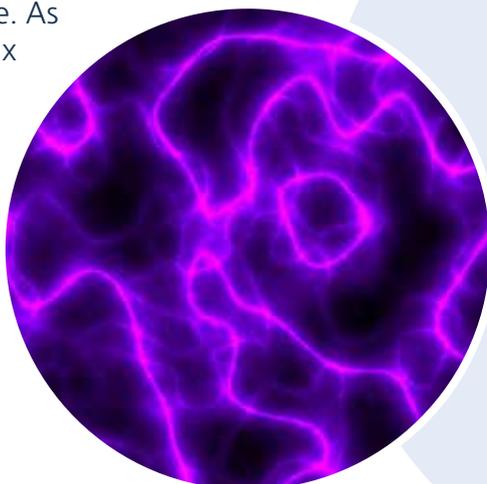
Industrial Science

Ionix – new materials for new applications

Piezoelectric materials share the unique ability to generate electrical charge from mechanical stress. If you squash it, you can make electricity; vice versa, if you apply electricity they generate mechanical strain. A wide range of naturally occurring materials have this property, but for industrial applications synthetic materials are used, with their properties tuned to meet the application. The range of applications are broad, from cigarette lighters to loudspeakers, inkjet printers to ultrasounds, piezoelectrics permeate our daily lives and represent a growing annual \$15bn market.

“Piezoelectric materials are ubiquitous in industrial and commercial sensing and actuation, but until recently they were limited to relatively low temperature environments. We set out to understand what the limiting factors were at the atomic scale, by studying new and existing materials with novel in-situ crystallography experiments and using this understanding to design materials that can operate reliably in challenging environments.” **Tim Stevenson.**

Tim Stevenson is Development Director at Ionix Advanced Technologies, a spin-out from the University of Leeds. The group used several instruments at the ISIS Neutron and Muon Source, run by the Science and Technology Facilities Council on behalf of the UK, to help develop a range of new materials that can perform in these challenging environments without compromising on performance. As of 2018 Ionix employs 17 full-time staff and



offers a range of products based on their unique piezo-ceramics to the oil and gas energy, nuclear and aerospace sectors.

Examining the lifetime of Laundry Detergent Pods with Procter & Gamble

An Industrial-Academic collaboration of scientists have been using neutron reflectometry at the ISIS Neutron and Muon Source to investigate surface segregation in water-soluble polyvinyl alcohol (PVA) films found in common household laundry detergent pods.

A laundry detergent pod is a common household product containing concentrated laundry detergent encapsulated in a dissolvable biodegradable polymer disc. The detergent is the soap (a mixture of surfactants with cleaning properties), whilst the water-soluble pouch it sits in is generally made from (polyvinyl alcohol) PVA or a derivative of PVA.

Over the past four years, a team from Durham University and Procter & Gamble have been studying the surface segregation behaviour of different types of surfactants (cationic, non-ionic and more recently, anionic) in water-soluble PVA films. The aim of their research is to use neutron

“The increased contrast, resolution and speed of data capture gained from using neutrons and high intensity X-rays respectively was vital in the development of our product. Crystallography as a function of applied electric, magnetic and mechanical fields provided the insights we needed to understand why existing materials failed and how we can refine their properties, so they can perform in more demanding environments.”

Tim Comyn, Technical Director at Ionix

technology to understand how to increase the lifetime and improve performance of these popular laundry products.

Scientists at Procter & Gamble and Durham University used the SURF and INTER instruments to measure the migration of two deuterated surfactants (d-SDS and d-C12hE5) in PVA systems with and without glycerol. This allowed them to gain a greater understanding of the effect of common solvents on the lifetime of household liquid tabs.

MedImmune – Revealing Adsorption qualities of a novel class of bio-therapeutics

A collaboration of scientists from the University of Manchester and MedImmune LLC have used neutron reflection at ISIS to investigate the interfacial adsorption of a monoclonal antibody at the solid/water interface.

Their results give unprecedented insight into the mechanics of a trending topic in immunology. Since their development in the 1970s, monoclonal antibodies (mAbs) have assumed their role as a vital player in the field of bio-therapeutics. Over the past decade, they have become the dominant recombinant therapeutic proteins used

in the clinic, applicable in the treatment of cancer and autoimmune diseases such as Crohn's and Rheumatoid arthritis.

Neutron reflectometry was the technique of choice in this experiment as it is a powerful tool that can reveal the thickness and composition of multiple adsorbed protein layers. SURF is a high flux, high resolution reflectometer which allows scientists to gather structural information on adsorbed protein layers in timely, reproducible, precise experiments. It is a world-leading instrument for liquid interface research, with the added benefit that it can offer horizontal sample geometry to users.

Combined with spectroscopy ellipsometry data, neutron reflectivity has allowed the researchers to piece together a mechanistic interpretation of the adsorption process. By collaborating with scientists from the Formulation Sciences department of MedImmune – the global biologics research and development arm of AstraZeneca – the team was able to exchange ideas and make use of cutting-edge facilities. Partnerships like this one demonstrate the value of academic-industrial relations within the scientific community.

“As we aim to continuously improve our products for consumers, it is critical to understand all parameters that can influence the shelf-life and the performance of our products. In Unit Dose, understanding how the detergent interacts with the film is therefore at the forefront of our research interests, and the level of detail revealed by Neutron Reflectometry has proven invaluable to describe surfaces at a molecular level.”

Florence Courchay, P&G



Lubrizol: Improving the efficiency of engine fuel delivery – one neutron at a time

Scientists from City, University of London and Lubrizol Limited have been using neutrons from ISIS to test the role that modern additives play in reducing flow losses – and therefore increasing the efficiency of fuel injectors in engines using diesel or biodiesel.

The team used SANS (small-angle neutron scattering) to investigate variations in surfactant aggregation in additives and their concentration dependence. SANS studies using SANS2D at the ISIS Neutron and Muon Source revealed significant differences between the micellar structures of the traditional additive, which has been added to diesel fuels for over 30 years, and a newly developed additive.

BP – Inhibiting the growth of the world's largest gas resource

Natural gas hydrates are ice-like structures, in which gas molecules, are trapped inside water molecules that form under conditions of high pressure and low temperature. These abundant compounds exceed our resource of conventional gas reserves by at least an order of magnitude and naturally occur in the ocean bed and permafrost regions. Whilst there is interest in natural gas hydrates as a potential untapped energy resource they currently cause considerable problems to both the energy sector and the environment.

Firstly, natural gas hydrates that escape to the surface are powerful greenhouse gases. Methane, commonly present in natural gas hydrates, is 21 times more powerful than carbon dioxide as a greenhouse gas. In addition, natural gas hydrates pose a severe problem in oil and gas pipelines. If water and natural gas cool in the pipes, hydrates may form which can block the line. Deep oil and gas extraction can also

disturb sites containing volatile natural gas hydrates, posing a danger to those nearby.

Given these damaging consequences there is much interest in understanding the mechanisms by which gas hydrates form to help with the design of future inhibitor technologies. Researchers from UCL, ISIS Neutron and Muon Source and BP Exploration Operating Co. Ltd have utilised neutron scattering techniques at ISIS Neutron and Muon Source and molecular dynamic simulations to study a natural gas hydrate - methane hydrate.

This research will help in the design of future inhibitor technologies that could stop the damaging environmental and industrial consequences of these abundant natural compounds.



“ Our SANS results were able to confirm the presence of micelles in solvents similar to that of diesel fuel. Of particular interest was the discovery that different deposit control additives formed different micellar structures and that this has implications for fuel flow through injectors. Determining the presence of micellar structures at the very low concentrations relevant to fuel additives was only possible with advancements in small-angle neutron scattering technology and the increased sensitivity offered by the instrument SANS2D. Our long-standing and successful collaboration with ISIS continues to provide new insights into fuel and lubricant technology. ”

Dr Kieran Trickett, Manager of Strategic Research, Research and Development, Lubrizol Limited

Environment

Unlocking the climate secrets of clouds

Related publication: M. W. A. Skoda et al. "Simultaneous neutron reflectometry and infrared reflection absorption spectroscopy (IRRAS) study of mixed monolayer reactions at the air–water interface" *RSC Adv.* 54(2017), 34208

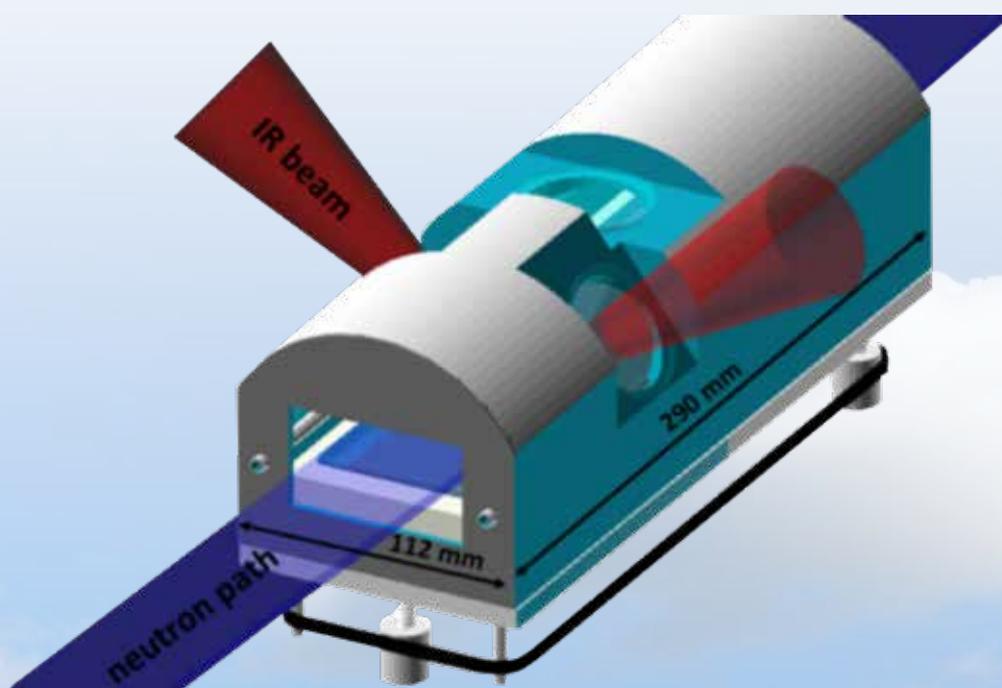
DOI: 10.1039/c7ra04900e

Instrument: INTER

Funding: NERC, University of Reading, ISIS/ SCENARIO DTP facility development studentship

 Max Skoda (ISIS Neutron and Muon Source) Christian Pfrang (University of Birmingham) Benjamin Thomas (Reading University)

The largest area of uncertainty in our understanding of climate change is the way in which small particles in the atmosphere (aerosols) interact with clouds. Many aerosol particles, particularly microscopic water droplets, attract surfactants (found in cleaning products and cooking oils), which can coat aerosols in a thin film and radically alter the way they grow and forms clouds. A new technique developed at ISIS, combining neutron reflectometry (NR) with infrared reflection absorption spectroscopy (IRRAS), allows detailed studies of the way the surfactants act in multi-surfactant configurations. When the neutron signal is unable to detect one of the film components, or to distinguish between two components, the infrared signal provides the extra detail necessary to obtain a complete picture. This collaboration between Reading University and ISIS Neutron and Muon Source demonstrates how simultaneous NR-IRRAS can substantially enhance future studies of increasingly complex surfactant mixtures and their atmospheric surface reactions.



Sketch of reaction chamber with neutron and Infrared Spectroscopy (IR) beam paths indicated. Figure 1 (b) from M. W. A. Skoda, B. Thomas, M. Hagreen, F. Sebastiani and C. Pfrang, *RSC Adv.*, 2017, 7, 34208 DOI: 10.1039/C7RA04900E - Published by The Royal Society of Chemistry.

Studying shale structure for CO₂ storage

Related publication: K. L. Stefanopoulos et al. "Neutron Scattering Measurements of Carbon Dioxide Adsorption in Pores within the Marcellus Shale: Implications for Sequestration" *Environ. Sci. Technol.* 51(11) (2017), 6515–6521

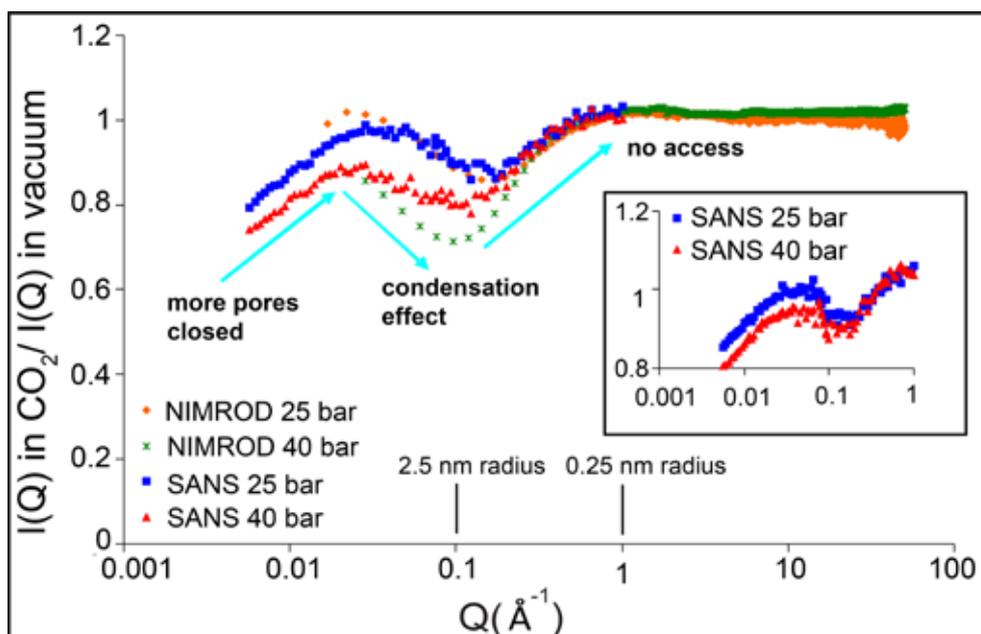
DOI: 10.1021/acs.est.6b05707

Instrument: NIMROD

Funding: European Commission under the seventh Framework Programme through the 'Research Infrastructures' action of the 'Capacities' Programme.

 Leslie F. Ruppert (U.S. Geological Survey)

The production of natural gas from shale is increasing in the US, and under consideration elsewhere in the world. Researchers are also investigating the potential of shale beds for storing carbon dioxide (CO₂), to reduce greenhouse gas emissions. The key to both these processes is an understanding of how gases are adsorbed into and sweep out of pores within the shale. Shale contains a network of pores and fractures of various sizes. Research published in *RSC Advances* used neutron scattering techniques on Nimrod, as they can distinguish between pores that are open, or accessible, and pores that are closed. The results suggest that the large numbers of micropores in shale are closed and are unavailable for CO₂ storage, a finding that is important for the development and refinement of CO₂ storage methods.



Ratio of scattering intensity in CO₂ at 22 °C and 25 and 40 bar compared to vacuum (SANS and NIMROD) for the Marcellus Shale with flat background removed. Inset: Ratio of scattering intensity in CO₂ at 60 °C and 25 and 40 bar (SANS) compared to vacuum, flat background removed. Image credit: K. L. Stefanopoulos et al. *Environ. Sci. Technol.* 51(11) (2017), 6515–6521 DOI: 10.1021/acs.est.6b05707

Understanding diffusion in industrial catalysts

Related publication: M. E. Potter et al. "Understanding the Role of Molecular Diffusion and Catalytic Selectivity in Liquid-Phase Beckmann Rearrangement" *ACS Catal.* 7(4) (2017), 2926-2934

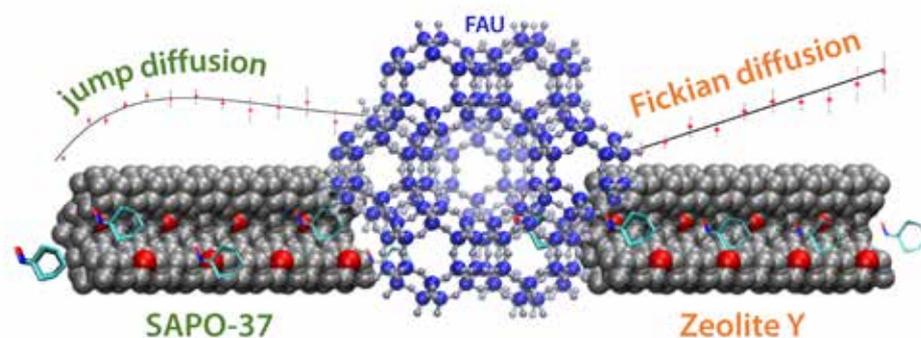
DOI: 10.1021/acscatal.6b03641

Instrument: OSIRIS, MAPS

Funding: EPSRC, UK Catalysis Hub, STFC, ISIS Neutron and Muon Source

 Robert Raja (Southampton University)

An international group of scientists has used quasi-elastic and inelastic neutron scattering at ISIS to uncover crucial differences in substrate diffusion and active-site interactions in zeotype catalysts for nylon manufacture (an industry valued at \$14 billion USD for 2019). With complementary solid-state nuclear magnetic resonance and probe-based Fourier-transform infrared spectroscopy (FTIR), they have been able to provide an insight into the role of the active site in the mechanistic and reaction pathways, and hence rationalise the activity of industrial, solid-acid catalysts. Their results will play a vital role in designing future catalysts for sustainable industrial processes.



Neutron spectroscopy has revealed contrasting diffusive behaviour in faujasitic catalysts for the Beckmann rearrangement, thus highlighting the importance of framework topology and active site interactions in catalyst design.

Heritage

Understanding Viking sword-making techniques

Related publication: A Fedrigo et al. "Extraction of archaeological information from metallic artefacts—A neutron diffraction study on Viking swords" *Journal of Archaeological Science: Reports* 12 425-436 (2017)

DOI: 10.1016/j.jasrep.2017.02.014

Instrument: INES

 Anna Fedrigo (ISIS Neutron and Muon Source)

The Vikings have a well-deserved reputation as fearsome warriors, and their weapons were indispensable tools for their plundering raids. Swords from this era often showed a decorative pattern on the surface, produced by pattern-welding - welding together thin strips of iron and steel that were twisted and forged in various ways. More than two thousand Viking swords have survived until today, often badly corroded. An international group of scientists used neutron diffraction at ISIS to perform a non-invasive investigation of three Viking swords from the National Museum of Denmark. They were able to characterise the blades in terms of composition and the manufacturing processes involved, and their study shows how the effects of past conservation treatments can either help or obstruct the extraction of archaeological information.



Double-edged sword from the Viking Age belonging to the National Museum of Denmark. The blade is 'pattern-welded', made by forge welding together thin strips of iron and steel, producing a decorative pattern on the surface.



Analysing copper bolts from sunken wrecks

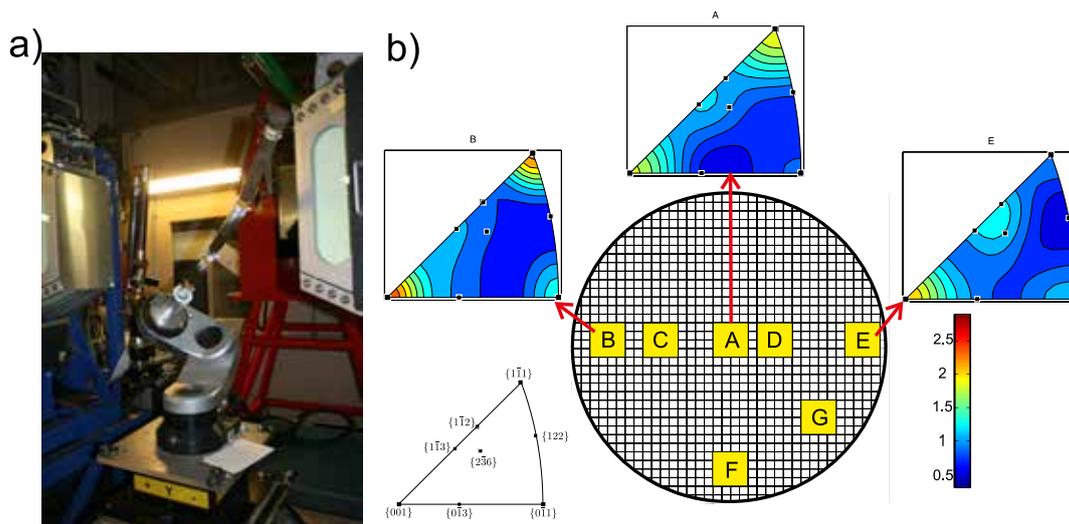
Related publication: F. Malamud et al. "Spatially resolved texture analysis of Napoleonic War era copper bolts" *J. Appl. Cryst.* 50(2017), 1359-1375

DOI: 10.1107/S1600576717011761

Instruments: ENGIN-X

 **Florencia Malamud** (Laboratorio de Física de Neutrones)

A team of scientists from the Open University, University of Oxford, Centro Atómico Bariloche Argentina and ISIS has used ENGIN-X and a new texture analysis methodology to non-destructively study texture variations across cross-sections of copper bolts taken from the wrecks of three ships from the eighteenth and early nineteenth centuries: HMS Impregnable, HMS Amethyst and HMS Pomone. Previous research has shown that during the Napoleonic war era, all copper bolts used by the Royal Navy were made of impure copper of a similar composition but their different methods of manufacture can be distinguished by the overall texture. By analysing the texture distribution across the bolts, the scientists were able to gain a greater understanding of the methods involved in their manufacture. These results are an important step in increasing our understanding of the introduction and evolution of copper fastenings in Royal Navy warships.



a) Experimental setup for the HMS Impregnable copper bolt using the Cybaman goniometer at ENGIN-X diffractometer

b) Explored positions across the bolt cross-section and inverse pole figures from three measurement volumes in the HMS Impregnable bolt. All use the same colour scale in mrd.

Engineering

Investigating stress-strain response in shape memory alloys

Related publication: A Reul et al. "In Situ Neutron Diffraction Analyzing Stress-Induced Phase Transformation and Martensite Elasticity in [001]-Oriented $\text{Co}_{49}\text{Ni}_{21}\text{Ga}_{30}$ Shape Memory Alloy Single Crystals" *Shap. Mem. Superelasticity* 4(2018), 61-69

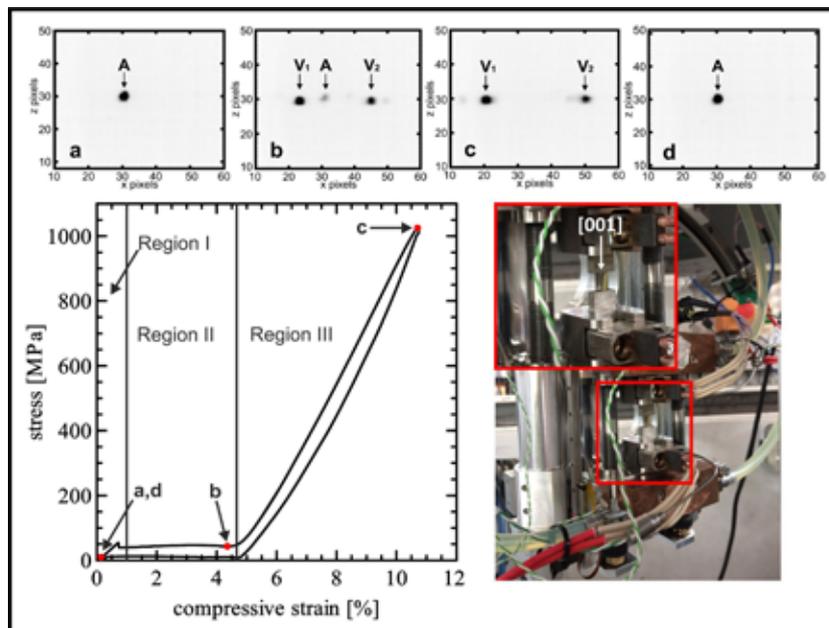
DOI: 10.1007/s40830-018-0156-1

Instrument: SXD

Funding: Deutsche Forschungsgemeinschaft

 Thomas Niendorf (University of Kassel)

High-temperature shape memory alloys (HT-SMAs) have numerous potential applications, including as solid-state actuators or damping devices for high temperature use in the automotive and aerospace sectors. As conventional binary Ni-Ti SMAs only exhibit fully reversible transformations at temperatures up to about 100 °C, and suffer from microstructural instability, researchers have been investigating new alloys with enhanced properties. An international team of researchers used *in situ* neutron diffraction experiments on SXD, using a newly-installed testing setup on Co-Ni-Ga single crystals. Their aim was to reveal the nature of the stress-strain response seen in the deformation curves up to 10% macroscopic strain, and their results show that the martensite phase is able to withstand about 5% elastic strain, which significantly increases the overall deformation capability of this alloy system.



The stress-strain response of [001] oriented $\text{Co}_{49}\text{Ni}_{21}\text{Ga}_{30}$ reveals excellent shape memory properties under compression (lower left). The underlying fully reversible martensitic transformation between austenite (A) and internally twinned martensite (V1 and V2) can be deduced from the diffractograms obtained from *in situ* neutron diffraction (upper row). The photograph highlights the newly installed miniature loadframe at the SXD (lower right).

Understanding copper corrosion in oil

Related publication: R. J. L. Welbourn et al. "Corrosion and inhibition of copper in hydrocarbon solution on a molecular level investigated using neutron reflectometry and XPS" *Corrosion Science* 115 (2017), 68-77

DOI: 10.1016/j.corsci.2016.11.010

Instruments: Inter

Funding: EPSRC and BP

 Becky Welbourn (ISIS Neutron and Muon Source)

The corrosion of copper in oil is an expensive problem for industry, particularly when it results in the failure of transformers or bearings. The damage can occur through dissolved oxygen (or air) or corrosive forms of sulphur. Several types of sulphur are present in crude oil, some of which react with copper. As it is not easy to remove all sulphur from oil, corrosion inhibitors are often added to the oil mixture to protect copper surfaces. Previous research has concentrated on how corrosion inhibitors work in water-based mixtures, but a team of UK researchers has used X-ray photoelectron spectroscopy (XPS), plus neutron reflection on the INTER reflectometer, to study the behaviour and molecular structure of three organic additives adsorbed from oil onto a copper surface. Researchers discovered that molecules that form dense coverage on the surface do not necessarily provide greater protection compared to less dense layers, implying that the chemistry of surface binding is more important. Their results offer a greater chemical understanding of the corrosion process, and may lead to better corrosion inhibitors.



Picture credit: pixabay

Fundamental Research

Examining the interplay between magnetism and topology

Related publication: L. M. Schoop et al. "Tunable Weyl and Dirac states in the nonsymmorphic compound CeSbTe" *Sci. Adv.* 4(2018), eaar2317

DOI: 10.1126/sciadv.aar2317

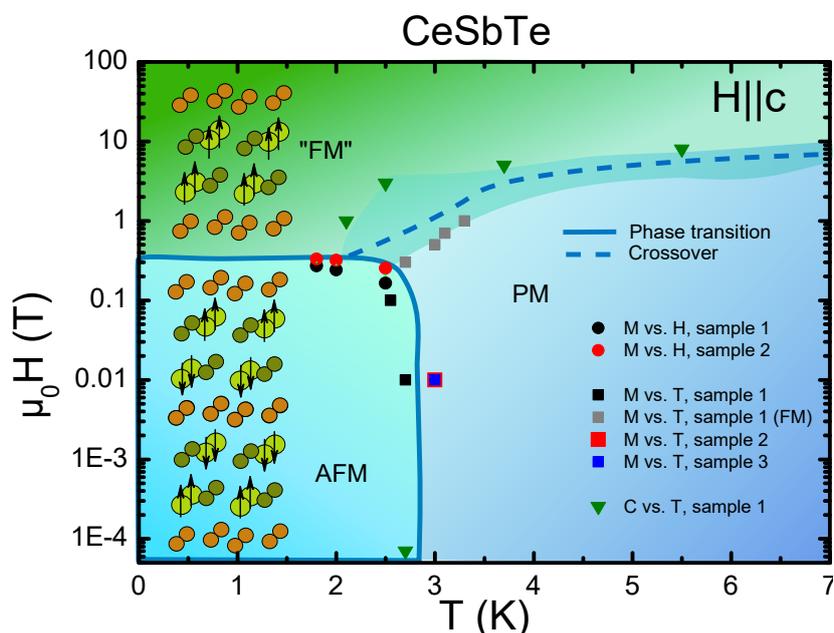
Instrument: WISH

Funding: The Max Planck Society, the Nanosystems Initiative Munich, and the Center for Nanosciences

 Leslie M. Schoop (Princeton)

The 2016 Nobel prize in physics was awarded to physicists who used the mathematical concept of "topology" to explain the exotic behaviour of certain materials. There is increasing interest in these "topological" materials, which may hold the key to next generation computing devices based on spintronics. Materials that exhibit long-range magnetic order in combination with topologically nontrivial band structures are particularly sought after.

An international team of researchers used powder neutron diffraction data collected on the WISH instrument, alongside other experiments, to demonstrate that a rich variety of different topological states can exist in a single material, CeSbTe. Their discovery introduces a realistic and promising platform for studying the interplay of magnetism and topology.



Magnetic phase diagram of CeSbTe. Three different regions can be observed within a low field limit. The magnetic structures of the different phases are shown in the respective regions. Different colours indicate different samples and different symbols indicate different measurement techniques. Image reproduced from L. M. Schoop et al. *Sci. Adv.* 4(2018) DOI: 10.1126/sciadv.aar2317

Using neutrons to examine correlated electron systems

Related publication: E. A. Goremychkin et al. "Coherent band excitations in CePd₃: A comparison of neutron scattering and ab initio theory" *Science* 359(2018), 186-191

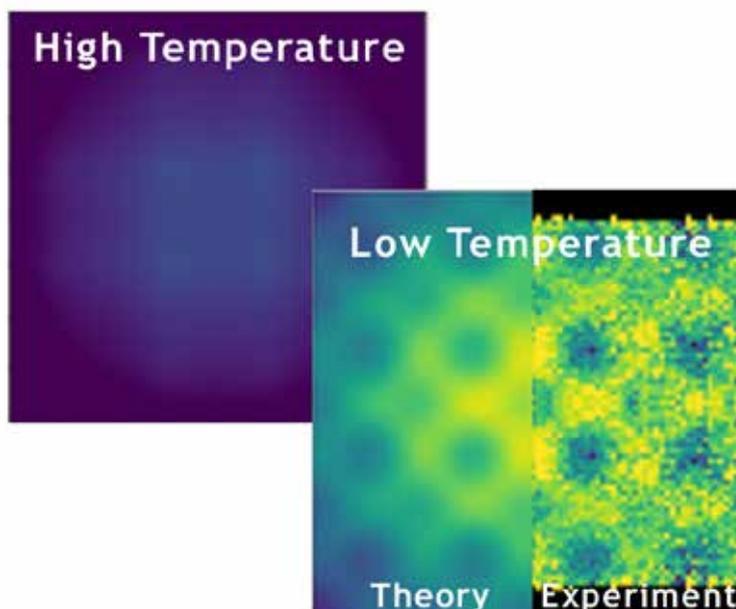
DOI: 10.1126/science.aan0593

Instrument: Merlin

 Raymond Osborn (Argonne National Laboratory)

For more than 50 years, scientists have been studying strongly correlated electron systems, in which electron-electron interactions are too strong to be ignored, and which give rise to useful properties such as superconductivity or magnetism. Following the development of a new generation of inelastic neutron scattering (INS) spectrometers, such as Merlin, it is now possible to probe electron interactions with unprecedented detail. A team of researchers used Merlin to show how the behaviour of correlated electron systems changes with temperature, demonstrating that neutrons can overcome the limitations of other techniques.

The team used their studies of CePd₃, a cerium-palladium compound, to produce a comprehensive comparison of experiment and theory, confirming that the anomalous properties of this class of materials can be predicted by the latest theoretical advances. The insights gained into the properties and functionality of these materials will open up their potential to be used in novel ways



Dynamic magnetic susceptibility of CePd₃ at high and low temperature.

Solving a tantalising Tantalum mystery

Related publication: M. Klanjšek et al. "A high-temperature quantum spin liquid with polaron spins" Nature Physics 13(2017), 1130–1134

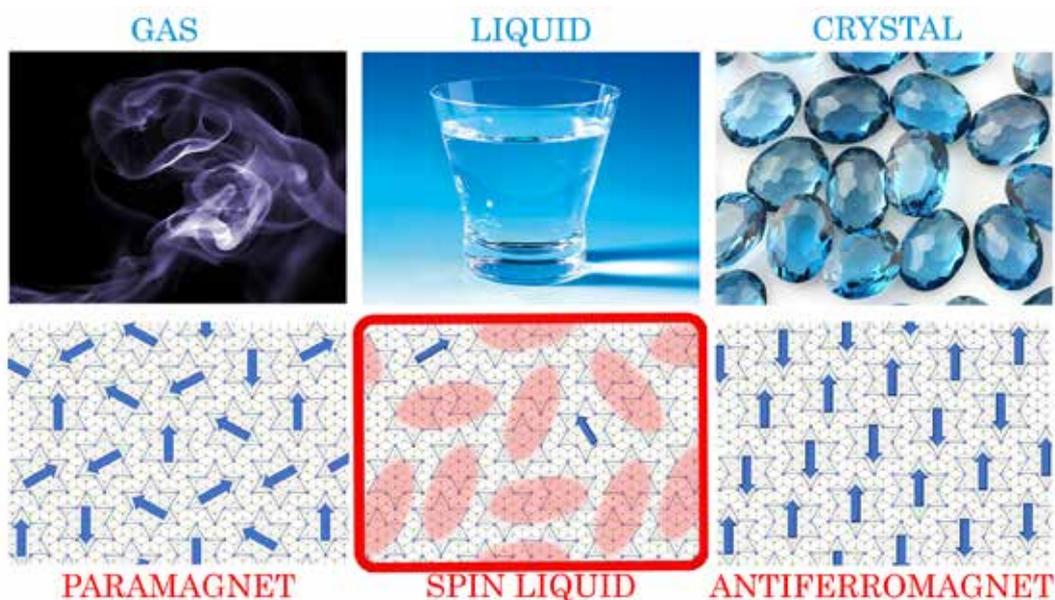
DOI: 10.1038/nphys4212

Instrument: MuSR

Funding: Slovenian Research Agency, ERC AdG Trajectory

 Denis Arčon (University of Ljubljana)

Nobel laureate Paul W. Anderson proposed that high-temperature superconductivity is related to an exotic quantum state now known as quantum spin liquid, in which magnetic moments behave like a liquid and do not freeze or order even at absolute zero. They are promising materials for topological quantum computers, which would be based on the particle-like excited states found in quantum spin liquids. Tantalum (IV) sulphide (1T-TaS₂) is an important model system with semiconductor properties, but scientists have been searching for an explanation of its unusual magnetic properties for more than 40 years. A team of Slovenian researchers undertook the first muon-spin-relaxation (μ SR) measurements on polycrystalline 1T-TaS₂ on the MuSR instrument, probing the magnetic properties of the low-temperature spin state and the physics behind the quantum spin liquid on a triangular lattice. Their findings confirmed the prediction of QSL in 1T-TaS₂, which has been unresolved for over 40 years, but also raise questions about the nature of emergent states out of QSLs.



A comparison of well-known aggregate states (gas, liquid, solid) with the corresponding analogies in magnetism: paramagnet, spin liquid and antiferromagnet.

Probing the underlying physics in quantum spin ladders

Related publication: S. Ward et al. "Bound States and Field-Polarized Haldane Modes in a Quantum Spin Ladder" Phys. Rev. Lett. 118(2017), 177202

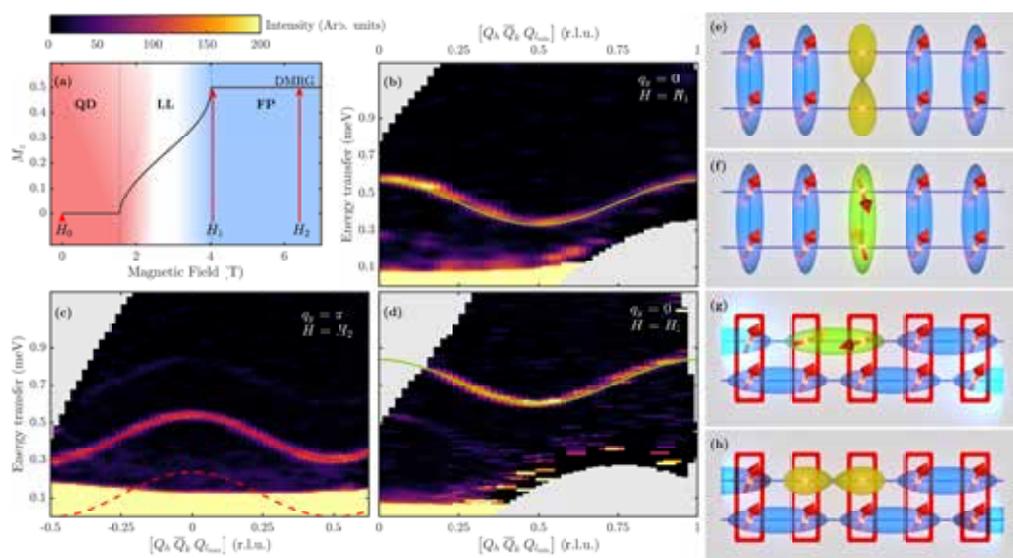
DOI: 10.1103/PhysRevLett.118.177202

Instrument: LET

Funding: SNF, ERC, DFG, Royal Society

 Rob Bewley (ISIS Neutron and Muon Source) and Tatiana Guidi (ISIS Neutron and Muon Source)

One-dimensional (1D) systems exhibit a range of unusual and interesting phenomena, and the challenge for scientists is to understand the underlying physics that causes them. An international team of researchers has used high-resolution inelastic neutron scattering on the time-of-flight spectrometer LET to investigate bis-piperidinium copper tetrachloride (BPCC), a quantum spin-ladder material which consists of two coupled spin-1/2 chains. They were able to measure two kinds of novel magnetic excitation, bound states at zero field and fully field-polarized Haldane modes. They further demonstrated that the magnetic response in BPCC can be explained accurately by state-of-the-art numerical (DMRG and series-expansion) methods. Their work provides a systematic understanding of the magnetic excitations in a broad family of gapped 1D quantum magnets, including ladder, alternating-chain, and Haldane systems.



Excitations in fully polarized BPCC. (a) Magnetization of BPCC (from DMRG) superimposed on the field-induced phase diagram; LL denotes the Luttinger-liquid and QD the quantum disordered phase. (b) SdQ;omegaP measured at $H_1 \approx 4.067$ T $\approx H_1$ and (d) $H_2 \approx 6.141$ T, both in the $q_y = 0$ sector. (c) SdQ;omegaP measured at H_2 in the $q_y = \pi$ sector. Green and red solid lines are, respectively, fits to the triplet ($q_y = 0$) and singlet ($q_y = \pi$) modes using Eq. (2). The dashed line in panel (c) indicates the position of the singlet at H_1 (not measured due to dominant nuclear incoherent scattering at low energies). (e) Schematic representation of a FP two-leg ladder with one rung-singlet excitation. (f) FP ladder with one rung-triplet (t0) excitation. (g) FP Haldane chain in the auxiliary-spin representation containing one leg-singlet and (h) one leg-triplet excitation.

Energy

Natural gas hydrates: fuel or foe?

Related publication: S. J. Cox et al. "Formation of Methane Hydrate in the Presence of Natural and Synthetic Nanoparticles" J. Am. Chem. Soc 140 (9)(2018), 3277-3284

DOI: 10.1021/jacs.7b12050

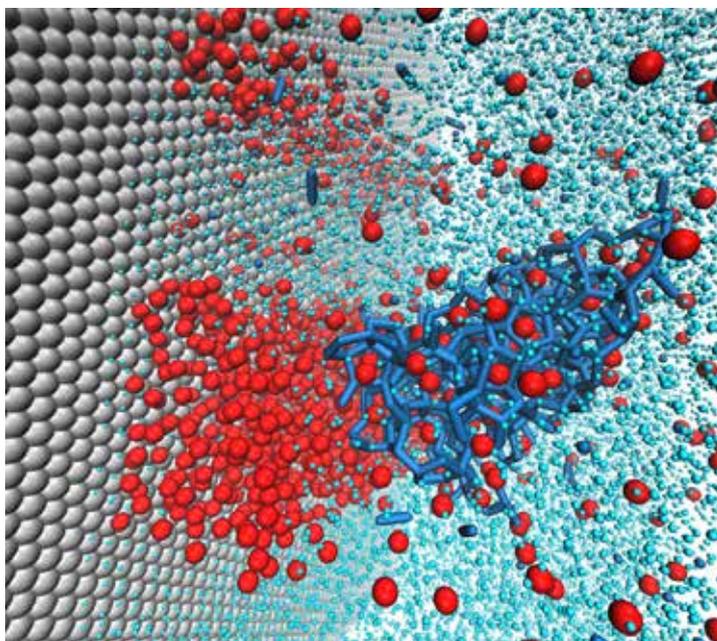
Instrument: NIMROD and SANDALS

Funding: European Research Council under the European Union's Seventh Framework Programme, BP Exploration Operating Co. Ltd

 Neal T. Skipper (UCL) and Angelos Michaelides (UCL)

Natural gas hydrates are ice-like structures that form at high pressure and low temperature. They consist of hydrogen-bonded water cages, which can stabilise the adsorption of gas molecules like methane. These abundant compounds occur naturally in the ocean bed and permafrost regions, and are a potential, untapped energy source. However, when they escape to the surface they are powerful greenhouse gases, and if they form in gas pipelines they can cause blockages.

Researchers from UCL, ISIS and BP Exploration Operating Co. Ltd have used neutron scattering techniques on NIMROD and SANDALS along with computer simulations to study the effect of dissolved solid impurity particles on the formation of methane hydrate. Their results show that, in contrast to the formation of other materials, the formation of methane hydrate is not affected by a wide range of impurity particles. This finding will inform the design of future inhibitor technologies aimed at preventing the damaging environmental and economic effects of natural gas hydrates.



Snapshot from a computer simulation showing the initial stages of methane clathrate formation (Credit: Steve Cox).

Enhancing performance in important industrial catalysts

Related publication: C. I. Hiley et al. "Pair Distribution Function Analysis of Structural Disorder by Nb⁵⁺ Inclusion in Ceria: Evidence for Enhanced Oxygen Storage Capacity from Under-Coordinated Oxygen" J. Am. Chem. Soc. 140(2018), 1588–1591

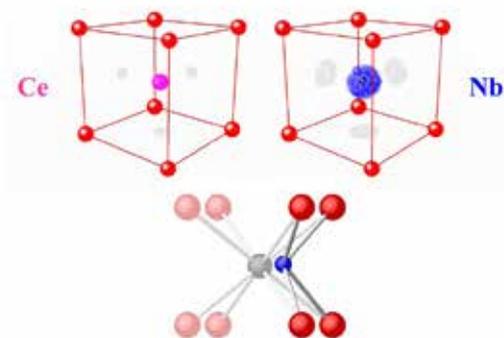
DOI: 10.1021/jacs.7b12421

Instruments: GEM, Polaris

Funding: Johnson Matthey plc, Science City Advanced Materials project "Creating and Characterizing Next Generation Advanced Materials" with support from Advantage West Midlands.

 Richard I. Walton (University of Warwick)

Ceria, cerium dioxide, has numerous applications in catalytic processes such as automotive emission control and hydrogen purification. Research is currently focusing on improving the oxygen storage capacity of the catalyst for new and emerging energy and environmental applications, and finding new methods for synthesising ceria. The inclusion of other metals can produce drastic improvements in the properties of ceria. A team of researchers has achieved partial substitution of cerium with niobium by also including sodium, via a low-temperature hydrothermal route. This process leads to thermally robust materials with oxygen storage capacities much greater than pure ceria. Neutron scattering on the GEM and Polaris instruments at ISIS was used to show how local structure may be dramatically disrupted by inclusion of substituent cations in this important class of materials, explaining their enhanced reducibility.



Displacement of Ce and Nb in their cubic environment of 8 oxygens (red spheres) determined by modelling of neutron scattering data. The lower image shows a typical asymmetric Nb environment compared to the ideal site for the cation in CeO₂, giving uncoordinated oxygen that explains the enhanced reducibility.

Exploring the next generation of solar cell materials

Related publication: K. L. Brown et al. "Molecular orientational melting within a lead-halide octahedron framework: The order-disorder transition in $\text{CH}_3\text{NH}_3\text{PbBr}_3$ " Phys. Rev. B 96(2017), 174111

DOI: 10.1103/PhysRevB.96.174111

Instruments: IRIS MAPS

Funding: EPSRC, STFC, the Royal Society, and the Carnegie Trust for the Universities of Scotland

 Stewart Parker, Sanghamitra Mukhopadhyay and Victoria Garcia Sakai (ISIS Neutron and Muon Source)

Lead-halide organic-inorganic perovskites consist of an organic molecule inside an inorganic host framework. These materials are of considerable interest due to their exceptional photovoltaic properties, which offer the potential of improved solar panels. The behaviour of the organic molecule is thought to be key to understanding the overall properties of the material, particularly the way in which it rotates within the framework. Although the structure and dynamics of these materials have been extensively studied, the exact nature of this rotation is not yet understood. A team of researchers from the University of Edinburgh, Imperial College London and ISIS used a combination of inelastic neutron scattering, Raman spectroscopy, and quasielastic neutron scattering to study the temperature dependent dynamics of the organic molecule in $\text{CH}_3\text{NH}_3\text{PbBr}_3$. Their results confirm the strong role of hydrogen bonding and a coupling between molecular and framework dynamics.



Image credit: Pixabay

A new method for synthesising oxyhydride materials

Related publication: O. S. Fjellvag et al. "Thermal and Structural Aspects of the Hydride-Conducting Oxyhydride La_2LiHO_3 Obtained via a Halide Flux Method" *Inorg. Chem.* 56 (18) (2017), 11123–11128

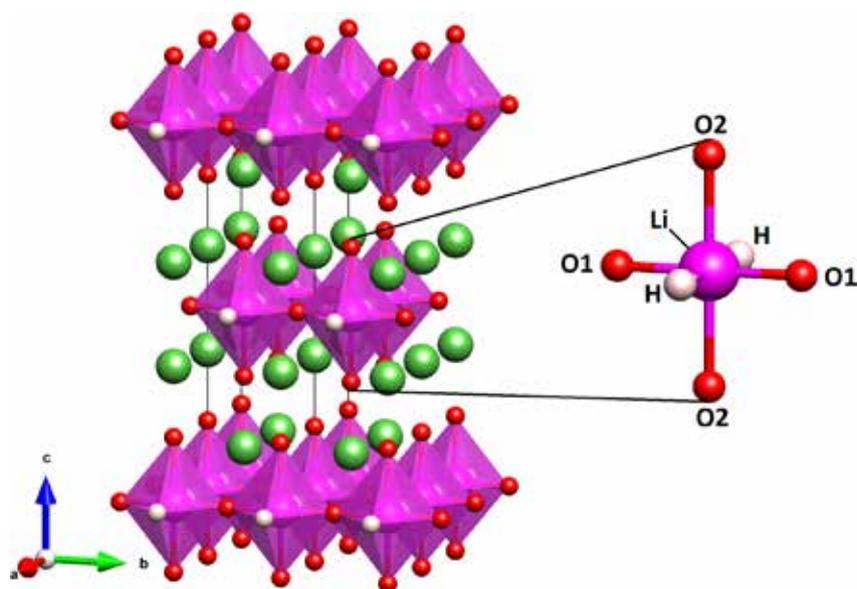
DOI:10.1021/acs.inorgchem.7b01409

Instruments: Polaris, IRIS

Funding: The Faculty of Mathematics and Natural Sciences, University of Oslo, via the Strategic Research Initiative program

 Anja O. Sjastad (University of Oslo)

Hydrogen-conducting materials have been widely studied for various technological applications, including proton conductors, high-temperature solid oxide fuel components and metals for hydrogen storage. Oxyhydrides, in which oxide and hydride anions share the same anionic lattice, are relatively rare compounds, and their synthesis is challenging. A team of researchers from the University of Oslo has used powder neutron diffraction experiments on Polaris and quasi-elastic neutron scattering measurements on Iris to develop a new method of synthesising La_2LiHO_3 that allows the production of larger quantities. They also reported, in detail, the conditions favouring high-quality high-yield samples of this material, which will be of considerable importance for further studies into its properties and potential practical applications in real devices.



The crystal structure of orthorhombic (*Immm*) La_2LiHO_3 as determined by x-ray diffraction. The atomic species are represented as lanthanum (green), lithium (pink), hydrogen (white), and oxygen (red).

Bioscience

Neutron studies of cellulose fibres

Related publication: C. Araujo et al. "Hydrogen Bond Dynamics of Cellulose through Inelastic Neutron Scattering Spectroscopy" *Biomacromolecules* 19(2018), 1305–1313

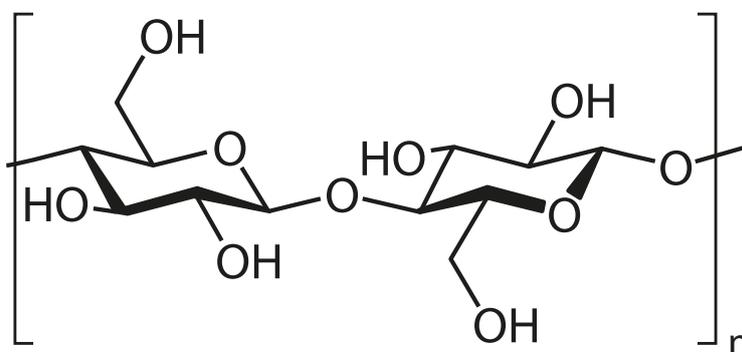
DOI: 10.1021/acs.biomac.8b00110

Instrument: TOSCA

Funding: FCT/MEC, FEDER

 Mariela Martins Nolasco (University of Aveiro)

Cellulose is a fascinating biopolymer and a never-ending source of new, sustainable materials. It is attracting increasing attention in different fields owing to its abundance, biodegradability and unique physicochemical properties. Chemical modification of cellulose, and the properties of the materials thereby produced, depends on the structure of the fibrils that make up cellulose fibres, and a team of Portuguese researchers has used neutrons to characterise the structure and packing of cellulose fibrils and their bundles. Inelastic neutron scattering (INS) spectroscopy is particularly useful for the study of the dynamics of hydrogen atoms and hydrogen-bond networks, and their results provide a sound basis for future use of INS spectroscopy in the characterisation of functionalised cellulose fibres and composite materials.



Cellulose bond

The Liquid of Life

New insights into planet formation using NIMROD

Related publication: S. Gärtner et al. "Micrometer-sized Water Ice Particles for Planetary Science Experiments: Influence of Surface Structure on Collisional Properties" *The Astrophysical Journal* 848(2017)

DOI: 10.3847/1538-4357/aa8c7f

Instrument: NIMROD

Funding: Open University, STFC, Royal Society International Exchange Award, EU COST Action, Our Astrochemical History, TU Braunschweig, DLR

 Sabrina Gaertner (ISIS Neutron and Muon Source) and Helen Jane Fraser (The Open University)

More than 3600 planets have been discovered outside of our Solar System since 1992, and yet the processes leading to the formation of these exoplanets are not yet fully understood. Dust aggregation is known to be a key step in planet formation, but dust on its own is not very sticky. Models and observations suggest that water can act as a "glue" to help dust form planets. A team of astrochemists used neutron scattering on NIMROD, in combination with cryo-SEM (scanning electron microscopy), to characterise ice particle analogues used in laboratory collision experiments, and their results suggest that the ice surface structure is fundamental to whether icy particles stick or not. Further investigations of the surface layer are needed, so that the influence of ice physics on collisional outcomes may be incorporated into more sophisticated models of planet formation and accounted for when interpreting collision experiments.



Sabrina Gaertner on NIMROD, image credit: STFC

Neutrons shed light on Martian channel formation

Related publication: S. Lenton et al. "Highly compressed water structure observed in a perchlorate aqueous solution" *Nature Communications* 8(2017), 919

DOI: 10.1038/s41467-017-01039-9

Instrument: SANDALS

Funding: EPSRC

 Lorna Dougan (University of Leeds) Alan K. Soper (ISIS Neutron and Muon Source)

As water is widely regarded as a prerequisite for life, the search for extra-terrestrial life generally starts as a search for water. Although water does not remain in liquid form in the Martian climate, there is growing evidence that flowing water was once present on the surface of our neighbouring planet. NASA's Phoenix Mars Lander discovered perchlorate in Martian soil, and more recently the Mars Express orbiter revealed the presence of a liquid water 'lake' below the planet's south polar ice cap. A team led by Dr Lorna Dougan at the University of Leeds has used neutron diffraction on SANDALS to study the structure of magnesium perchlorate aqueous solution, an analogue of Martian water. They found that magnesium perchlorate had a major impact on water structure in solution, and could explain how these salt solutions remain liquid in the low and widely varying humidity environment of the Martian surface.

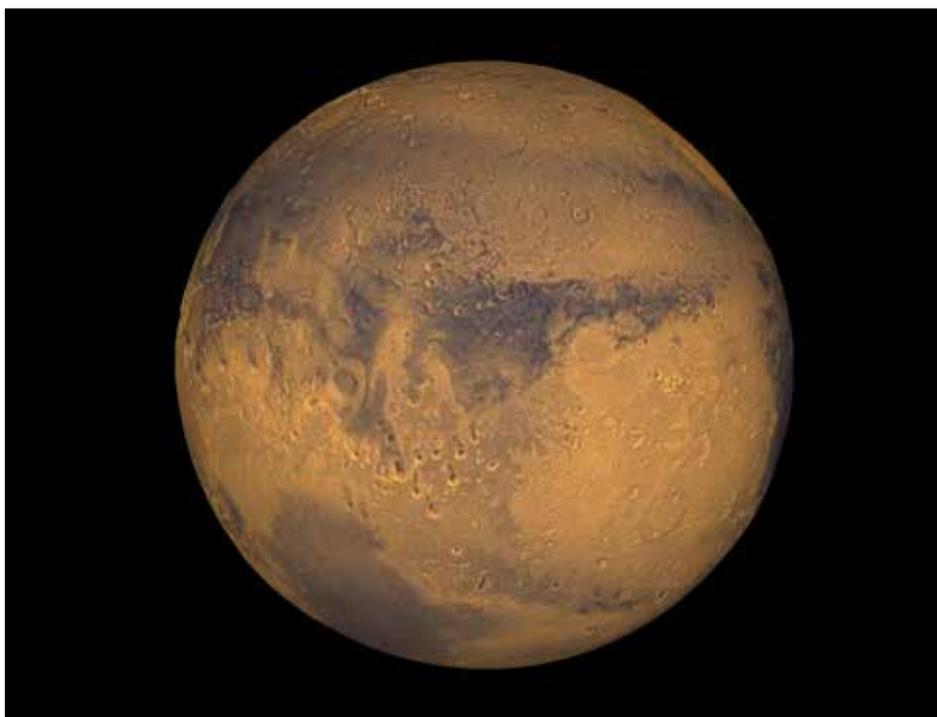


Image credit: NASA

Under pressure: neutron diffraction helps unlock the secrets of water's phase diagram

Related publication: J. J. Shephard et al. "Doping-induced disappearance of ice II from water's phase diagram" *Nature Physics* 14(2018), 569-572

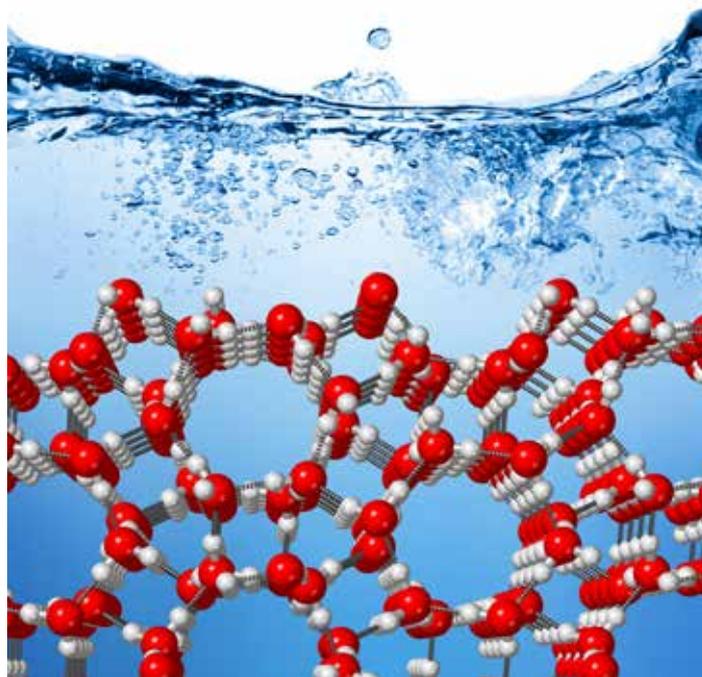
DOI: 10.1038/s41567-018-0094-z

Instrument: PEARL

Funding: The Royal Society, The Leverhulme Trust

 Christoph G. Salzmann (UCL)

Ice takes on many different forms, depending on the pressure at which it crystallises. These forms are summarised using a phase diagram, which shows the preferred physical states of water at different temperatures and pressures. Researchers from UCL and ISIS have used high-pressure neutron diffraction on PEARL to investigate the impact of ammonium fluoride impurities on water's phase diagram. Their surprising results showed that the addition of this impurity caused a particular phase of ice, known as ice II, to completely disappear whereas the other phases were unaffected. The knowledge of this effect will be of importance to any study where ice coexists with other materials in nature, for example on icy moons. The disappearance of ice II also highlights its topologically frustrated nature which could be the origin of some of the well-known anomalies of water's phase diagram.



The crystal structure of ice II floating in liquid water. Oxygen and hydrogen atoms are represented by red and white spheres, respectively.

Applied Materials

Muons measure the lifetime of electron-hole pairs

Related publication: K. Yokoyama et al. "Photoexcited Muon Spin Spectroscopy: A New Method for Measuring Excess Carrier Lifetime in Bulk Silicon" *Phys. Rev. Lett.* 119(2017), 226601

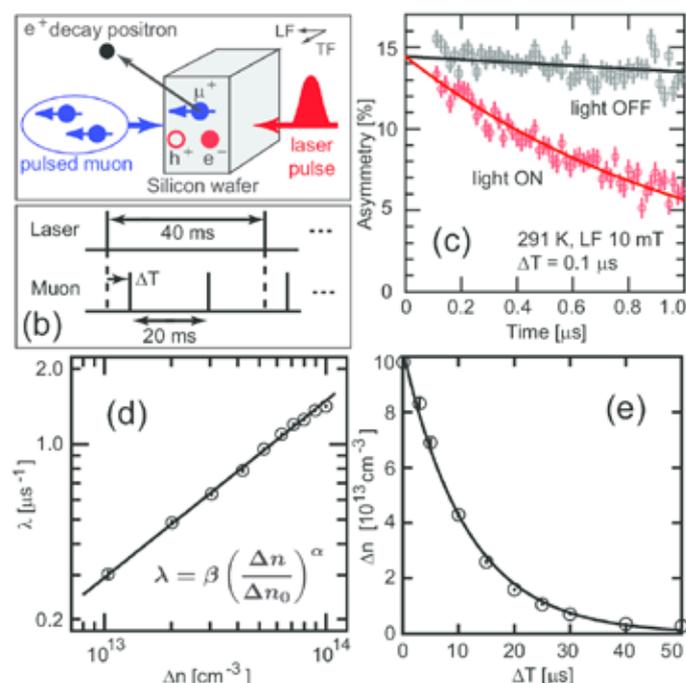
DOI: 10.1103/PhysRevLett.119.226601

Instrument: HiFi

Funding: European Research Council

 Koji Yokoyama (ISIS Neutron and Muon Source)

Silicon wafers are one of the workhorses of the electronic age, widely used in integrated circuits and many photosensitive devices. Understanding the behaviour of electrons and holes, and controlling their dynamics, is key to their success. How long these electron-hole pairs live impacts their performance in solar cells, and their lifetime is also used as an indicator of cleanliness in chip manufacturing. These "bulk" lifetimes represent the purity and intrinsic quality of the wafer. Traditional measures of carrier lifetime are strongly influenced by the surface condition – without proper cleaning, wafer surfaces are normally full of impurities. A recent upgrade to the HiFi muon spectrometer allows samples to be excited with a high-energy laser, and a group of scientists have used this new technique to overcome the difficulty and directly probe the bulk carrier lifetime. The study will be extended to new class of semiconductors, such as the emerging photovoltaic materials.



Schematic diagram of the experimental geometry and timing diagram of laser and muon pulse. Pulse duration (FWHM) of the laser and muon pulse are ≈ 16 and ≈ 70 ns respectively. (c) μ SR time spectra for light OFF (black squares) and ON (red circles, $\Delta n = 4.7 \times 10^{13} \text{ cm}^{-3}$). 5×10^6 events are averaged for each spectrum. Fit parameters are $A(0) = 14.44(3)\%$, $\lambda' = 0.068(2) \mu\text{s}^{-1}$ for light OFF, and $\lambda = 0.94(2) \mu\text{s}^{-1}$ for light ON. (d) λ as a function of Δn . The fit gives $(\alpha, \beta [\mu\text{s}^{-1}], \Delta n_0 [\text{cm}^{-3}]) = [0.68(4), 1.46(4), 8.9 \times 10^{13}]$. (e) Carrier decay curve. The fit gives $\Delta n(0) = 9.4(4) \times 10^{13} \text{ cm}^{-3}$ and $\tau = 11.1(9) \mu\text{s}$. More information can be found in: "Photoexcited Muon Spin Spectroscopy: A New Method for Measuring Excess Carrier Lifetime in Bulk Silicon", *Phys Rev Lett* 119, no. 22 (2017): 226601.

Neutrons illuminate stress/strain in high-temperature superalloys

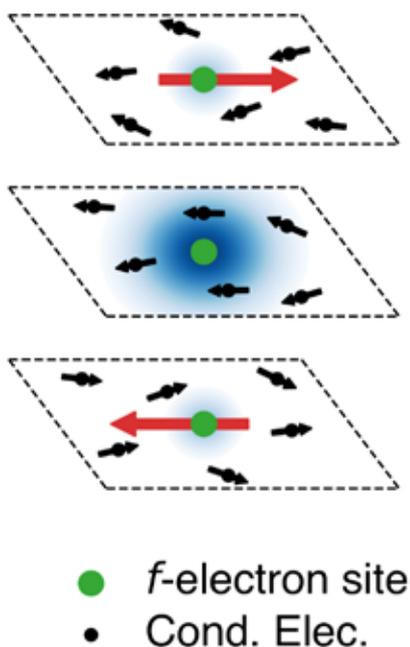
Related publication: D. M. Fobes et al. "Tunable emergent heterostructures in a prototypical correlated metal" *Nature Physics* 14(2018), 456-460

DOI: 10.1038/s41567-018-0060-9

Instrument: LET

 Marc Janoschek (Los Alamos National Laboratory)

Superconductivity, and other desirable properties, can arise (or be greatly enhanced) at the interface between two different materials. Electronic textures emerge spontaneously in bulk materials due to competing atomic-scale interactions, from which functional interfaces can arise. The control of these electronic textures would enable a top-down approach for designing new generations of devices. An international team of researchers has used high-resolution neutron spectroscopy on LET to probe the prototypical strongly correlated metal CeRhIn₅, revealing competition between magnetic frustration and easy-axis anisotropy—a well-established mechanism for generating spontaneous superstructures. The resulting self-assembling interfaces have major advantages; they are intrinsically clean, and relevant parameters such as the interface thickness can be tuned in-situ via external parameters such as magnetic field or temperature. Their work demonstrates that strongly-correlated electron materials are a promising route to producing tunable and emergent heterostructures, the basis for applications in adaptive electronics.



A spontaneously emerging interface in a quantum material is shown. In the top and bottom layers the atoms carry a magnetic moment (red arrow) that points in opposing directions. The center layer is akin to an electronic interface, in which the atoms do not carry magnetic moments because they are screened by the magnetic moments of the surrounding electrons (black arrows).

The structural and magnetic properties of thin-film yttrium iron garnet

Related publication: A. Mitra et al. "Interfacial Origin of the Magnetisation Suppression of Thin Film Yttrium Iron Garnet" Scientific Reports 7(2017), 11774

DOI: 10.1038/s41598-017-10281-6

Instrument: POLREF

Funding: European Union Seventh Framework Programme, EPSRC

 B. J. Hickey (University of Leeds)

Recent research in spintronics to develop efficient devices using spin currents has focused on magnetic insulators. Yttrium iron garnet (YIG) is a ferrimagnetic insulator with properties that make it ideal for use in spin pumping, spin transfer torque and spin Hall magnetoresistance measurements and applications. Spin currents can propagate over relatively long distances in YIG making it an ideal material for the emerging field of *magnonics*, where spin wave excitations can be exploited to transfer and process information in nanostructures. Unusual, and undesirable, magnetic behaviour is observed in thin films (<100nm) which also varies with temperature. The origin of this behaviour has remained elusive. A team of researchers, led by the University of Leeds, have used a variety of techniques to study the structural and magnetic properties of single crystal thin-film YIG. Polarised neutron reflectivity (PNR) measurements performed on the POLREF beamline have spatially resolved the magnetic profile of the layer to reveal an interdiffused region with magnetic and temperature dependent properties distinct to the bulk of the film. These results are of direct relevance to the large body of research in insulator-based magnonics.

Sniffing out hydrogen leaks

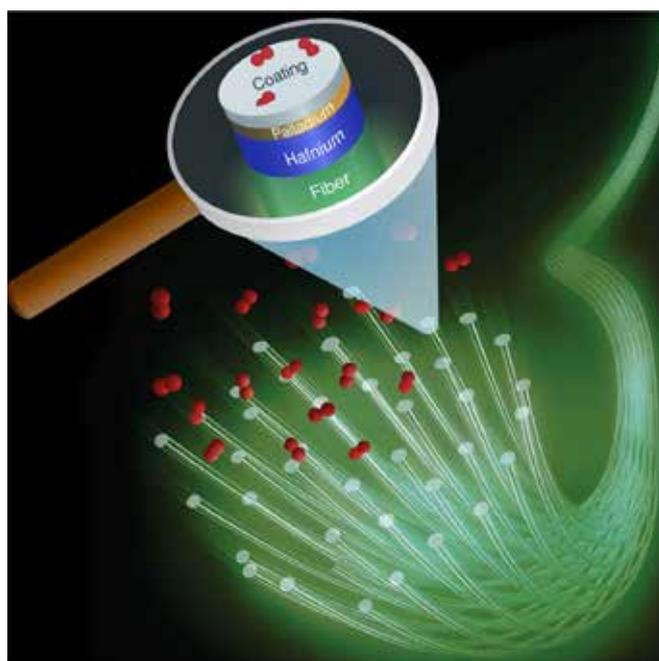
Related publication: C. Boelsma et al. "Hafnium—an optical hydrogen sensor spanning six orders in pressure" *Nature Communications* 8(2017), 15718

DOI: 10.1038/ncomms15718

Instrument: Offspec

 Bernard Dam (Delft University of Technology)

Hydrogen stands a good chance of being one of the replacements for fossil fuels as an energy carrier in the near future. It is clean, as water vapour and heat are the only by-products of combustion, and you can make as much of it as you want using just water and another energy source (for example solar energy). There are several hurdles that must be overcome before the vision of a 'hydrogen economy' can become a reality, one of which is finding a reliable way of detecting gas leaks. Researchers from Delft University of Technology, Catholic University of Leuven and ISIS have used neutrons on Offspec to help develop an extremely sensitive hydrogen sensor that can detect even the smallest of leaks with a proven hydrogen partial pressure range from 104 to 10⁻² Pa. This discovery brings us one step closer to safely using hydrogen as a low carbon emission energy carrier.



Placing a thin layer of hafnium on top of an optical fibre, before heating the fibre with a warm-up LED may solve the issue of hafnium working best at a temperature of around 120°C. A thin Pd layer is needed to allow for dissociative hydrogen absorption by the Hafnium. Credit: Christiaan Boelsma, Delft University of Technology.

Spontaneous decay of a soft optical phonon

Related publication: C. Stock et al. "Spontaneous decay of a soft optical phonon in the relaxor ferroelectric $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ " *Phys. Rev. Materials* 2(2018), 024404

DOI: 10.1103/PhysRevMaterials.2.024404

Instrument: Merlin

Funding: EPSRC, STFC, Carnegie Trust, Royal Society of London, Royal Society of Edinburgh

 Russell Ewings (ISIS Neutron and Muon Source) Chris Stock (Edinburgh University)

Phonons and magnons are elementary excitations that correspond to well-defined deformations of nuclear and magnetic lattices. These excitations are normally long-lived for harmonic potentials, but in some cases they spontaneously decay, resulting in unusually short lifetimes. Relaxors are anharmonic systems that are characterized by a broad, frequency-dependent peak in the temperature dependence of the dielectric permittivity. The perovskite $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ (PMN) is one of the most studied relaxors. An international team of researchers using the Merlin neutron spectrometer has found that specific phonon lifetimes in $\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ are unusually short within well-defined ranges of energy and momentum. Their results suggest that the well-known relaxor "waterfall effect" is a form of quasiparticle decay analogous to those observed in quantum magnets and fluids.

A computer-generated roadmap to new materials

Related publication: C. Collins et al. "Accelerated discovery of two crystal structure types in a complex inorganic phase field" *Nature* 546(2017), 280-284

DOI: 10.1038/nature22374

Instrument: HRPD

Funding: EPSRC

 Matthew. J. Rosseinsky (University of Liverpool)

Discovering new materials is a challenging process, as their boundless potential combinations of atoms, a great many of those combinations will not result in materials that are stable, and which can be synthesised. Researchers at the University of Liverpool developed a computer-guided strategy to speed up the discovery of new materials by identifying regions of compositional space likely to yield new materials. Their algorithm uses knowledge of crystal chemistry to suggest probe structures which are used to approximate the composition energy landscape and identify promising regions of chemical composition. Their calculations led them to the experimental discovery of two new materials, one of the structures was determined using neutron powder diffraction on HRPD, together with X-ray powder and electron diffraction to confirm the crystallographic symmetry. The structure obtained is a triclinic, 64-fold super structure of perovskite containing 102 atomic sites, without the high-resolution data the structure would have been insoluble due to the high degree of pseudo symmetry. This combined approach will accelerate the systematic discovery of new materials for many applications, including energy generation and storage.

International Collaborations

The ISIS Neutron and Muon Source has many international partnerships and collaborations, some of which have been ongoing for many years. These collaborations not only create new opportunities for researchers from partner countries to use ISIS neutron and muon instruments, but also provide additional resources, such as instrument upgrades, which benefit the whole ISIS user community. Two particular collaborations are highlighted here.

ISIS and RIKEN, Japan

ISIS has had a very long-standing partnership with RIKEN in Japan for muon science. In the early 1990's, RIKEN constructed the RIKEN-RAL Muon Facility at ISIS, consisting of four experiment ports for pure and applied muon studies. The first agreement between RIKEN and ISIS was signed in 1990, under which RIKEN built, owned and operated the muon facility for both Japanese and UK users. ISIS and RIKEN have just signed the fourth collaboration agreement, under which ownership and operations of the facility pass to ISIS, the facility will be refurbished, and a Japanese user programme run by RIKEN will also continue.



Kazunori Mabouchi (RIKEN) and Adrian Hillier (ISIS) marking the hand-over of the RIKEN-RAL Muon Facility to ISIS following the signing of a new agreement.

Indonesia and the Newton programme

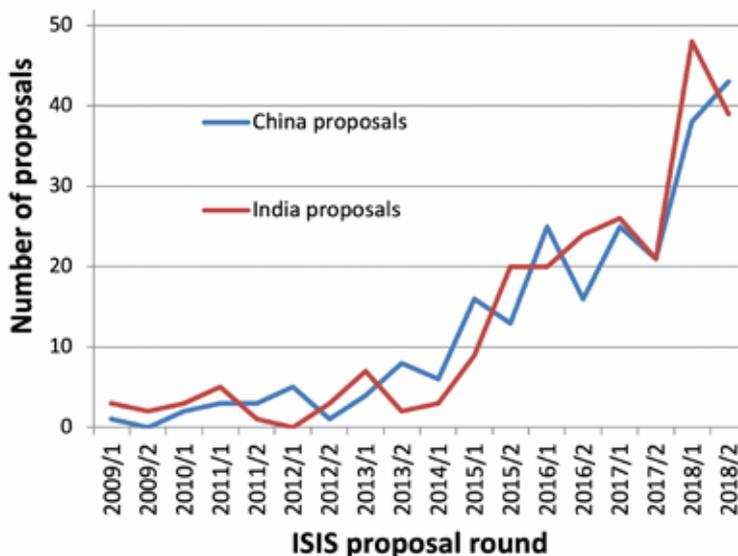
Indri Adilina (Indonesian Institute of Sciences) is based at ISIS for one year as part of the UK Government-funded Newton Programme. She is using ISIS neutron instruments to study catalytic processes for the production of useful fuels from biomass as a way of reducing our dependency on fossil fuels.



Indri Adilina

ISIS and India

ISIS also has a very long-standing partnership with India, which began in 1983, and which, more recently, has seen ISIS and India signing a new agreement for collaboration. The agreement with the Indian Department of Science and Technology, made through the Jawaharlal Nehru Centre for Advanced Scientific Research, gives access for Indian scientists to the ISIS instrument suite and contributes to the development of the Zoom small angle scattering instrument on the Second Target Station. Proposals to use ISIS from Indian scientists have trebled over the past few years thanks to this agreement and to UK Government Newton Funding for Indian scientists.



The Indian Minister for Science and Technology and Earth Sciences, Dr Harsh Vardhan and Director of ISIS, Professor Robert McGreevy.

Technology



Technology

Source Operation and Performance

This report covers the accelerator and target stations performance and beam delivery for the science programme in the period April 2017 – March 2018, corresponding to Cycles 17/1 through 17/4.

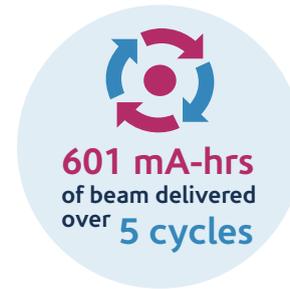
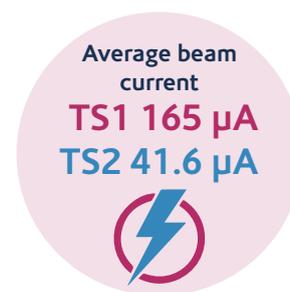
Cycle 17/1 2 May – 2 June (30 days)

Cycle 17/2 19 Sept – 19 Oct (29 days)

Cycle 17/3 14 Nov – 20 Dec (35 days) – TS1 only

Cycle 17/4 6 Feb – 26 March 2018 (47 days)

ISIS delivered 601 mA-hrs of beam over these five cycles. The accelerator delivered 141 days for the user programme (with TS1 running for 141 of these and TS2 for 101). Taking into account instrument down-time, plus calibration and commissioning time, the fully-scheduled instruments delivered 2971 days to the user programme (see section 3). The source reliability for the user programme was 85.6%¹. A summary of the performance is given in table 1.1 and a comparison with previous years is presented in Table 1.2. Figure 1.1 shows the average ISIS beam current and figure 1.2 the integrated current over the last twenty five years. Figure 1.3 shows details of the performance of the accelerator and target stations for all five cycles on a day by day basis.



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

Table 1.1: Performance in 2017/2018 Cycle by Cycle

Cycle	17/1	17/2	17/3	17/4
	2 May – 2 June 2017	19 Sept – 19 Oct 2017	14 Nov – 20 Dec 2017 (TS1 only)	6 Feb – 26 Mar 2017
Beam on target (hr)	631	568	589	989
Total beam current delivery for both targets (μ A-hr)	133840	122406	128786	215770
Combined beam current for beam on target (μ A)	212	215	219	218
- Target 1	171	175	219	183
- Target 2	41	40	0	35
Averaged combined beam current per hour (μ A)	212	217	191	225
Peak beam current over 24 hrs (μ A)	186	196	215	191

¹Off-time less than 1 hour.

Major Projects

ISIS Neutron and Muon Source has an ongoing programme of developments to ensure the continuation of cutting edge science.

ISIS Supporting the European Spallation Source

Staff at ISIS Neutron and Muon Source have been busy continuing their important contributions to several areas of the €1.8Bn European Spallation Source (ESS), currently being built near Lund in southern Sweden.

Loki is a SANS instrument currently in detail design and progress has been made by ISIS to develop boron detectors. Procurement of Loki components is due to start in early 2019.

FREIA is a reflectometer currently in concept design with analysis and development work being carried out to verify concepts.

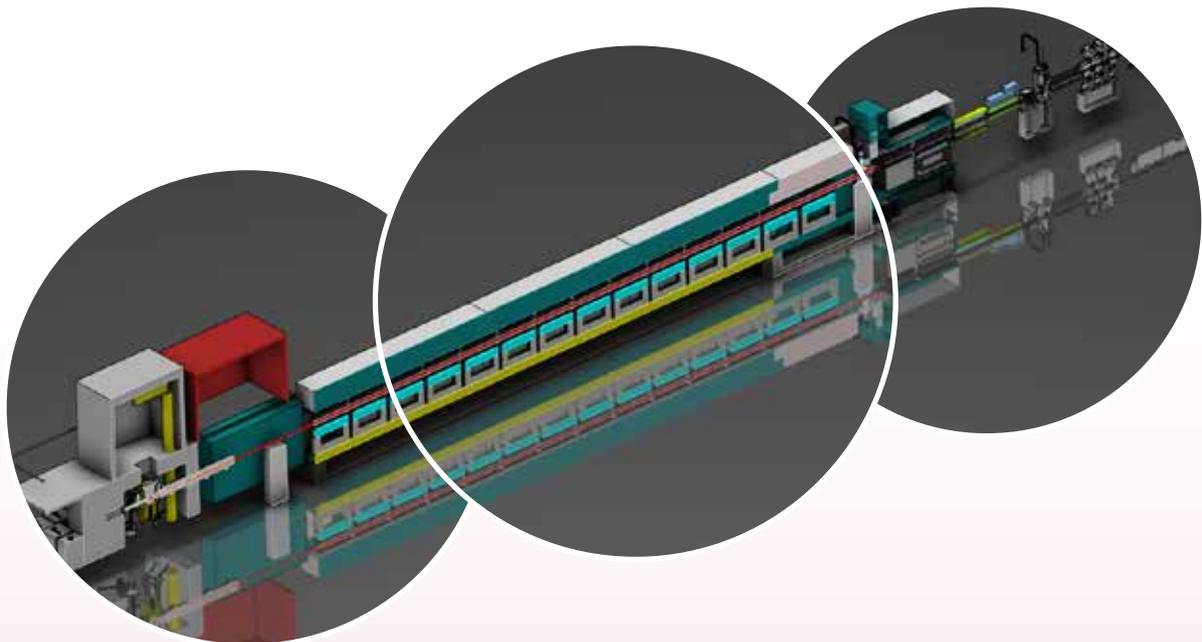
VESPA is a spectrometer currently being designed in conjunction with CNR Italy.

ISIS have designed chemistry laboratories for the ESS that are due for construction in Lund this year.

MICE Update

The journey that started in 2001 with the founding of the Muon Ionization Cooling Experiment (**MICE**) has come to fruition. MICE, based at ISIS, has demonstrated the cooling of muon beams with lithium hydride and liquid hydrogen absorbers. This technique will enable the preparation of a beam of subatomic particles known as muons ready for acceleration to high energy.

High energy muon accelerators have never been built before, but they could have a big impact on the world of fundamental physics and answer important questions about the nature of the universe. At present, the data from MICE is being analysed. Several publications are in preparation.



VESPA is a spectrometer currently being designed in conjunction with CNR Italy.

Linac accelerator tank 4 replacement project

The project to replace the vulnerable ISIS Linac tank 4 in 2020 is well underway. The 6 sections that make up the 12m tank were successfully delivered to the ISIS Accelerator workshop from the Netherlands in early 2018. The 2m sections were temporarily assembled for alignment testing on site and excellent results were achieved, confirming the specified high tolerances were maintained throughout machining, processing and transportation. The parts will be reassembled in a dedicated test area later on in the year and the drift tubes will also be installed and aligned to the tank. It is planned to condition the 12m tank up to full power and hold at an operational level for several weeks in order to build confidence that it will fulfil the demands of a typical ISIS machine cycle.

As the date to replace the existing linac tank fast approaches significant planning is also in progress. After more than 40 years of service the linac tank is radioactively active and careful plans are needed to ensure the area is not contaminated as the old tank is removed.

Target Station 1 Project

The Target Station 1 (TS1) Project seeks to develop and upgrade key elements of the target station, which has run for over 30 years without significant maintenance or development work.

Highlights from the last year include: placing orders for many of the large procurement contracts, creating several prototypes for key components and assemblies to test manufacturing routes and techniques and to allow design verification, and carrying out several packages of preparatory work including replacement of ventilation systems and control unit upgrades and more.

The neutronics analysis for the TS1 project has calculated the change in instrument performance and engineering relevant nuclear quantities such as nuclear heating. The calculations are performed using Monte Carlo radiation transport simulations of the proton beam and subsequent spallation neutron generation and moderation processes. This methodology has been extensively benchmarked against experimental results for the current ISIS TS1 which shows very good agreement for the instrument resolution and within a factor of two agreement for absolute neutron fluxes. The neutronics analysis for the TS1 project allows us to have confidence that the new target can be operated safely and that we can predict the effect on instrument performance.



All six sections of the 12m tank IV replacement temporarily assembled at RAL in April 2018.



Test tank: view with traditional and conical drift tubes.



As part of the TS1 Project this full-scale target, reflector and moderators (TRaM) mock-up has been constructed, complete with remote manipulator arms. The set up allows staff to test components and practice procedures in a representative environment.

Instrument Updates

TOSCA

Tosca is an indirect geometry spectrometer optimised for the study of molecular vibrations in the solid state. The instrument has been operational for more than two decades and recently underwent an upgrade to significantly increase the neutron flux available for experiments, enabling the instrument to further participate in strategic research areas such as CO₂ capture, catalysis and charge storage.

MAPS was the first chopper spectrometer to employ a large array of position sensitive detectors, and the first to be designed solely for the purpose of measuring excitations in single crystals. December 2017 saw the completion of the MAPS instrument modernisation programme, resulting in an order-of-magnitude increase in neutron flux that will open up significant new science possibilities on the instrument.

MAPS

GEM

The incident beam path of the GEM instrument has been upgraded during an extended winter shut down period, replacing the original beam defining jaws with independently-controlled in-vacuum collimators, removing the majority of the aluminium vacuum windows and re-surveying and re-aligning the beam. As a result we have increased the neutron flux on the sample by around 20% and reduced the instrument backgrounds.

The guide upgrade on MARI has been completed successfully and the detector electronics upgrade is progressing well. The first commissioning measurements have confirmed the expected order-of-magnitude increase in neutron flux. The full commissioning of the upgraded instrument is expected to be completed by the end of the year with the user program starting in early 2019.

MARI

OSIRIS

The silicon analyser upgrade project for the OSIRIS spectrometer has moved into the implementation phase with detailed engineering drawings and Monte Carlo simulations.

The vacant analyser side of the instrument will be occupied by a silicon analyser, which provides new capabilities in dynamic range for the user community.

IMAT is the new neutron imaging and diffraction instrument, designed and built for non-destructive analysis and in-situ testing in diverse disciplines such as engineering material science, hydrogen-related technologies, battery research, earth science and cultural heritage. IMAT is now open for imaging applications and allocates 50% of its time for the user programme, alongside which further commissioning work is being carried out and whilst two large diffraction detector arrays for strain and stress analysis are being prepared for installation next year.



Zoom will be a flexible, high count rate small angle scattering instrument with the ability to reach very small Q. It has entered the science commissioning stage, which has confirmed that the instrument capabilities are in accordance with the specifications. The motion control safety system was installed during the 2018 summer, and the instrument is open to users.

IRIS is a high resolution quasi-elastic and inelastic neutron scattering spectrometer. Developments have been made on its sample environment and data analysis, equipping IRIS towards becoming the gateway to QENS at ISIS. High-throughput capabilities and more automated capabilities (including software) provide a simpler and less labour-intensive user experience.



Target Station 1

Accelerators and Targets



Accelerators and Targets

The Accelerators and Experimental Operations divisions are responsible for developing and operating the ISIS machine. Over the past 12 months the divisions have been involved in a range of activities including new power drives for the RF cavities and new beam chopper prototypes as well as organising international conferences and a Particle Accelerator Careers Open Day. Here are some of the highlights.

Dipole Scintillators Installation Programme

Daniel Harryman and apprentice Jack Day, ISIS Diagnostics Section (image 1), installing new scintillating beam loss monitors inside a synchrotron dipole magnet. Over the past year, these monitors have been installed in each dipole to provide additional information during accelerator setup and operation, enabling fine tuning to reduce beam loss and reach higher beam intensities without damaging or activating other accelerator components.

BBQ Tune Measurement System & Collaboration with CERN

Will Frank, ISIS Diagnostics Section, with the recently installed Baseband Tune (BBQ) Measurement System, developed in collaboration with the Beam Instrumentation Group at CERN. The system uses signals from Beam Position Monitors to provide on-line measurements of beam oscillations in the synchrotron. Optimising and controlling these oscillations improves the quality, stability and lifetime of the beam, and can reduce beam loss during acceleration.

Synchrotron Magnets Vibration Monitoring System

Julian Brower and Asim Yaqoob (image 2) of the ISIS Performance Improvement Team, testing a vibration monitor installed on a synchrotron dipole magnet. These monitors, installed on dipoles and quadrupoles around the synchrotron, will enable condition monitoring of these critical magnets in real time; providing robust data previously unavailable and replacing the need for periodic manual tests.

Personnel Protection System

Mark Arnold and Elliot Taylor (image 3), ISIS RF Group, with new personnel protection system racks ready for installation into the outer synchrotron. The new racks incorporate upgrades and additional functionality to existing health and safety measures when staff are required to work in the synchrotron hall.



High Power Drive Amplifier Upgrade

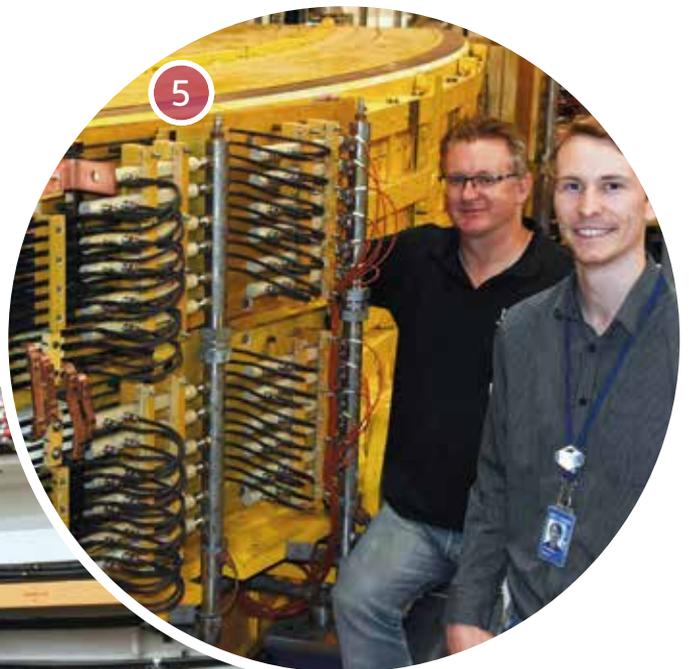
The RF Group's synchrotron section (image 4; left-right: Rob Mathieson, Neil Farthing, Dave Gibbs, Dave Allen, Noel Mcnamee & Andy Seville), with the newly installed High Power Drive (HPD) amplifier, fitted to the 2nd Harmonic RF Cavity in straight 6 of the synchrotron. The upgraded HPD is designed to provide additional power to the accelerating cavities, enabling more consistent operation at higher intensities and also reducing downtime on ISIS.

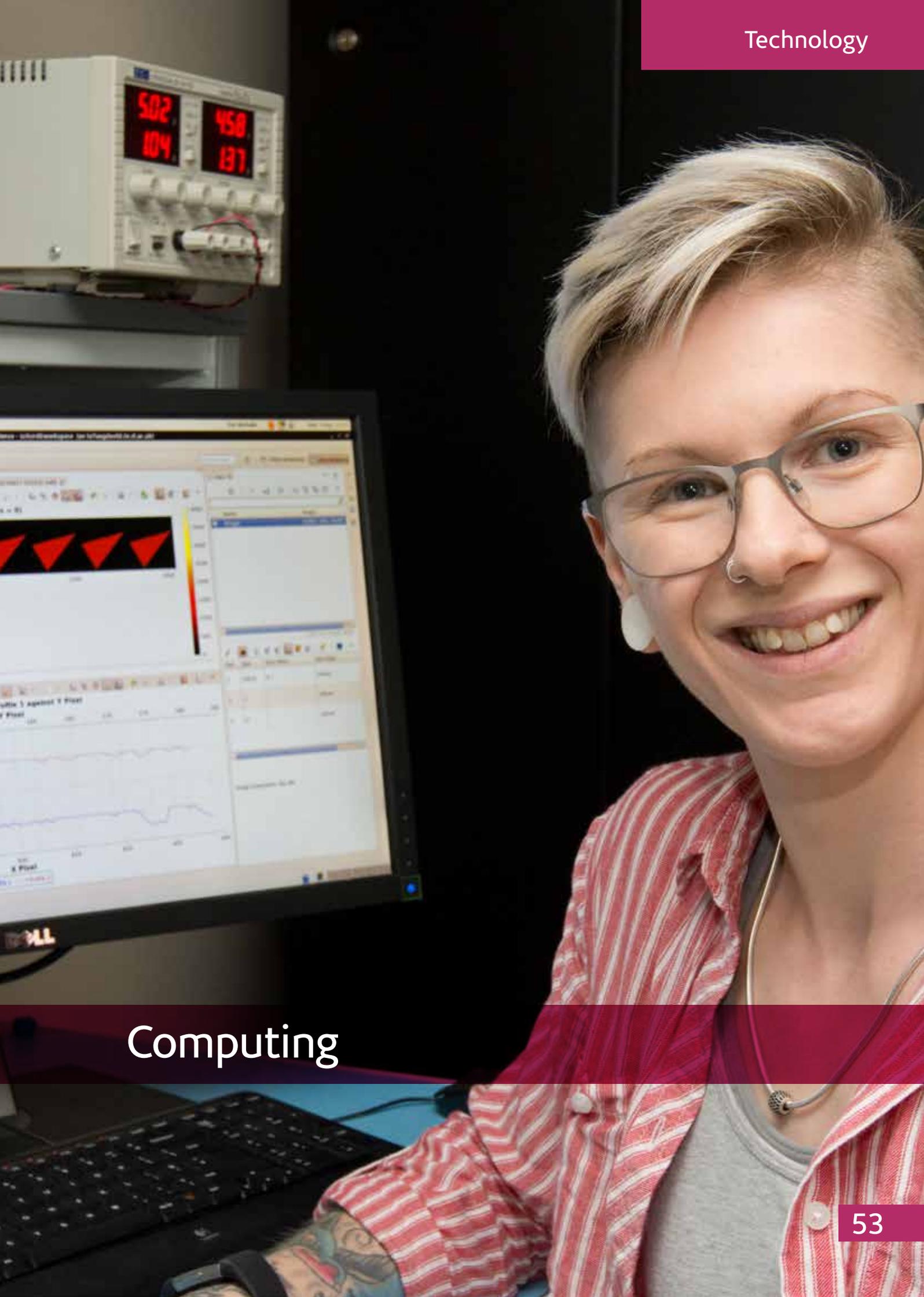
Mica Dipole Coils

Oliver Newell, Jim Loughrey, and Jon Speed (image 5), next to a synchrotron main magnet dipole coil with mica impregnated insulation. Electrical faults in dipole coils have caused significant downtime in recent years, which has been mitigated by reducing their operating voltage, requiring ISIS to be run at lower beam energy. Mica insulation has a higher withstand voltage than the existing glass insulation, meaning the new coils will lead to fewer dipole faults and re-enable consistent 800 MeV operation.

Linac Tank 4

Six sections of a new accelerating tank for the ISIS Linac (pictured here in the R78 workshop), totalling 12 metres in length, were assembled at RAL during 2018 for alignment and fit checks. The new tank is scheduled for installation in 2020 to replace the existing Linac tank 4, which has been in use since 1976.





Computing

Computing

Several groups are responsible for developing and operating computing to support the needs of the facility and its users. Over the past 12 months the groups have continued to develop instrument control capabilities, enhance data reduction software, provide data cataloguing and storage, and deliver the computing infrastructure, software and IT support to both business and science.

The Ada Lovelace Centre

Development of computational facilities to enable ISIS users to get the most out of their data is a very important activity. This includes the Mantid data analysis and visualisation framework which is in use across the ISIS instrument suite as well as at other facilities world-wide. It also includes developing further data analysis infrastructure in collaboration with Diamond Light Source, the Central Laser Facility and the Culham Centre for Fusion Energy. All four facilities, together with STFC's Scientific Computing Department, have formed the Ada Lovelace Centre (ALC) with the aim of working together to develop data processing, computer simulation and data analytics. The ALC has just received an initial £4M of funding for development of infrastructure to give facility users access to data, modelling codes and computational resources, as well as cataloguing and archiving facilities and exploration of deep learning and artificial intelligence methods for facility data analysis and data mining.

Mantid

As the now widely used Mantid data processing software is maturing its priorities changes, as specified by its user community. One such change is towards better stability and reliability. This year this was achieved through the implementation of automated testing of several Mantid Graphical User Interfaces (GUIs). GUIs are one of the most difficult part of a software to test well; the approach taken by Mantid is to adopt the so-called software engineering pattern called MVP, which stands for Model-View-Presenter.

In October 2008 the first seven TS2 instruments entered the user programme. As the number of users and experiments has grown over the last 10 years so

has the demand for more automation and web-based applications. To ensure we have the software engineers we need to both develop these new systems and maintain and support existing systems, we have built up a diverse team at various stages in their career. This year we have welcomed two new experienced team members, two graduates, two apprentices and two sandwich students.

The online proposal systems have been improved, giving users more control over their personal data. We have made it easier to see what is needed in the experiment risk assessment, and ensured the ISIS website remains fit-for-purpose including improving how users find the computing-related information when they need it.



Ada Lovelace, pioneering computer scientist



Skills

Developing the skills of our staff and wider scientific community is vital to maintaining our status as a world-leading research facility. We also have a key role to play in inspiring the scientists and engineers of the future. We offer a wide range of hands-on training, offer around 150 placement opportunities and have an active public engagement programme.

Placements



24
Graduate
Students



39
co-sponsored
PhD students



21
vacation
students



work experience
placements



16
undergraduate
sandwich
students



Apprentice
placements



4011 total
visitors, including
2381 schools,
students, and
public visitors



Staff talks

Inspiring the next generation



Inspiring the next generation

2017–2018 has been another active year for public engagement at ISIS Neutron and Muon Source, with the facility welcoming over 2300 school students, teachers and members of the public for talks, workshops and tours of the experimental halls. A further 2000 members of the public have engaged with ISIS science and engineering at off-site events, with ISIS staff and students heading out to local schools, festivals and fairs, reaching new audiences and inspiring the next generation of scientists and engineers.

Opening its doors to the public for several large events a year, ISIS sees hundreds of visitors flooding into the facility to hear about the cutting edge science and engineering that goes on, from superconductors and soaps to ancient swords and Amati violins. Public access days are always very popular, and participation in large events such as the European Researchers Night, Stargazing at RAL, the Institute of Engineering and Technology Open Day and Oxfordshire Science Festival have captured new audiences. School activities including Education Access Days, Particle Physics Masterclass, Chemistry at Work, Science in

the Park and Science in Your Future have excited hundreds of pupils from across the country about ISIS science and engineering. 2017 also saw ISIS hosting a summer Open Day, with almost 500 visitors touring target station 2, taking part in hands-on science and engineering activities, making slime and crystal gardens, and enjoying demonstrations using liquid nitrogen, flame tubes and robotic arms!

For 2018 - the Year of Engineering - ISIS has expanded its portfolio of engineering-focused activities. Events including Exploring Engineering days, the ISIS Schools Accelerator Day and Apprentice Open Days have inspired secondary school pupils about engineering at ISIS and STFC. This year ISIS staff participated in the Engineering Education Scheme, working with local school pupils over a 6 month period on a real engineering challenge at ISIS, designing and building a prototype of a second shutter on the ISIS ChipIR instrument.



Developing the student community



Developing the student community

The student community continues to lie at the heart of ISIS Neutron and Muon Source. More than 75 co-sponsored PhD students, vacation and sandwich students worked at the facility in 2017–2018. In addition, there were nearly 1000 visits from PhD students to ISIS for experiments. The facility seeks to encourage and grow the student community in three key ways: training courses, supervision and on the job training.

Training Events

2017–2018 saw a range of training events aimed at students including the ISIS Neutron Training Course, the ISIS Muon Training School, ISIS Student days and a variety of more specialised talks and courses

Student Conferences

Each year ISIS organises 2 student-specific meetings: the ISIS Student Meeting held in October and a satellite student day at the UK Neutron & Muon Science and User Meeting (NMSUM). These provide opportunities for students to present their research to their peers, chair the meeting sessions and challenge them to ask questions of each other, as well as network with students who also spend significant time at large scale facilities. Students are educated on a variety of topics ranging from catalysis to strain mapping. 2017/18 saw increased attendance at both events and excellent presentations, showcasing the very diverse research with the ISIS community.

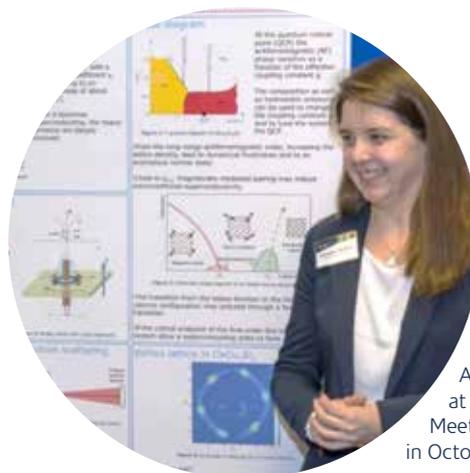
Supervision

ISIS staff are also co-supervisors of many PhD students, in addition to managing sandwich students, apprentices or graduates within ISIS. PhD student co-supervision is always done in partnership with a university collaborator and students will spend an extended period at the facility – at least one year over their PhD period.

On the job training

ISIS had 1020 visits by PhD students (607 unique PhD visitors) in the 16/17 year who came to run experiments at the facility. These students benefit from the training experience that this provides, in terms of experiment planning, learning about the neutron or muon techniques, experience with sample environment equipment and computing and interacting with more experienced ISIS staff.

ISIS provided some 7000 PhD student training days in the 16/17 year.

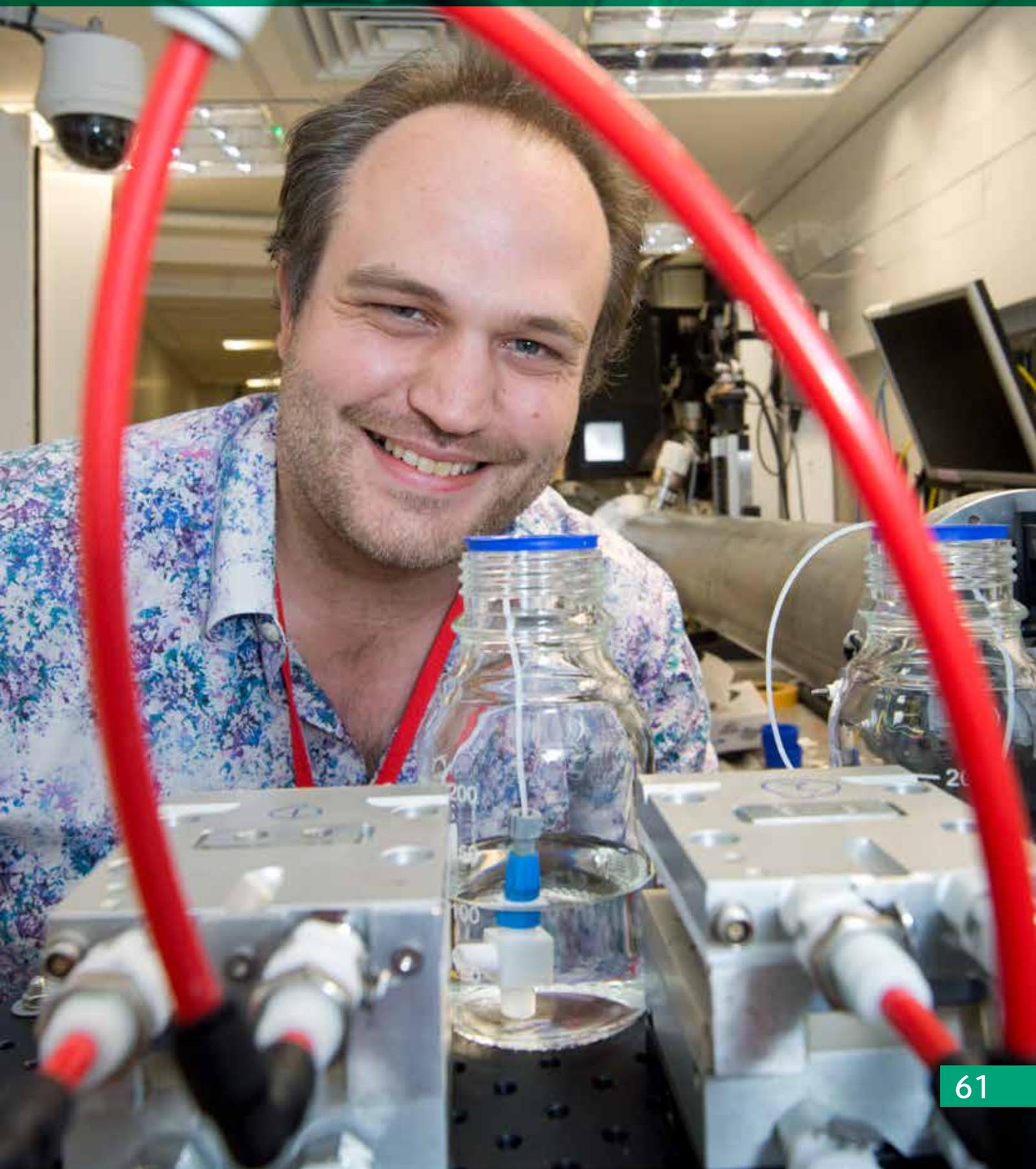


A poster presentation at the ISIS Student Meeting which took place in October 2017 in Abingdon.



Students at the 2017 ISIS Student Meeting in Abingdon.

Developing the wider neutron community



Developing the wider neutron community

ISIS Neutron and Muon staff organise, or have major input in organising, many different events, workshops, conferences, user groups and seminars for the neutron and muon community. In addition, ISIS staff deliver many talks at a variety of meetings, including presentations at conferences and workshops, departmental seminars and more. A few highlights from the last year can be found below.

Muon Training School

ISIS Neutron and Muon Source runs a biennial training school on how to use muons as a research tool. These include a variety of lectures and workshops on the muon techniques given by experienced researchers, and also the chance to perform muon experiments. The school welcomed 30 attendees over 5 days in March.

Neutron Training School

The annual ISIS Practical Neutron Training Course is aimed at PhD and post-doctoral researchers who have little or no experience of neutron scattering, but whose future research program aims to make use of neutron scattering techniques at ISIS. There were 35 at the school, which ran over 10 days in late February.

Neutrons Matter Workshop

The seventh international workshop on electron-volt neutron spectroscopy was held in November 2017 in Rome, Italy. The workshop celebrated the partnership between CNR and STFC in scientific research at ISIS Neutron and Muon Source, focusing on recent developments in electron-volt neutron spectroscopy. The conference proceedings have recently been published in Journal of Physics: Conference Series.

Muon Spectroscopy User Meeting - Future Developments and Site Calculations

This meeting was held to mark a new agreement between ISIS and RIKEN for future operation of the RIKEN-RAL facility and to highlight the developing plans for a major upgrade of the ISIS MuSR spectrometer. The event was held in July 2018 in Abingdon with talks focused on the scientific opportunities associated with these new developments.

PNCMI 2018

The 12th International Conference on Polarized Neutrons for Condensed Matter Investigations took place in July 2018. The conference covered the latest condensed-matter investigations using polarised neutrons and state-of-the-art methodologies and techniques of polarised-neutron production and utilisation for novel instrumentation and experiments.

UK Neutron and Muon Science and User Meeting

The UK neutron and muon science and user meeting is an opportunity to hear about the latest science from ISIS Neutron and Muon Source and ILL, plus updates from the facilities and other matters of interest to neutron and muon users. The meeting comprised of a dedicated student day, a science day and a user meeting, and was held at the University of Warwick. In 2017 it attracted the highest number of attendees ever – over 260 attendees.



Attendees at the 2018 Muon Training School



Dr Igor Zaliznyak, Brookhaven National Laboratory, USA, speaking at the PNCMI conference on the 4th July 2018.



Delegates at the PNCMI conference.

Developing our people



Developing our people

ISIS has several initiatives to support our staff, from the thriving graduate and apprentice schemes to encouraging further study by part-time PhDs to professional memberships. In addition formal recognition of ISIS staff member expertise is given by other institutions through visiting or honorary appointments, professorships or lectureships.

Congratulations to Dr Devashibhai Adroja, has been promoted to IM scientist.

Dr Devashibhai Adroja has been promoted to STFC Individual Merit Fellow in recognition of his work on magnetic materials using inelastic neutron scattering and muon spectroscopy.

Prof Jacqui Cole awarded Senior Research Fellowship in Data Driven Molecular Engineering of Functional Materials

The Royal Academy of Engineering has awarded Jacqui Cole, who has a joint appointment with Cambridge University and ISIS, a 5-year Fellowship under their Research Chair and Senior Research Fellowship scheme.

Jacqui Cole is Head of Molecular Engineering at Cambridge and has a long history of collaboration with the Science and Technologies Facilities Council (STFC). ISIS is the founding external partner to Molecular Engineering at Cambridge. The Royal Academy of Engineering award enables Jacqui to welcome a new external partner, BASF, the world's largest chemical company, to join the collaboration.



Dr Devashibhai Adroja



Prof Jacqui Cole

Case study: Claire completes the final year of her degree during her year in industry

Placement student Claire Wilde recently completed the final year of her Chemistry degree by distance learning alongside her year in industry at ISIS. Traditionally sandwich students return to university for a year after their placement has finished to complete their degree. We catch up with Claire to see how she juggled work and study at ISIS Neutron and Muon Source.

What have you done during your year in industry?

I work in the muon group at ISIS Neutron and Muon Source. I make online learning materials which are then used as pre-course materials for the Muon Training School. This is a training school that the muon group at ISIS run every 2 years to help PhD students and post docs learn about muon spectroscopy.

Tell us some of your highlights from your year in industry...

I really enjoyed the muon training school as I got to speak to the students who actually used my materials which was a really big highlight for me. The feedback has been really positive; on a survey to students who used my resources over 90% of them said they found them useful.

I also got to go to the SINE2020 conference in Italy to present my work as SINE2020 partially fund my placement.

Has your placement helped you decide what you want to do when you graduate?

This year I've been doing my final year by distance learning at the same time as my placement, I'm actually graduating a few days after my placement ends. My manager and senior line manager have both been really flexible throughout the year.

I always thought I'd definitely work in lab, but I've really enjoyed this placement. Though I'll be starting work in a lab at a pharmaceutical company called Aptuit after graduating I don't want to rule anything out long term.

Has the placement year been what you expected?

It's been a lot harder than I thought balancing university and work! But I've enjoyed it a lot more than I thought I was going to. As I didn't know very much about muons before starting my placement I thought I would struggle a lot more than I did. I think I've surprised myself by how much I've learnt this year.

Would you recommend doing a placement at ISIS to other students?

Yes definitely! One of the great things about it here is there are lots of other placement students, if you have any struggles there is a support system there. Placement students here also have a good relationship their managers; I meet with my manager at least once a week. I would say it's a positive environment to work in too. I feel like I've had a more positive experience than my friends doing placements at other companies.



Claire Wilde stands outside Target Station 1.

Case study: Developing new skills

Name: Emma Hancock

Job: Apprentice Software Developer

Tell us a little bit about your background and about what you do?

I didn't become interested in software development until I had left school and started learning it for myself at home. I then decided that I would get an apprenticeship so that I could learn the skills I needed whilst working at something I enjoy. I am currently doing a degree apprenticeship in Software Development, rotating around different departments so that I can gain extensive knowledge of the different areas.

Why did you choose to do an apprenticeship?

I wanted to learn whilst doing a job so that I could put everything that I am learning into practice, and so I could also gain valuable experience of the industry.

What is your favourite project you have worked on?

So far my favourite project has been the scheduler. There are so many different layers to how the scheduler works, all in different coding languages so I have learnt so much!

Where do you hope your career will take you in the future?

I hope that once I have finished my degree apprenticeship I can get a full time job here. I want to continue to learn as much as I can.

How does your job make a difference?

People all over the world use the scheduler to check when they are coming here to use our equipment. It helps them book to come to ISIS, their transport and accommodation.

What would your advice to young people who'd like a career like yours?

Try and get work experience in the industry so that you have a greater knowledge of what you are doing. Try to keep working on your skills – it will help you in the future when applying for jobs in the industry.

Finally, do you have any heroes who have inspired you?

Someone who I look up to is Lyndsey Scott, because she has helped to break the stigma around women working in engineering. She is a famous supermodel who works for massive brands like Louis Vuitton and Victoria's Secret, but it also a software developer. I think she has helped to make people realise that being a software developer doesn't just mean you sit by yourself behind a computer, she reminds people that it doesn't matter what gender you are or what you look like, there is always a way for you to make a difference in technology.



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Science and Technology Facilities Council, Rutherford Appleton Laboratory,

Harwell Oxford, Didcot, Oxfordshire OX11 0QX, UK

T: +44 (0)1235 445592 F: +44 (0)1235 445103 E: isisuo@stfc.ac.uk

www.isis.stfc.ac.uk