

# ISIS Neutron and Muon Source Annual Review 2019



### The ISIS Neutron and Muon Source

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](mailto:isisuo@stfc.ac.uk)

[www.isis.stfc.ac.uk](http://www.isis.stfc.ac.uk)

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ISIS Director, Prof Robert McGreevy	01235 445599
User Office	01235 445592
ISIS Facility Web pages	<a href="http://www.isis.stfc.ac.uk">http://www.isis.stfc.ac.uk</a>

ISIS production team: Andrew Collins, Sara Fletcher and Rosalind Davies

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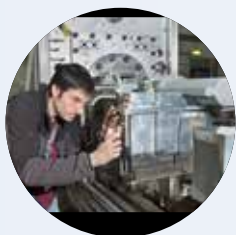
Industrial Science – in 2018/9 60 companies used neutrons and muons to support their research, including Toyota, Tata Steel, Cobham RAD Europe, Johnson Matthey.

[Find out more on Page 7](#)



Our Impact Awards showcase some of the contributions our users make to science, society and the economy.

[Read more on Page 15](#)



Our long shutdown starts in 2021 with a programme of work to extend the life of the facility for many years to come.

[Read about the developments on Page 53](#)



ISIS is committed to inspiring the next generation of scientists and engineers, which we deliver through a strong public engagement programme.

[Read about some of our activities on Page 67](#)



Over 800 PhD students carry out experiments at ISIS every year. The facility seeks to encourage and grow the student community through networking events, training courses, supervising and on the job training.

[Read more on Page 69](#)



# Foreword

## Welcome to the ISIS Neutron and Muon Source Review for 2019!

ISIS is approaching the end of its 35th year of operation. At this 'age' it is inevitable that some of the people who made major contributions in the early days of the facility, and indeed over many years, will have passed away. During the past year we have unfortunately lost several such friends and colleagues. Alan Leadbetter was a central figure in UK large facility science, being ISIS director, then director of the Daresbury Laboratory and finally of the Institut Laue Langevin. Uschi Steigenberger spent most of her career at ISIS, moving from instrument scientist to group leader to division head before becoming director in 2012. She was also a strong, and early, supporter of careers for women in science and technology. Don Paul (Warwick University) was one of the best known users of ISIS and ILL, active in supporting the facilities and the UK user community through serving on different committees and panels, including chairing our annual user meeting a number of times. Sten Eriksson (Chalmers Technical University) was a pillar of the

Swedish user community and for 15 years the driving force behind the ongoing Sweden-ISIS collaboration, including significant funding for development of POLARIS and IMAT.

I have little doubt that they would all be excited about our plans for the future of ISIS. With several European neutron facilities closing this year, and with no sign that neutrons and muons will outlive their usefulness, we need to plan for at least another 35 years. In order to ensure continuing reliable operation, in 2021 we will start a long shutdown for the replacement of the entire TS1 target/moderator system and of Linac Tank IV. Following this work our focus will shift to the (imaginatively named) Endeavour project for upgrading our instrument suite, and to the early development work needed to prepare for a possible future new ISIS (so far unimaginatively named) ISIS-II. Surprising as it may seem, if we want to have a new facility available in 20 years we really do need to start work now!

*Robert McGreevy,  
Director of the ISIS Neutron and Muon Source*



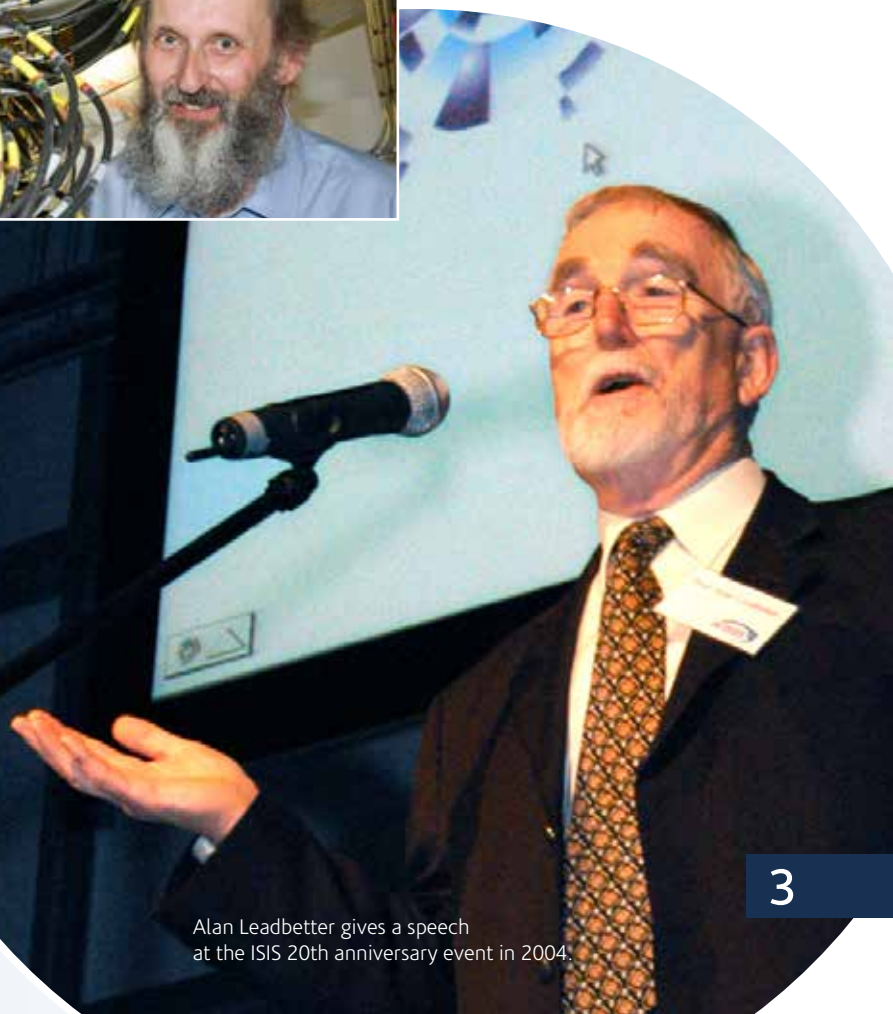
Sten Eriksson at ISIS.



Dr Uschi Steigenberger's leaving presentation at ISIS on 24th October 2012.



Don Paul, long-time ISIS user, who passed away this year.



Alan Leadbetter gives a speech at the ISIS 20th anniversary event in 2004.

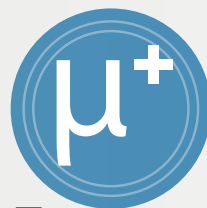
# The ISIS Neutron and Muon Source

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.

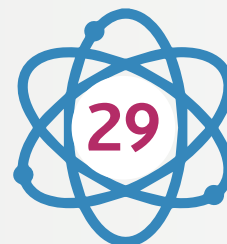
We are part of the global research structure, providing tools for over 1700 scientists a year to use our suite of 34 instruments.

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.



**5 Muon instruments**



**Neutron instruments**



Members of the public, schools and other visitors



**825 PhD students visited as users**  
(456 UK, 369 Intl)  
4800 days of student training



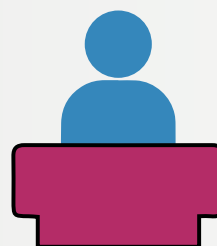
**new users 32%**



**unique research visitors 1771**



**1505 proposals received from 32 countries**



**3478 user visits**



**Companies**

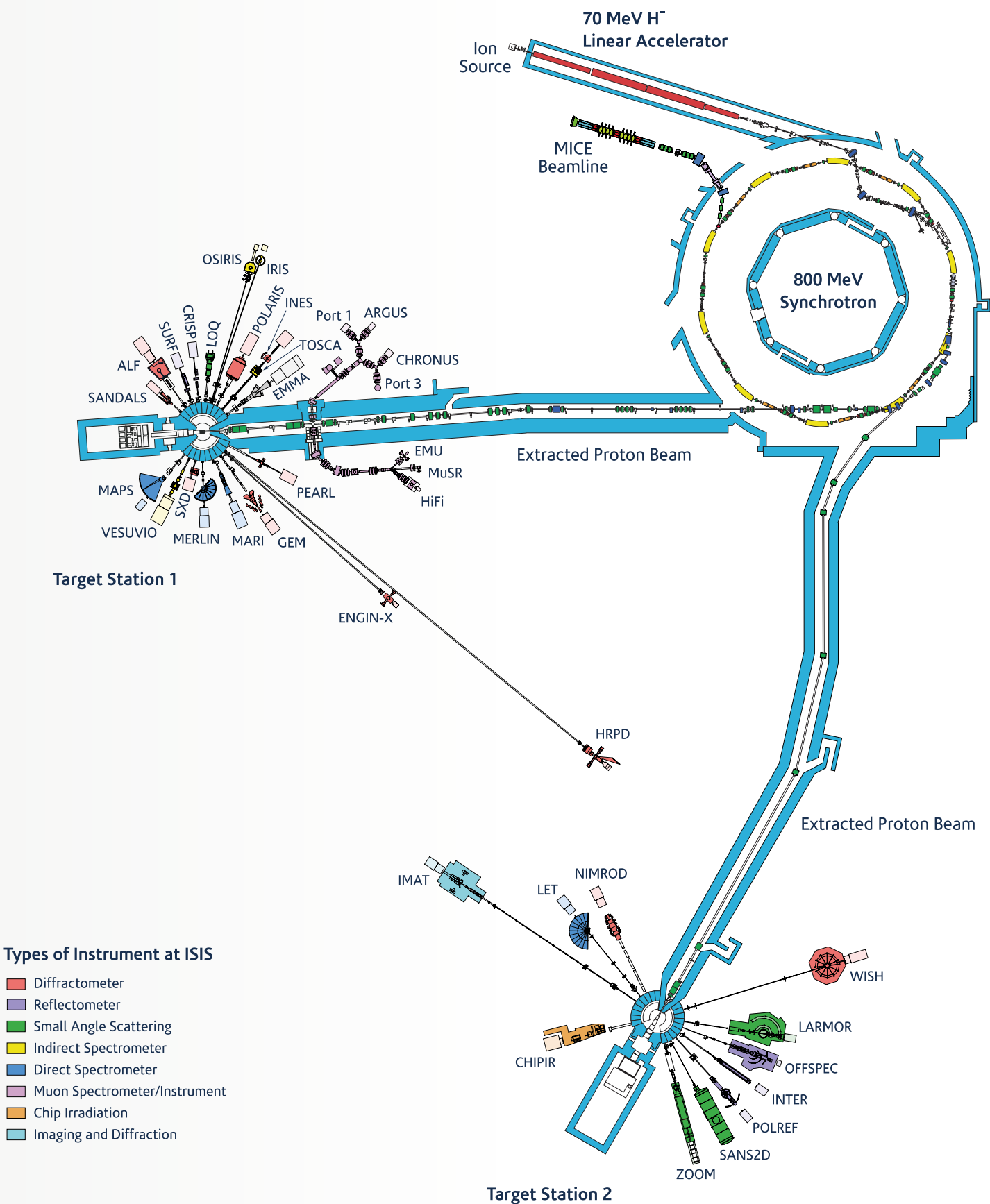
Represent a variety of industrial areas, including chemicals/plastics, healthcare, automotive, materials, aerospace, engineering, energy, petrochemical and other high-tech companies.



**Journal publications**



**358 Xpress proposals**



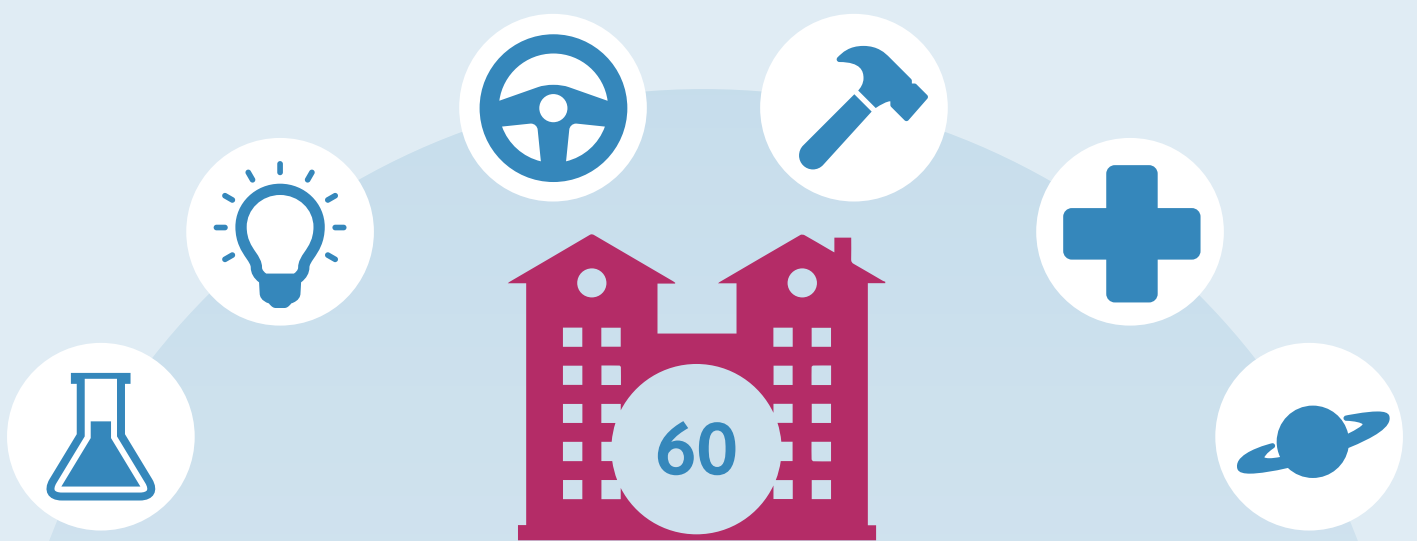
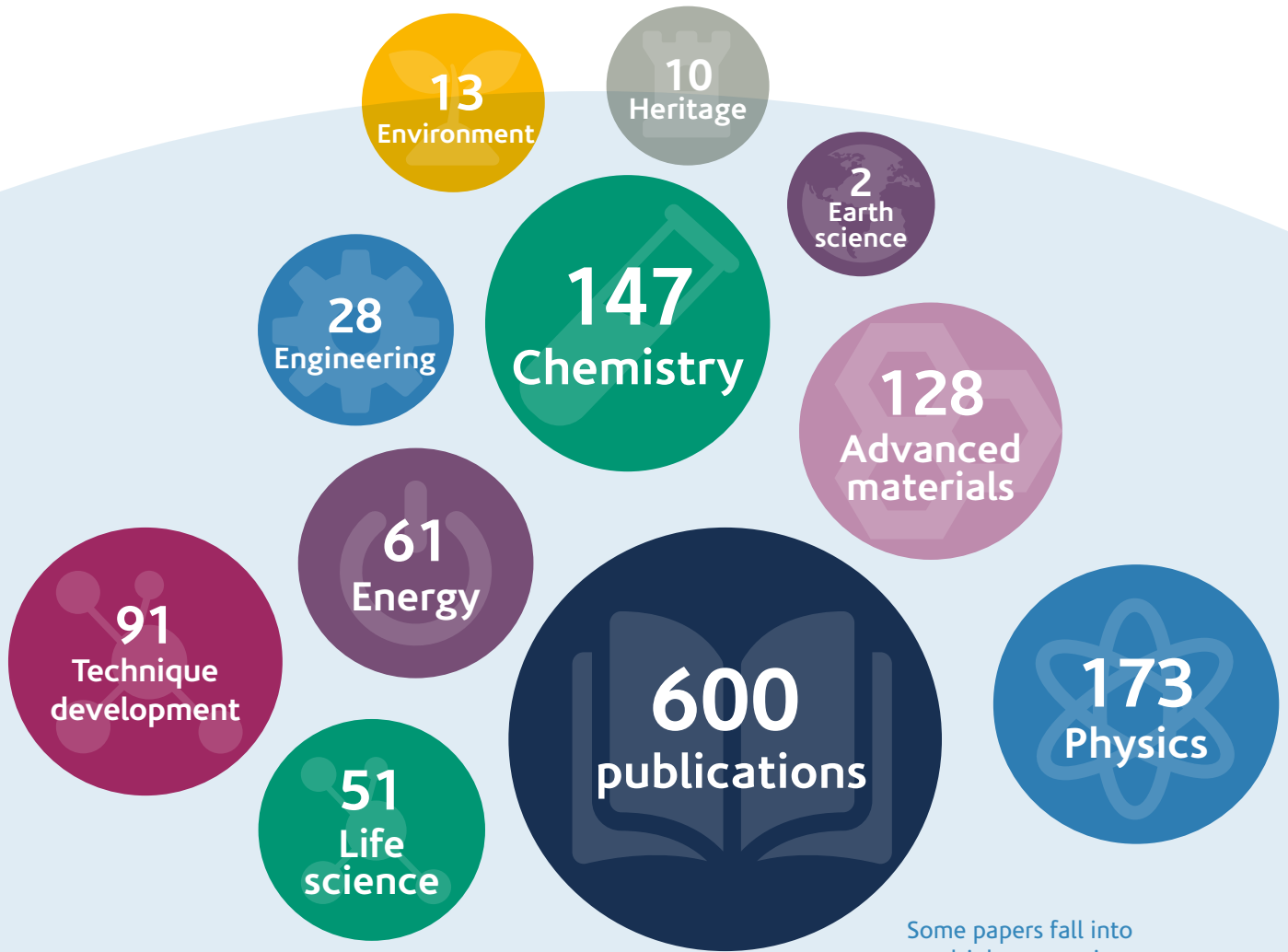
# Science at ISIS



## Science at ISIS

Science at ISIS spans a wide range of scientific disciplines, from pharmacology, cultural heritage, engineering, chemistry and fundamental research. The facility is used by over 1,700 scientists every year from both academia and industry. This section gives a snapshot of ISIS research over the past year.





# Industrial Science



## Industrial Science Highlight: Cobham use ChiPlr to bring a product to market



Cobham RAD Europe Ltd have brought a new product to market thanks to STFC's Bridging for Innovators (B4I) programme, which enabled them to access the unique capability offered by the ChiPlr beamline at ISIS for cosmic radiation testing.

Cobham's 'Aviator S' device is intended primarily for communicating flight data between the aircraft and the ground, but potentially has a secondary role through its Passenger Information and Entertainment Services (PIES). With this device, airline passengers would be able to stay in touch with social media and emails without interrupting the aircraft's operations.

Even though this device is not safety-critical to the aircraft's operation, it still needs to pass vigorous testing before it can be used commercially. One of these tests is the resilience of the device to neutrons generated by cosmic rays. Being based on the Harwell Campus made coming to ISIS the obvious choice.

"Having access to a world-class neutron facility like ISIS, here in the UK, is a huge advantage for Cobham. The alternatives are located in North America so there is a significant cost advantage in using ISIS for the testing and qualification of our aerospace equipment."

**Dr Richard Sharp, Managing Director, Cobham RAD Europe Ltd**

ChiPlr tests the effect of many years of exposure to cosmic neutrons in just one day. By using ChiPlr, Cobham were able to identify any issues caused by the radiation and ensure changes were made so the equipment met the standards required.

The beamline access required to accelerate the productivity of this business was provided through STFC's B4I programme, which helps companies to overcome product, manufacturing or process performance issues. Working closely with STFC research and innovation experts, companies can develop projects that address specific innovation challenges to accelerate business productivity.

"Access to funding under the B4I scheme enabled us to carry out much more extensive testing of our system than would have been feasible otherwise," Richard explains. "The support provided by the ChiPlr team was fantastic and helped us produce a market-leading system, with full confidence in its reliability in the natural aerospace radiation environment."




## Industrial Science Highlight: Toyota – studying $\text{MgH}_2$ as a hydrogen storage material

**Related publication:** “Desorption reaction in  $\text{MgH}_2$  studied with in situ  $\mu^+\text{SR}$ ”, Sustainable Energy Fuels, 2019, 3, 956-964.

DOI: 10.1039/C8SE00568K

Instruments: EMU

**Funding:** Marie Skłodowska-Curie Action, International Career Grant through the European Commission, Swedish Research Council (VR), Carl Tryggers Foundation for Scientific Research, Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan and Japan Society for the Promotion Science (JSPS).

 Jun Sugiyama, Izumi Umegaki, Mitsuru Matsumoto, Kazutoshi Miwa, Hiroshi Nozaki, Yuki Higuchi, Tatsuo Noritake (all Toyota Central Research & Development Laboratories), Ola K. Forslund (KTH Royal Institute of Technology), Martin Månsson (KTH Royal Institute of Technology), Stephen Cottrell (ISIS), Akihiro Koda (J-PARC), Eduardo Ansaldo (University of Saskatchewan) and Jess H. Brewer (University of British Columbia, TRIUMF)

An ideal hydrogen storage material for use in vehicles would be able to absorb and desorb hydrogen gas reversibly without its capacity fading, preferably at room temperature. Magnesium hydride ( $\text{MgH}_2$ ) is a promising hydrogen storage material because of its relatively low cost and high density of hydrogen by weight and volume. However, the energy needed for decomposition to release hydrogen leads to a high hydrogen desorption temperature ( $T_d$ ) and a slow reaction rate.

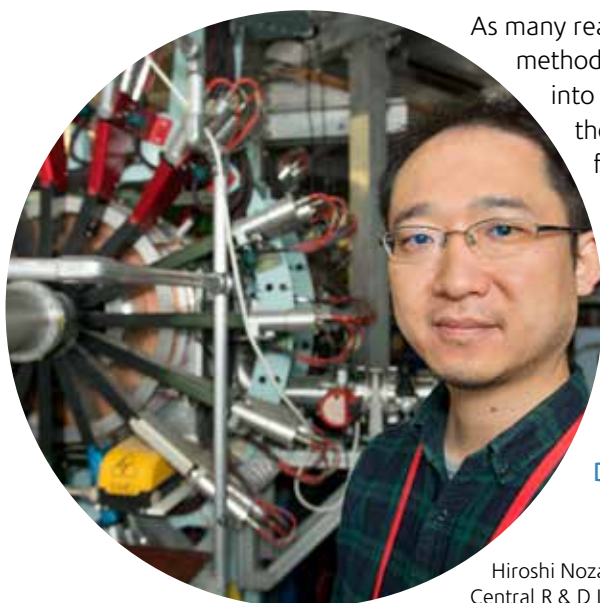
In order to study the mechanism determining the desorption temperature of hydrogen storage materials, researchers from Toyota came to ISIS to measure positive muon spin rotation and relaxation ( $\mu^+\text{SR}$ ) in  $\text{MgH}_2$ . They were able to study the sample over the relevant temperature range, monitoring the pressure in the sample cell (due to desorbed  $\text{H}_2$ ) in parallel with the  $\mu^+\text{SR}$  measurements with the help of the pressure and furnace group at ISIS.

These were the first in situ  $\mu^+\text{SR}$  measurements to observe such a reaction in solids, and aimed to clarify the role of hydrogen diffusion in solid  $\text{MgH}_2$  in determining the hydrogen desorption temperature. By combining their results with those from their experiments at other facilities, they revealed that hydrogen starts to diffuse in  $\text{MgH}_2$  well below this temperature. This indicates the important role of hydrogen diffusion in accelerating the desorption reaction by removing the reaction product ( $\text{H}_2$ ) from the reaction system.

As many reactions occur via mass transport in solids, this new method of in situ  $\mu^+\text{SR}$  experiments will provide clear insights into many reaction mechanisms. In addition to studying the material of interest, the group have paved the way for many more experiments to come.

“ISIS provides a stable and intense pulsed muon beam, which is essential for our work. In addition, we expect a support from a well experienced pressure and furnace group, because we need to heat the sample above around 800 K during the in situ  $\mu^+\text{SR}$  experiment.”

Jun Sugiyama, Toyota Central Research & Development Laboratories



Hiroshi Nozaki, Toyota Central R & D Labs Inc, Japan, on the EMU instrument at ISIS



## Industry Collaboration: Johnson Matthey joint research fellowship

Specialty chemicals and technology company Johnson Matthey (JM) place a high value on cutting-edge research and development. Already regular users of neutron diffraction beam time at ISIS, JM realised a lot more could be done using neutrons and muons and so, in early 2018, they teamed up with ISIS and formed the Johnson Matthey/ISIS Research Fellow position.

The position is a 50/50 collaboration, filled by Dr Hamish Cavaye, who is based at ISIS as part of the Molecular Spectroscopy Group. Half of Hamish's time is spent performing the duties of a beamline scientist, including being a local contact for visiting users on the TOSCA and MAPS beamlines and working on his own programme of research. The other half of Hamish's time is dedicated to liaising and working with JM staff to identify challenges that could be solved using neutron and muon techniques. In his first year in post, seven different joint JM proposals for neutron beam time were successful.

One of the major areas of JM's business is "Clean Air", which includes automotive catalysts and exhaust filters. With colleagues at JM, Hamish has been investigating the use of neutron radiography and tomography on IMAT to identify how and where soot particles are deposited within exhaust particulate filters. These measurements are currently forming part of the commissioning experiments for the new high-resolution camera on IMAT.

Another area of interest to JM is energy generation and storage, including both fuel cell and battery technologies, which Hamish has been working with a number of different groups from JM on. One group has used INTER to investigate the behaviour of fuel cell materials under different conditions of use, informing the researchers about physical aspects of these materials and how they interact with their working environments. Battery materials have been investigated even more widely, with experiments taking place on TOSCA, OSIRIS, and MARI, with *in-situ* measurements forming a focus for the future. The neutron scattering experiments have opened up a wealth of new characterisation information previously unattainable with offline techniques and which will lead to improvements in material design and understanding.



Dr Hamish Cavaye,  
Johnson Matthey and ISIS

## Industrial Science Highlight: Tata Steel – Nano-steels studied to improve their efficiency for the automotive industry

**Related publication:** “VC-Precipitation Kinetics Studied by Small-Angle Neutron Scattering in Nano-Steels”, Materials Science Forum, Vol. 941, pp. 236-244, 2018.

**DOI:** 10.4028/www.scientific.net/MSF.941.236

**Instruments:** Larmor

**Funding:** Dutch Technology Foundation and by Tata Steel through its contribution to the Materials innovation institute M2i.

 Chrysoula Ioannidou, Zaloa Arechabaleta (Delft University of Technology), Arjan Rijkenberg (Tata Steel), Robert M. Dalgliesh (ISIS), Ad A. van Well and S. Erik Offerman (Delft University of Technology).

Researchers from Tata Steel and TU Delft have used Small-Angle Neutron Scattering (SANS) to investigate the formation of crucial precipitates inside Nano-steels, with the aim to reduce the need for critical raw materials in these advanced materials.

The automotive industry is continuously looking for opportunities to improve fuel economy and to reduce steel consumption. Nano-steels are a new generation of Advanced High Strength Steels that can provide a combination of properties such as high strength and formability, making them ideal for lightweight automotive applications.

Nano-steels consist of a soft ductile ferrite steel matrix strengthened by nanometre-sized precipitates. To reach the high level of precipitation strengthening needed, considerable amounts of micro-alloying elements such as vanadium and niobium are added. The key challenge in the development of Nano-steels is to investigate options for suitable alloys with less of these critical raw materials, which maintain the excellent mechanical properties for these steels. Therefore, there is a demand for further knowledge of the role of these micro-alloying elements on the precipitation kinetics.

SANS is a powerful tool for studying the precipitation kinetics in steels as it can measure the volume fraction, size distribution and density of precipitates in the nanometre size range. Recently, the technique has attracted a lot of interest in this field of research because of its ability to provide quantitative data over a large bulk sample volume. This research used SANS experiments on Larmor to investigate the precipitation kinetics at 650°C in a vanadium-containing alloy related to a Nano-steel of interest. The researchers were able to track the size of the vanadium-containing precipitate particles as they grew with time.

“We used Small-Angle Neutron Scattering to obtain quantitative data on the VC-precipitation kinetics. The Larmor instrument (developed by ISIS and TUDelft) at ISIS provided the opportunity to measure the precipitate-size-distribution with high resolution in large sample volumes.”

Chrysoula Ioannidou, TU Delft




*Suspension for automotive applications made of Nano-steel,  
Credit: Chrysoula Ioannidou, TU Delft*

## Our people



### From Post-doc to Individual Merit Scientist

 Chris Frost

#### Industry Liaison Manager

Dr Chris Frost works on the Chiplr instrument and as Industry Liaison Manager, and this year gained his Individual Merit promotion.

#### Background

It was during a summer placement at the Institut Laue-Langevin in Grenoble, France, whilst still an undergraduate at Trinity College Cambridge, that I discovered neutron scattering. A few years later, with a bachelor's degree and PhD in superconductivity, I began working at ISIS as a PostDoc and never looked back. During almost twenty years at ISIS, I progressed from PostDoc, to Instrument Scientist on MAPS, to Group Leader with ISIS Industry Liaison Manager as one of my responsibilities.

#### Projects

Currently, I am working on the Chiplr instrument, one of the first dedicated facilities outside of the US to look at how silicon microchips respond to cosmic ray neutron radiation. The instrument is therefore of significant strategic importance for the European electronics industry.

Using Chiplr, our users perform electronics testing at highly accelerated rate, with a measurement of just one hour being equivalent to exposing microchips to high-energy neutrons for hundreds to thousands of years in the real environment. Such accelerated atmospheric neutron testing is designed to mimic the single event effects that can disrupt electronics, and allow industry to develop strategies, designs and methods to mitigate their effects to ensure that those systems do the job they are supposed to do in a resilient and reliable way, before they hit the market.

Bringing the Chiplr instrument online was one of my proudest achievements. Having spent a number of years working with industry conceiving the idea and a number of years with engineers building the instrument, to see it turn into something that is of key strategic importance to the electronics industry in the UK and Europe is a great achievement.

#### Future

By developing a completely different kind of instrument to others at ISIS, many new users have come to the facility doing experiments that are new to the UK. Some of these have even been with applications that I was not expecting.

**Through my role as Industry Liaison Manager, I am working to help break the barriers and perceptions about the application of neutron scattering between industry, academia and the facilities to try to increase the number of industrial collaborations with ISIS users and to grow the direct industrial work with ISIS through the ISIS Collaborative Research and Development scheme.**

# Impact Awards





## The 2019 Impact Awards

After its success in 2018, ISIS users were invited to apply for the second ISIS Impact Awards for facility users, celebrating the scientific and socio-economic impact generated by the user community. These three separate awards recognise the diverse ways research using neutrons and muons can advance knowledge, improve quality of life and impact on the economy. The 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.



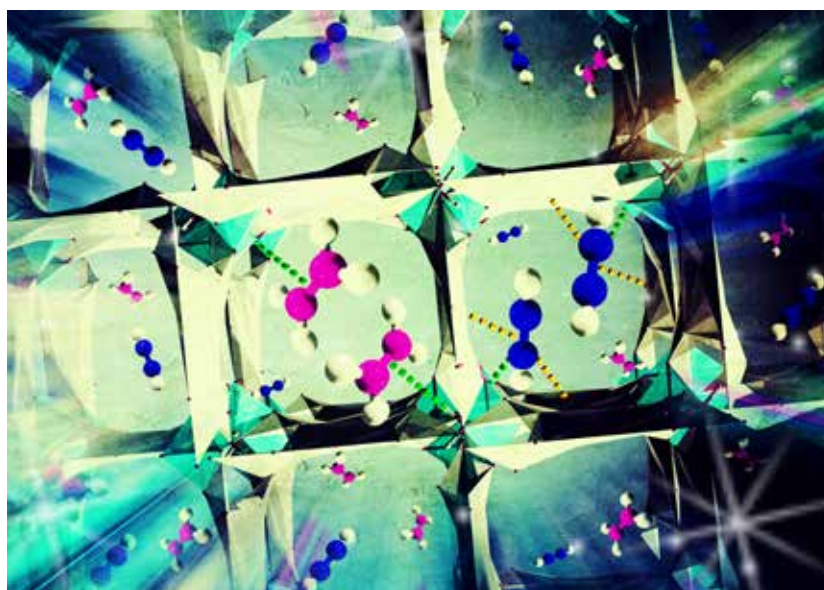
### Science Impact Award: Dr Sihai Yang

The winner of the ISIS Science Impact Award demonstrated the value of neutron techniques for the development of functional materials for applications in the energy, environmental and well-being sectors. Dr Sihai Yang (University of Manchester) has been using neutrons to investigate a wide range of porous materials based on metal-organic frameworks, metal oxides and phosphates, and zeolites.

Porous materials containing **nano-sized cavities** (1-5 nm), the walls of which are decorated with various active sites, can form **unique functional platforms** to study and re-define the chemistry of guest molecules within confined space and on active sites. Dr Yang's research group uses neutron scattering techniques with the aim to determine **what happens to the guest molecules inside these materials**, and find out how and where the guest molecules interact with the walls of the cavities. Such knowledge will allow the design of successive generations of porous materials with enhanced functionality. Their work at ISIS since 2015 has generated **26 joint publications** with ISIS scientists.

Dr Yang and his group have made a series of breakthroughs on the development of robust metal-organic materials for **highly efficient clean-up of SO<sub>2</sub> and NO<sub>2</sub>**. These materials show record-high adsorption capacity and selectivity of SO<sub>2</sub> and NO<sub>2</sub>. More importantly, the **captured gases are fully recovered** for use in other chemical processes, and the host materials are regenerated for the next cycle of use.

For **biomass conversion**, it is critical but challenging to develop a detailed mechanistic understanding of how a catalyst functions. Dr Yang's work has strengthened the links between neutron scattering and catalysis, **promoting new discovery and knowledge in a wider range of heterogeneous catalysis**. Their recent success has the potential to lead to huge reductions in the energy consumption of bio-refineries by developing **new efficient catalysts**, and hence reduced costs for biomass-derived materials - promoting their widespread applications.



*A framework structure of MFM-300 materials for gas separation.*



## Society Impact Award: Professor Maria Paula M. Marques

The winner of the ISIS Society Impact Award is a project that shows the value of neutron spectroscopy for clinically relevant research, particularly aiming at improving cancer patients' prognosis and quality of life.

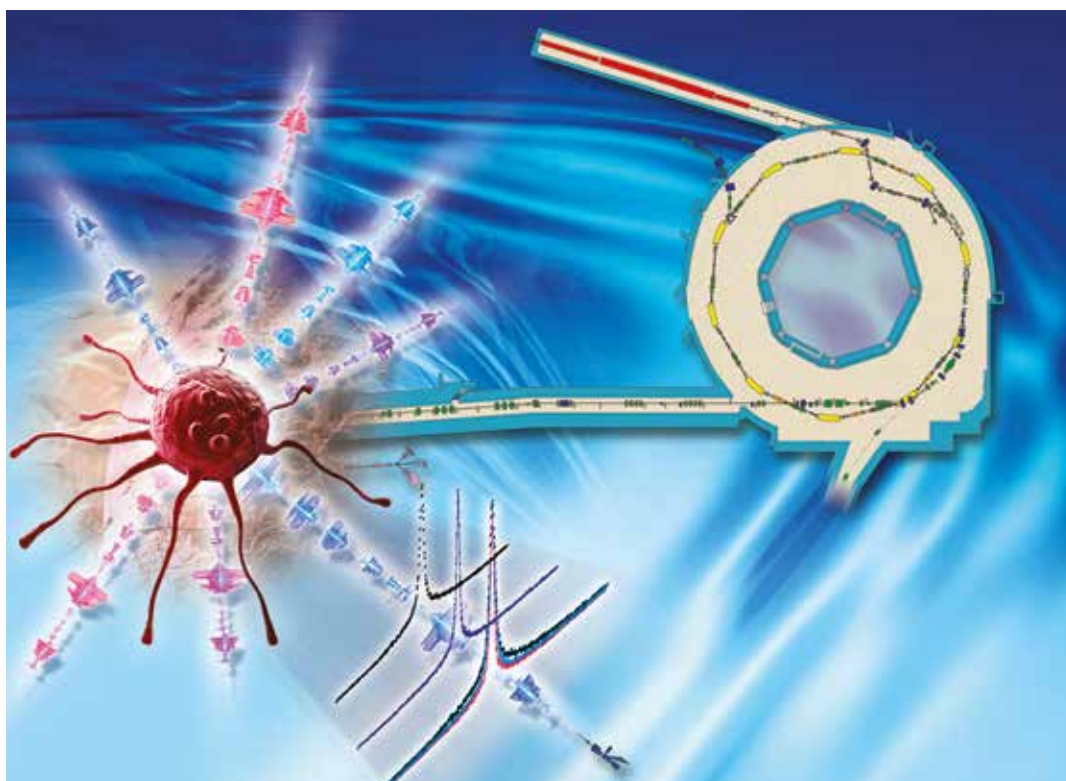
Professor Marques and her team from Coimbra University, Portugal, use neutron scattering techniques (inelastic and quasi-elastic) to study the **changes happening inside the cell as it undergoes drug treatment**. Their work focusses on the water inside the cell, and how this 'intracellular water' could be used as a target for anticancer drugs.

The water inside the cells has different properties to water outside the body – it maintains the three-dimensional architecture and functional conformation

of the molecules required for normal cellular activity. Just **small variations** in the structure or dynamics of intracellular water could trigger inhibition of cell growth and eventually cell death.

The team used inelastic and quasi-elastic neutron scattering techniques as a **direct probe of the behaviour of the different types of cellular water, in the presence and absence of a drug**. For these experiments, the team developed a new experimental procedure where cells were grown and drug-incubated immediately before neutron data acquisition.

The measurements were very successful in highlighting **drug-induced differences in intracellular water mobility**. These studies constitute an innovative approach for chemotherapeutic research, aiding the interpretation of a drug's mode of action within the cell and enabling the identification of alternative therapeutic targets. Looking at water as a promising chemotherapeutic target may pave the way for the development of **improved anti-tumour drugs with multiple sites of action**, i.e. multi-targeted as opposed to single-targeted agents, leading to an enhanced efficiency and minimised acquired resistance during treatment.



Reproduced from M. P. M. Marques et al. "Intracellular water – an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons" *Phys. Chem. Chem. Phys.* 19 (2017), 2702-2713 DOI: 10.1039/C6CP05198G with permission from the PCCP Owner Societies.



### Economic Impact Award: Dr Indri Adilina

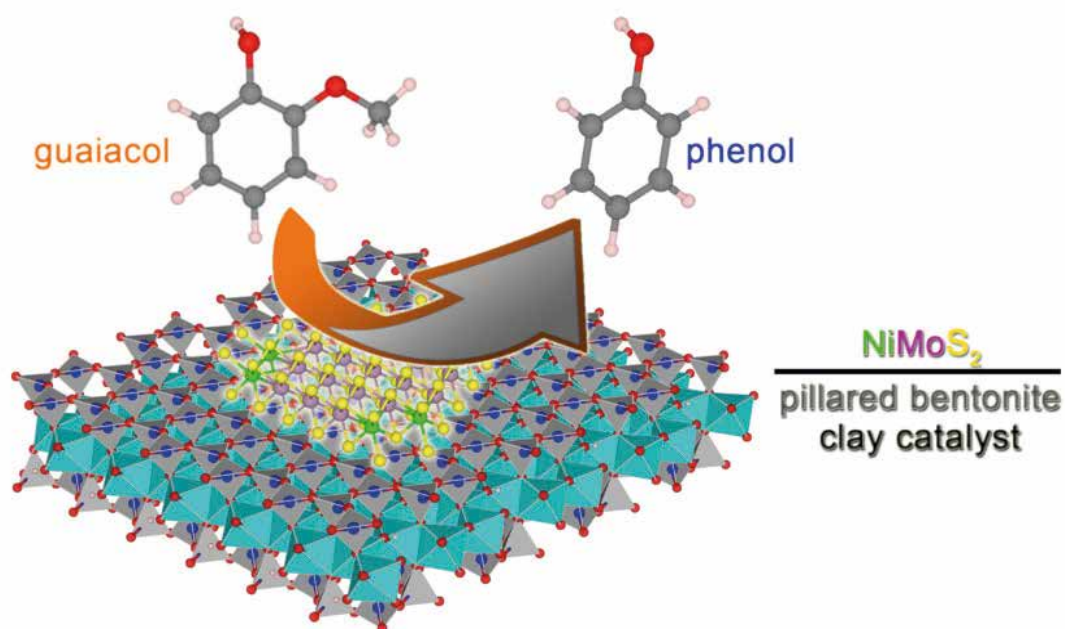
The winner of the ISIS Economic Impact Award is a project that aims to reduce Indonesia's reliance on fossil fuels, whilst creating a partnership that has increased the expertise of the Indonesian scientific community.

Indonesia is the world's largest producer of **palm oil** creating more than 35 million tonnes annually. The industry is hugely wasteful with the oil extracted making up as little as 10% of the total biomass produced – meaning the remaining **90% of that biomass is classified as waste**.

Indri and her group from LIPI, Indonesia, aim to establish a viable method of using palm oil **biomass waste in place of the palm oil itself** to meet government targets for biofuel use without affecting the local food industry. However, significant advances in catalysis are required to convert the **bulky feedstock into high value biofuel**. With the unique properties of neutrons, they have been able to **understand the interactions** between the chemical compounds in biomass waste and the catalyst, giving important information for the **catalyst design and optimisation** strategies.

From their work using INS and QENS, they have developed a new catalyst based on bentonite clay, a **renewable and abundant resource** in Indonesia, which can promote the chemical reactions that convert the heavy palm oil molecules into the lighter hydrocarbon molecules that make up fuels like gasoline and diesel.

Both the knowledge that the team has gained and the networks established in neutron science at ISIS will return with them to Indonesia, opening up research using **techniques that were previously unavailable**. This project is pioneering for users in Indonesia and the South East Asia region, and is funded through the UK Government's Newton Programme.





# Science Highlights





## Physics


### Neutron studies explain anomalies in a Weyl semimetal

**Related publication:** “Magnetic excitations in non-collinear antiferromagnetic Weyl semimetal  $Mn_3Sn$ ” *NPJ Quantum Materials*, Volume 3, Article number: 63 (2018)

DOI: 10.1038/s41535-018-0137-9

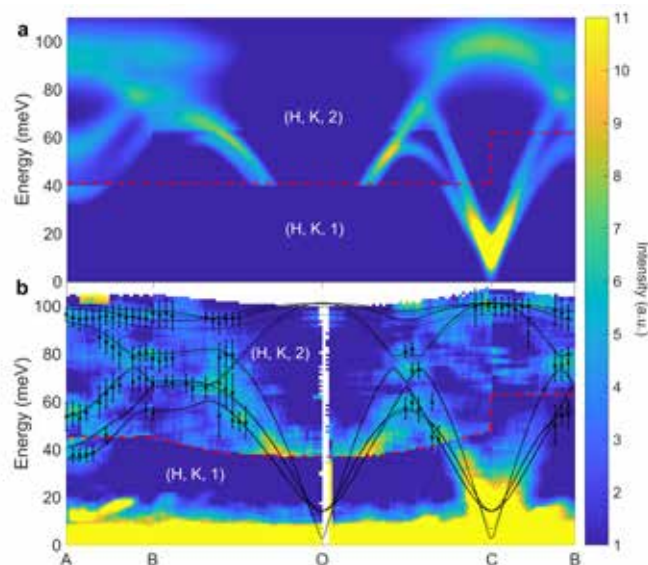
**Instrument:** MERLIN

**Funding:** The Institute for Basic Science (IBS-R009-G1), the Ministry of Education, Youth and sports of Czech Republic, the BME-Nanotechnology FIKP grant of EMMI (BME FIKP-NAT) and by the Hungarian National Scientific Research Fund (NKFIH). Support from the EPSRC under a service level agreement with STFC (core support for the CCP9 project).

 Pyeongjae Park, Joosung Oh (Institute for Basic Science, Seoul; Seoul National University), Klára Uhlířová (Charles University in Prague), Jerome Jackson (SCD, STFC), András Deák, László Szunyogh (Budapest University of Technology and Economics), Ki Hoon Lee, Hwanbeom Cho (Institute for Basic Science, Seoul; Seoul National University), Ha-Leem Kim (Seoul National University), Helen C. Walker, Devashibhai Adroja (ISIS), Vladimír Sechovský (Charles University in Prague), Je-Geun Park (Institute for Basic Science, Seoul; Seoul National University).

Weyl semimetals are solid-state crystals that carry electrical charge at room temperature due to the presence of particles called Weyl fermions.  $Mn_3Sn$  is a magnetic Weyl semimetal attracting considerable research attention. An international team of researchers has used inelastic neutron scattering on the MERLIN time-of-flight spectrometer to measure the full spin wave spectra of  $Mn_3Sn$  over a wide range of momentum and energy. They then used a linear spin wave theory to create a theoretical model that explains their results and is consistent with density functional theory calculations.

Their work, published in *NPJ Quantum Materials*, provides an unusual example of a topological phenomenon (the Weyl point) being removed by a slight change to the magnetic ground state, demonstrating the close coupling between the spin and electronic degrees of freedom in  $Mn_3Sn$ .



Inelastic neutron scattering data of  $Mn_3Sn$  over the full Brillouin zone at 4K, and calculated magnon spectra using a linear spin wave theory. Black solid and dashed lines on the data shows the calculated magnon dispersion relation. Error bars indicate one sigma of the magnon energy fitted by the data.

## Neutron spectroscopy of magnetic fluctuations in a charge-ordered antiferromagnet

**Related publication:** "Anharmonic Magnon Excitations in Noncollinear and Charge-Ordered  $\text{RbFe}^{2+}\text{Fe}^{3+}\text{F}_6$ ", *Phys. Rev. Lett.* 121, 087201

DOI: 10.1103/PhysRevLett.121.087201

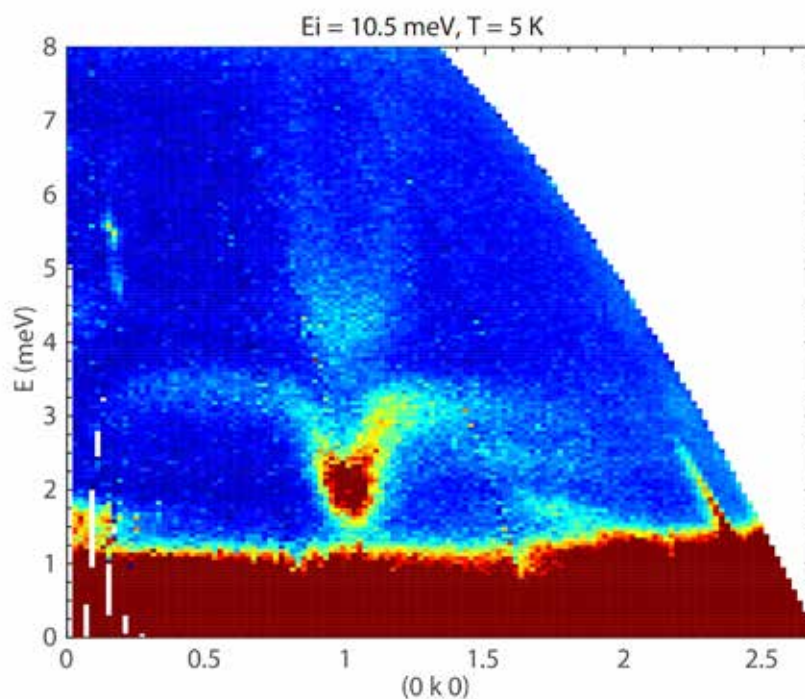
**Instrument:** MERLIN

**Funding:** EPSRC, STFC, and the Carnegie Trust for the Universities of Scotland.

 M. Songvilay (University of Edinburgh), E. E. Rodriguez (University of Maryland), R. Lindsay, M.A. Green (University of Kent), H.C. Walker (ISIS), J.A. Rodriguez-Rivera (NIST Center for Neutron Research; University of Maryland), and C. Stock (University of Edinburgh).

Quasiparticles are disturbances in a material that behave like particles, with momentum and position, and so can be regarded as particles. When they occur in condensed matter, they are generally long-lived and non-interacting. Magnon excitations in ordered magnetic lattices are a prototypical example, and understanding the conditions under which they break down will inform understanding of the low energy properties in a variety of systems including superconductivity, frustrated magnets and quantum liquids.

In work published in *Physical Review Letters*, an international team of researchers used neutron spectroscopy on MERLIN to demonstrate the breakdown of these excitations in  $\text{RbFe}^{2+}\text{Fe}^{3+}\text{F}_6$ , a classical magnet with noncollinear magnetic order in which spin geometry is key to establishing quasiparticle stability. They found that the separation of different  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  chains results in an orthogonal spin arrangement on the two magnetic sites, as well as separate spin-wave branches. Their results demonstrate that multi magnon processes can occur in magnets with a noncollinear spin arrangement.



Magnetic excitation spectrum recorded on MERLIN at  $T = 5\text{ K}$  with an incident energy of  $10.5\text{ meV}$ . The spectrum was measured along the  $(0\text{ k } 0)$  direction and illustrates two magnon modes associated to the  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$  magnetic sites.


## Probing helimagnetic correlations in a doped chiral magnet

**Related publication:** "Evolution of helimagnetic correlations in  $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$  with doping: A small-angle neutron scattering study" Phys. Rev. B 98, 184431

DOI: 10.1103/PhysRevB.98.184431

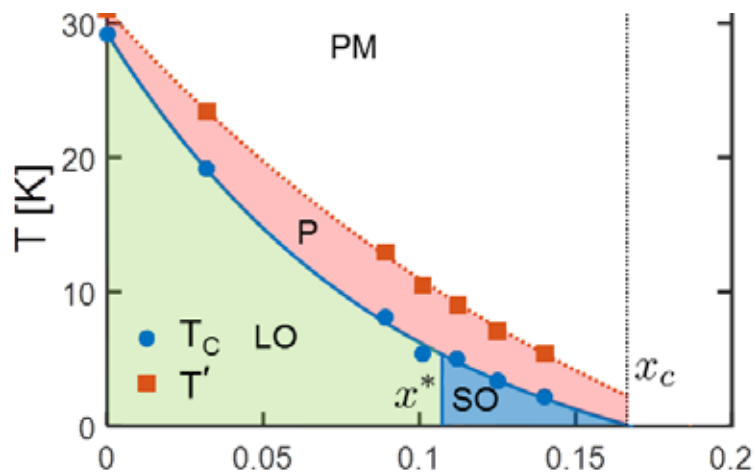
**Instrument:** Larmor

**Funding:** The Netherlands Organisation for Scientific Research (NWO)

 L. J. Bannenberg (Delft University of Technology), R. M. Dalgliesh (ISIS), T. Wolf, F. Weber (Karlsruhe Institute of Technology), and C. Pappas (Delft University of Technology).

New and exotic phases of condensed matter can be discovered by tuning the interactions in magnetic materials by pressure or chemical substitution. The most notable example in chiral magnetism is provided by the effect of hydrostatic pressure on the properties of the archetype chiral magnet MnSi. In research published in Physical Review B, an international team of researchers carried out a comprehensive small angle neutron scattering (SANS) study of the doping dependence of the helimagnetic correlations in  $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$ .

They used SANS measurements, performed on the time-of-flight instrument Larmor, to systematically study the evolution of the helimagnetic correlations as a function of both temperature and magnetic field. Their results show that the long-range helimagnetic order in  $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$  is suppressed with increasing iron content and disappears when  $x$  is increased to 0.11, above which only finite isotropic helimagnetic correlations persist. Magnetic fields gradually suppress and partly align these short-ranged helimagnetic correlations along their direction through a complex magnetisation process.



Magnetic phase diagram of  $\text{Mn}_{1-x}\text{Fe}_x\text{Si}$  illustrating the Fe concentration dependence of the critical temperature  $T_c$  and  $T'$ , which marks the onset of the (short-ranged) helimagnetic correlations in the precursor phase. LO indicates long-range helimagnetic correlations, SO short-range, helimagnetic correlations, P the precursor phase, and PM the paramagnetic phase.



## Muons find magnetic order in materials for spintronics and multiferroics

**Related publication:** "A 3D antiferromagnetic ground state in a quasi-1D pi-stacked charge-transfer system", *J. Mater. Chem. C*, 2018, 6, 12468

DOI: 10.1039/c8tc03709d

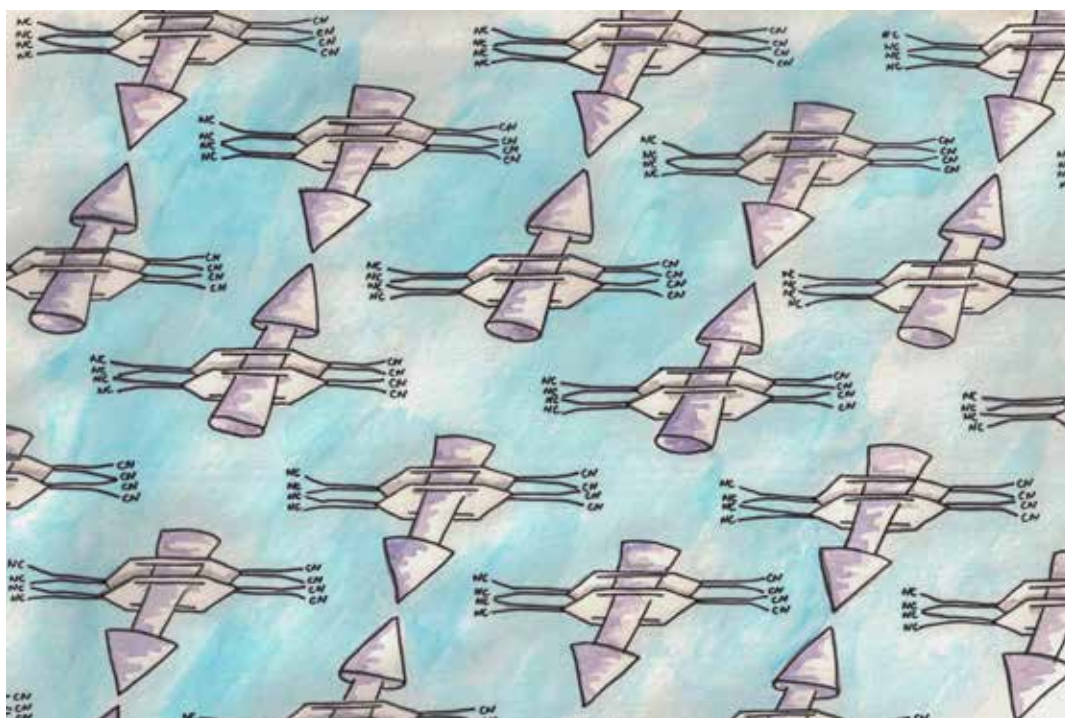
Instrument: CHRONUS

Funding: STFC

 Adam Berlie (ISIS), Ian Terry and Marek Szablewski (Durham University).

With rising interest in organic-based materials for spintronic and multiferroic applications, it is important to fully understand their electrical and magnetic properties and to identify correlations between their structural and physical attributes. Research led by ISIS, with collaboration from staff at Durham University, used muon spin spectroscopy to understand the anomaly seen in the magnetic susceptibility measurements of TEA(TCNQ)<sub>2</sub> (triethylammonium bis-7,7,8,8-tetracyanoquinodimethane). This allowed them to carry out an in-depth study of the magnetic transition in the material.

Previous work showed coupling between the magnetic and electronic properties occurring alongside a magnetic transition at around 120 K. However, the magnetism and magnetic ground state were not well understood. This work, published in the *Journal of Materials Chemistry C*, took a closer look at the ambiguous magnetic behaviour of TEA(TCNQ)<sub>2</sub>, and provided evidence of long range magnetic order. The molecules were ordered in a three-dimensional manner, in such a way that their magnetic moments were pointing in opposite directions to their nearest neighbour (known as 'Ising-like').



Artistic impression of two TCNQ molecules with magnetic moments in an Ising configuration.


## Iron meteorites allow us to probe the formation of our Solar System

**Related publication:** "Type I and type II residual stress in iron meteorites determined by neutron diffraction measurements" *Planetary and Space Science*, Volume 153, April 2018, Pages 72-78

DOI: 10.1016/j.pss.2017.12.015

**Instrument:** Engin-X

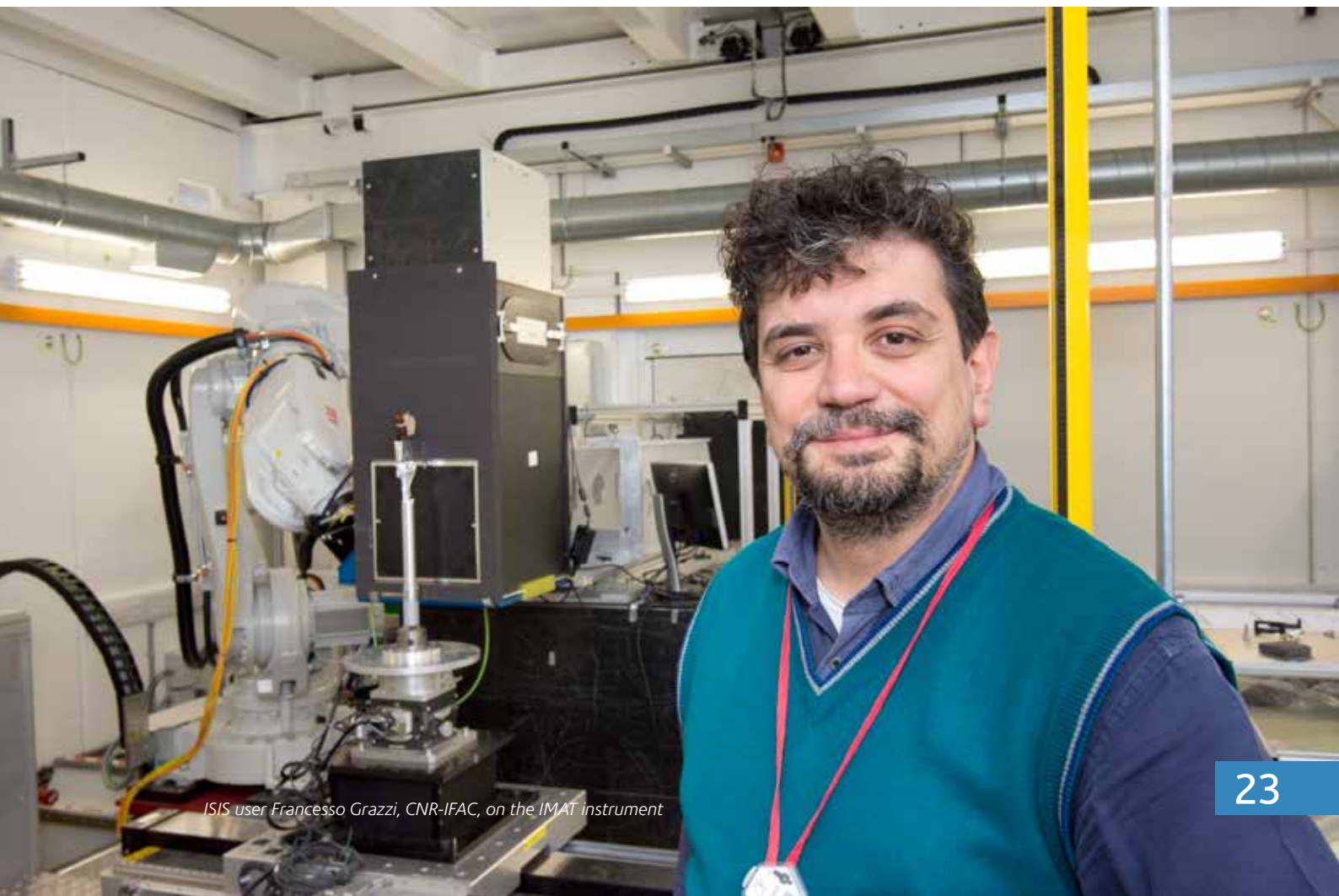
**Funding:** CNR-STFC

 Stefano Caporali (Università degli Studi di Firenze; Istituto dei Sistemi Complessi), Giovanni Pratesi (Università degli Studi di Firenze), Saurabh Kabra (ISIS), Francesco Grazzi (Istituto dei Sistemi Complessi).

Iron meteorites are thought to be fragments of the cores of ancient planet-like bodies that shattered in high-velocity impacts in the early stages of the formation of our Solar System. Iron meteorites are rare compared to stony meteorites. However, as they are easily recognised and more likely to be found as large pieces, they are plentiful in meteorite collections. Analysing the residual stresses in iron meteorites could be a powerful way to investigate the geochemical and geophysical conditions during the first stages of Solar System formation.

A team of Italian researchers used neutron diffraction measurements on ENGIN-X to analyse three different iron meteorites. They achieved, for the first time, a very careful and reliable quantification of the residual stress in a non-destructive way.

Their work, published in *Planetary and Space Science*, constitutes a robust and non-destructive method for the careful evaluation of the residual stress of metal artefacts. The systematic application of this new and powerful tool on a selected set of different groups of meteorites would provide fundamental clues about the early stages of formation of the Solar System planets.



ISIS user Francesco Grazzi, CNR-IFAC, on the IMAT instrument


### A neutron analysis of a promising magnonics material

**Related publication:** "Crystal structure and crystal growth of the polar ferrimagnet  $\text{CaBaFe}_4\text{O}_7$ "  
 Phys. Rev. Materials, 2018, 2, 054403

DOI: 10.1103/PhysRevMaterials.2.054403

**Instrument:** SXD and HRPD

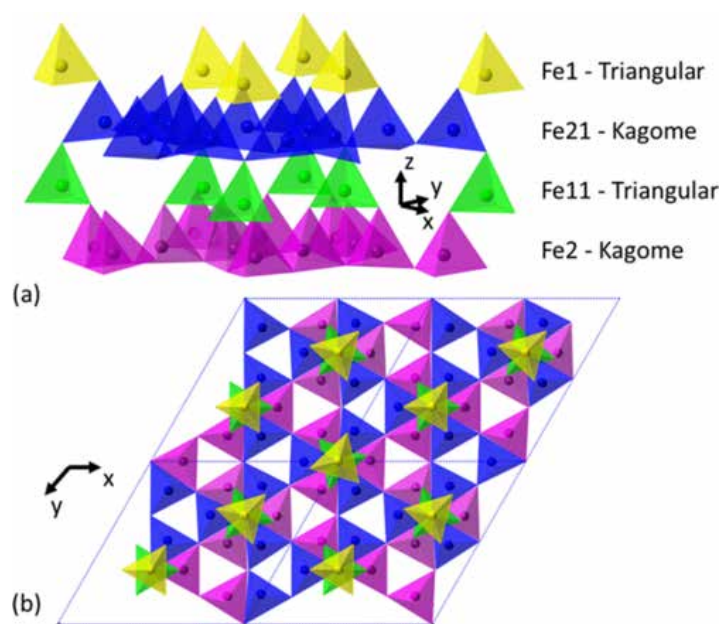
**Funding:** EPSRC

 R. S. Perry (University College London; ISIS), H. Kurebayashi (University College London), A. Gibbs, and M. J. Gutmann (ISIS).

Achieving the efficient use of electron spin for next-generation information technologies is a principal research aim for scientists in the field of spintronics. Spin waves in suitable materials can propagate over the length scale of millimetres with frequencies from GHz to even THz regimes and with a broad range of wavelengths from micrometres to nanometres. These properties can be controlled and tuned using an appropriate choice of magnetic materials, sample geometries, and excitation methods.

Materials suitable for spin transport tend to be chemically complex and challenging to synthesise, and few have been investigated. A recently-proposed approach is to use magnons, which are spin excitations in magnetically-ordered systems. In work published in *Physical Review Materials*, researchers from University College, London, and ISIS conducted a comprehensive analysis of the high-temperature crystal structure of the Swedenborgite  $\text{CaBaFe}_4\text{O}_7$ , a candidate for magnon transport. They collected single-crystal neutron-diffraction data with the single-crystal diffractometer (SXD), and additional data on the high-resolution powder diffractometer (HRPD).

They demonstrated that the growth of large crystals via the liquid phase is possible, opening the door to further investigations into the magnetic structure and dynamic response of this promising material.



(a) Triangular and Kagome layers of the Fe-O tetrahedra of the high-temperature  $P3$  (large cell) structure of  $\text{CaBaFe}_4\text{O}_7$ ,  
 (b) Projection along the  $z$  direction highlighting the interplanar order. Four unit cells are shown. The oxygen atoms exist at the vertices of the tetrahedra. The Ba and Ca atoms are situated between the planes and have been omitted for clarity.



## Using neutrons to measure the helix pitch for calculating the Topological Hall Effect

**Related publication:** "Helical magnetic structure and the anomalous and topological Hall effects in epitaxial B20" *Phys. Rev. B*, 2018, 97, 214406

DOI: 10.1103/PhysRevB.97.214406

Instrument: POLREF

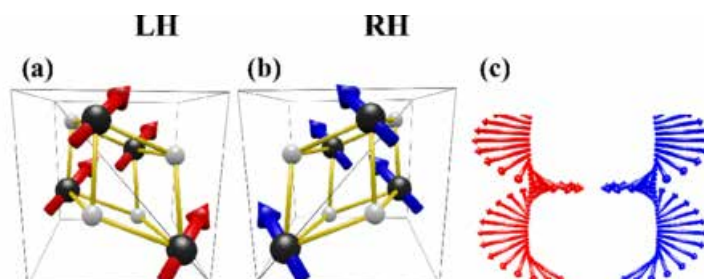
Funding: CNR-STFC

 Charles S. Spencer (University of Leeds), Jacob Gayles (Max Planck Institute for Chemical Physics of Solids; Johannes Gutenberg Universität Mainz), Nicholas A. Porter, Satoshi Sugimoto, Zabeada Aslam (University of Leeds), Christian J. Kinane, Timothy R. Charlton (ISIS), Frank Freimuth (Forschungszentrum Jülich), Stanislav Chadov (Max Planck Institute for Chemical Physics of Solids), Sean Langridge (ISIS), Jairo Sinova (Johannes Gutenberg Universität Mainz; Institute of Physics ASCR), Claudia Felser (Max Planck Institute for Chemical Physics of Solids), Stefan Blügel (Forschungszentrum Jülich), Yuriy Mokrousov (Johannes Gutenberg Universität Mainz; Forschungszentrum Jülich) and Christopher H. Marrows (University of Leeds).

Skyrmions are the focus of intense research for their potential applications in spintronics: next-generation electronic devices that exploit the spin degree of freedom. Skyrmions are curious magnetic systems and offer the possibility of new high-density, low-power magnetic storage devices.

Previous research has shown that the conditions required for the formation of skyrmions occur in a group of materials called B20 compounds, which naturally possess the necessary inversion symmetry in their crystal structure. In research published in *Physical Review B*, an international team of researchers used polarised neutron reflectometry (PNR) on the POLREF beamline to investigate the preliminary helical magnetic phase in B20 thin films.

Their pioneering use of PNR on POLREF allowed them to study the underlying helical magnetic structure, by determining the magnetic depth profile of the film. They were able to measure the helix pitch of the spiral: the distance in which it completes one 'twist'. They were also able to observe the changes in the helix pitch with increasing concentrations of cobalt. Their results provide a comprehensive data set for the magnetic properties of  $\text{Fe}_{1-y}\text{Co}_y\text{Ge}$  B20 films and demonstrate that it is possible to control the helix pitch, a crucial step towards developing working devices.



Chiral crystal structure of  $\text{Fe}_{1-y}\text{Co}_y\text{Ge}$ . B20 unit cell diagrams for (a) left-handed and (b) right-handed chiral crystals where the helical ground state propagates along the dashed line. The dark colored ion magnetic moments belong to  $\text{Fe}_{1-y}\text{Co}$  and the light colored ions to Ge. (c) Diagram of magnetic helix structure for left-handed and right-handed chirality.

## Life Science


## Secrets of peptide assembly unzipped at ISIS

**Related publication:** "Nanoribbons self-assembled from short peptides demonstrate the formation of polar zippers between  $\beta$ -sheets" *Nature Communications* volume 9, Article number: 5118

DOI: 10.1038/s41467-018-07583-2

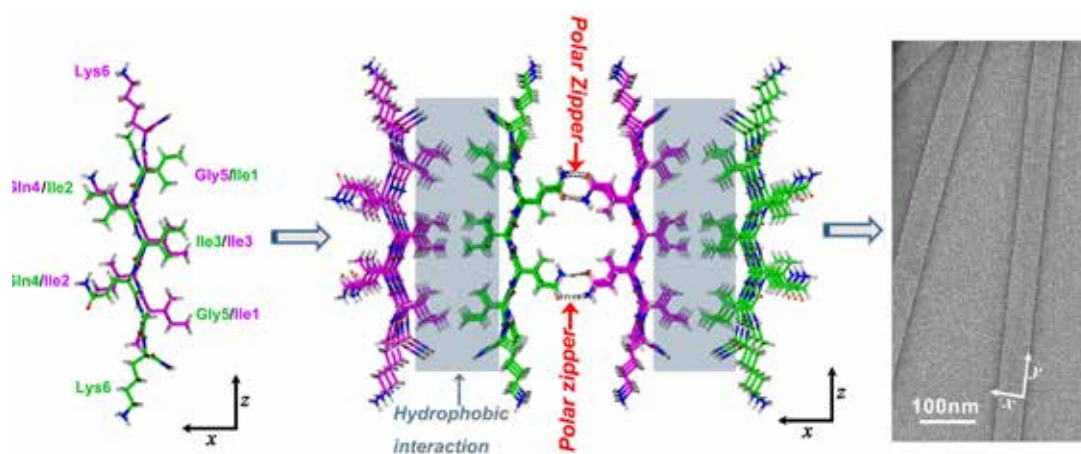
Instrument: SANS2D and LOQ

Funding: National Natural Science Foundation of China, EPSRC and Innovate UK

 Meng Wang, Jiqian Wang, Peng Zhou (China University of Petroleum (East China)), Jing Deng (Wuhan Institute of Physics and Mathematics), Yurong Zhao, Yawei Sun, Wei Yang, Dong Wang (China University of Petroleum (East China)), Zongyi Li, Xuzhi Hu (The University of Manchester), Stephen M. King, Sarah E. Rogers (ISIS), Henry Cox, Thomas A. Waigh (The University of Manchester), Jun Yang (Wuhan Institute of Physics and Mathematics), Jian Ren Lu (The University of Manchester) & Hai Xu (China University of Petroleum (East China)).

Peptide self-assembly exhibits some special features, including the 'polar zipper', proposed 25 years ago by Max Perutz. Shown to form between beta strands of peptides via side chain interactions, it may influence some types of neurodegenerative disease. New research, conducted by the China University of Petroleum and The University of Manchester, used neutron scattering to demonstrate a novel form of polar zipper between neighbouring beta sheets and not just between the strands within a beta sheet. Small angle neutron scattering on SANS2D and LOQ was used to make in situ measurements of the self-assembled nanostructures that formed in aqueous solution.

This research, published in *Nature Communications*, has provided ground-breaking insights into how peptides self-assemble. This could improve the development of peptide-based materials already used in artificial enzymes, antibacterial and anticancer agents, cell culture scaffolds and even biological semiconductors, with the added benefit of improved biodegradability and biocompatibility.



Schematic illustration of the self-assembly of  $\text{Ac-I}_3\text{XGK-NH}_2$  ( $X=Q, S, \text{ and } N$ ) into nanoribbons. Carbon atoms are shown as purple or green, oxygen as red, nitrogen as blue, and hydrogen as grey. Two  $\beta$ -strands pack in an anti-parallel mode with one-residue shifting. The formation of polar zippers (red arrows) at the polar interface between neighboring  $\beta$ -sheets. The nonpolar interface is colored grey. Right hand image TEM micrograph.


## Neutron scattering probes the intricacies of drug delivery

**Related publication:** "Increased rate of solvent diffusion in a prototypical supramolecular gel measured on the picosecond timescale", *Chem. Commun.*, 2018, 54, 6340

DOI: 10.1039/c8cc02962h

**Instrument:** LET

**Funding:** N/A

 Tilo Seydel (Institut Laue-Langevin), Robert M. Edkins (University of Oxford, University of Strathclyde), Christopher D. Jones (Queen's University Belfast), Jonathan A. Foster (Sheffield University), Robert Bewley (ISIS), Juan A. Aguilar (Durham University) and Katharina Edkins (Queen's University Belfast).

A key issue in modern healthcare is the development of new ways to safely deliver drugs to the areas of the body in which they are needed. With an aging population and ever more complex drug compounds, novel delivery vehicles are highly sought after. A team of researchers is developing a new material based on supramolecular gels with tailored long-term release kinetics. These gels are made of small organic molecules that can aggregate into one-dimensional fibres, mimicking the properties of larger molecules such as gelatin that are traditionally used to create gels. This gives them improved characteristics such as easier processing and reduced incompatibilities.

In work published in *Chemical Communications*, the researchers used quasi-elastic neutron scattering on LET to probe the diffusion behaviour of the liquid phase in a model supramolecular gel. Their results showed that the solvent diffuses faster in the gel network compared to the bulk solvent measured on the picosecond timescale and nanometer length scale. They attributed this to the breaking of the hydrogen bonding of the solvent by the surface of the hydrophobic gel fibres, and the lowering of the solvent viscosity directly around the fibres. The results of this study will inform future research on influencing the diffusion of drug molecules in supramolecular gels.





## Bacterial outer membranes and the potential for new antibiotics

**Related publication:** “Liquid crystalline bacterial outer membranes are critical for antibiotic susceptibility” PNAS, vol. 115, no. 32, E7587–E7594

DOI: 10.1073/pnas.1803975115

**Instrument:** INTER and CRISP

**Funding:** STFC, Newcastle University, and OJ-Bio Ltd.

 Nicolò Paracini (Newcastle University), Luke A. Clifton, Maximilian W. A. Skoda (ISIS), and Jeremy H. Lakey (Newcastle University).

Gram-negative bacteria, which are responsible for two-thirds of bacterial infections acquired in hospital, are surrounded by a protective outer membrane (OM). This OM severely limits the variety of antibiotic molecules effective against Gram-negative pathogens and, as antibiotic resistance increases, so does the need to solve the problem of permeating the OM.

Polymyxin B (PmB) is a last-resort antibiotic used to treat many hospital-acquired bacterial infections. Scientists from Newcastle University and STFC used neutron reflectometry on the INTER and CRISP reflectometers to reveal how PmB penetrates the outer membrane of Gram-negative bacteria. The OM has a dense outer layer of lipopolysaccharide (LPS), a glycolipid directly targeted by PmB.

The researchers studied the PmB–OM interaction *in vitro*, and their results (published in PNAS) showed that *in vivo* results are only reproduced when the LPS is in a liquid crystalline phase, which occurs at body temperature. These findings not only explain why PmB only works at, or above, body temperature but also support the fundamental notion that bacteria actively control the viscosity of their outer membranes as temperatures vary.

Polymyxin B (PmB) represents a currently rare type of antibiotic, which acts directly on the OM. Improving our understanding of its mode of action offers a distinct starting point for new antibiotic development.



The figure shows a cartoon of the model outer membrane used in the ISIS experiments with the neutron beam shown as green spheres. On the left, the intact bilayer model is shown below body temperature with the red PmB unable to penetrate. On the right is shown the effect of raising the temperature to induce the liquid crystalline phase whereupon the PmB insets and disrupts the membrane. This is what kills the bacteria and cures infections.

## Energy and Environment


### A novel sodium-rich double perovskite proves promising for new battery technologies

**Related publication:** "Na<sub>1.5</sub>La<sub>1.5</sub>TeO<sub>6</sub>: Na<sup>+</sup> conduction in a novel Na-rich double perovskite", Chem. Commun., 2018, 54, 10040

DOI: 10.1039/c8cc03367f

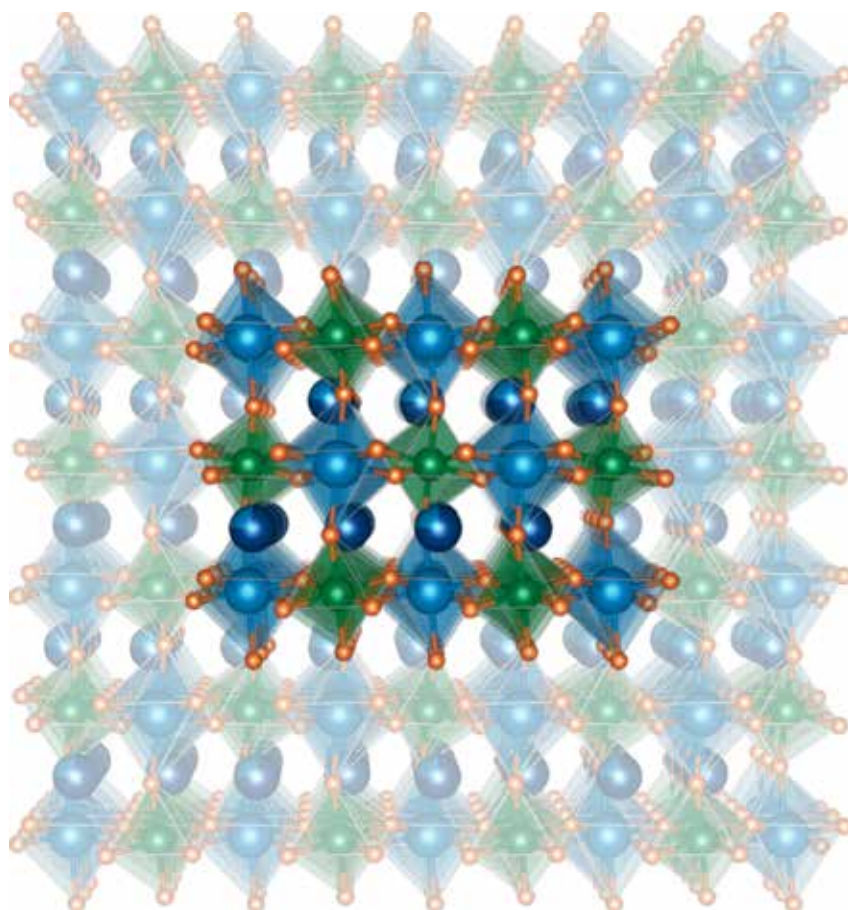
Instrument: EMU

Funding: EPSRC (EP/N001982/1)

 Marco Amores (University of Glasgow, University of Strathclyde), Peter J. Baker (ISIS), Edmund J. Cussen (University of Strathclyde) and Serena A. Corr (University of Glasgow).

With automotive applications increasing demand for batteries, and a need for more large-scale energy storage systems, there is a push to develop new battery technologies. Sodium-ion batteries are emerging as a leading alternative to lithium-ion, as sodium is both cheaper and more widely available than lithium. The use of organic liquid sodium electrolytes raises concerns over safety and the available operating voltage window, but solid-state electrolytes could increase safety and energy density, increase the number of cycles possible and facilitate the use of versatile battery cell geometries.

In work published in *Chemical Communications*, researchers now at the University of Sheffield and the ISIS used muon spin relaxation measurements on EMU to investigate the transport properties of a novel, sodium-rich double perovskite (Na<sub>1.5</sub>La<sub>1.5</sub>TeO<sub>6</sub>). Their results revealed a low activation energy barrier for sodium diffusion, demonstrating that this material shows great promise for use as an electrolyte in solid-state sodium batteries.



Crystal structure of the Na-rich double perovskite, Na<sub>1.5</sub>La<sub>1.5</sub>TeO<sub>6</sub>


## Understanding the performance of hydrogen storage materials

**Related publication:** "Synthesis and characterization of mixed sodium and lithium fullerides for hydrogen storage" International Journal of Hydrogen Energy, Volume 43, Issue 34, Pages 16766-16773

DOI: 10.1016/j.ijhydene.2018.03.210

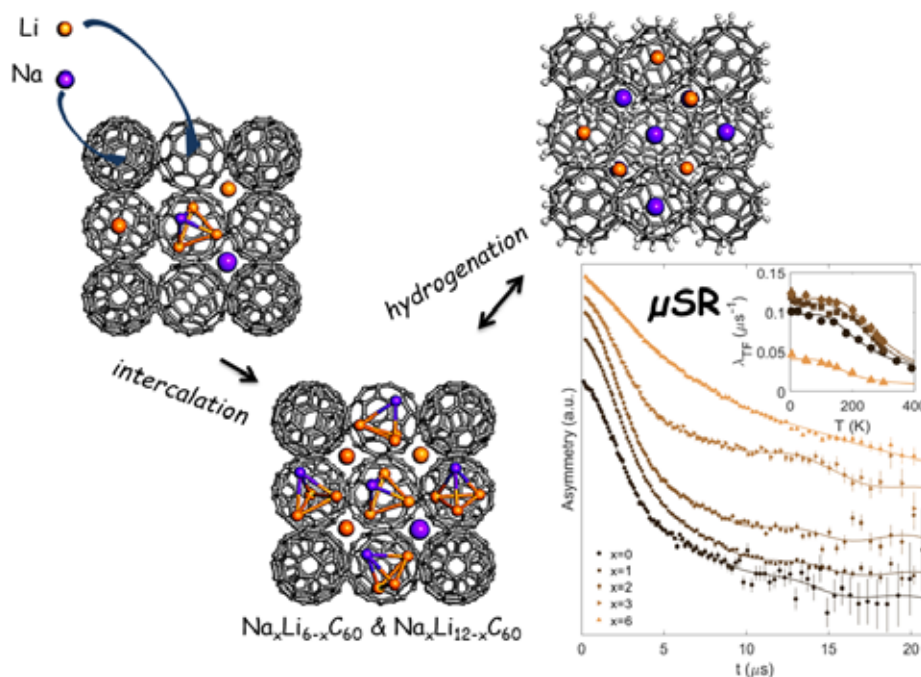
Instrument: EMU

**Funding:** EU Horizon 2020 Marie Skłodowska-Curie grant nr. 665593 and Cariplo foundation project nr. 2013-0592.

 Mattia Gaboardi (ISIS), Nicola Sarzi Amadè, Mauro Riccò (Università di Parma), Chiara Milanese, Alessandro Girella, Marta Gioventù (Università Degli Studi di Pavia), and Felix Fernandez-Alonso (ISIS; University College London).

There is renewed interest in intercalated fullerides in the field of energy storage, due to their performance as hydrogen-absorbing materials. An international team of researchers investigated sodium (Na) and lithium (Li) doping of Buckminster fullerene ( $C_{60}$ ). In general, sodium-doped  $C_{60}$  compounds have release hydrogen at a lower temperature. However, lithium-doped  $C_{60}$  compounds are lighter and can absorb larger quantities of hydrogen. In this work, the group investigated adding small amounts of sodium into a mainly lithium-doped  $C_{60}$  compound with the aim of balancing these benefits.

After characterisation of the structure of the mixed fullerides using X-ray powder diffraction and Raman spectroscopy, the group measured their hydrogen uptake and release. They found that the temperature of hydrogen release decreased as the amount of sodium was increased. The researchers then used muon spin relaxation experiments on EMU to compare  $Na_xLi_{6-x}C_{60}$  and  $Na_xLi_{12-x}C_{60}$  compounds. They found that, for  $Na_xLi_{6-x}C_{60}$ , the muonium has a preference for binding to the outside of the fullerene molecule, whereas for  $Na_xLi_{12-x}C_{60}$  (the fulleride with the higher lithium content) the muonium preferentially binds with the lithium atom. This is likely to lead to the formation of LiH, which will reduce the rate of hydrogen adsorption, explaining the improved properties of  $Na_xLi_{6-x}C_{60}$  when sodium is added to replace lithium.



Schematic of the hydrogen uptake and release of the intercalated fullerides, alongside muon spin relaxation results.




## Neutrons – a breath of fresh air for the offshore wind turbine industry

**Related publication:** “Residual stress measurements in offshore wind monopile weldments using neutron diffraction technique and contour method” *Theoretical and Applied Fracture Mechanics*, Volume 96, August 2018, Pages 418-427

DOI: 10.1016/j.tafmec.2018.06.001

Instrument: ENGIN-X

Funding: EPSRC

 Anais Jacob (Cranfield University), Jeferson Oliveira (The Open University), Ali Mehmanparast (Cranfield University), Foroogh Hosseinzadeh (The Open University), Joe Kelleher (ISIS), Filippo Berto (Norwegian University of Science and Technology).

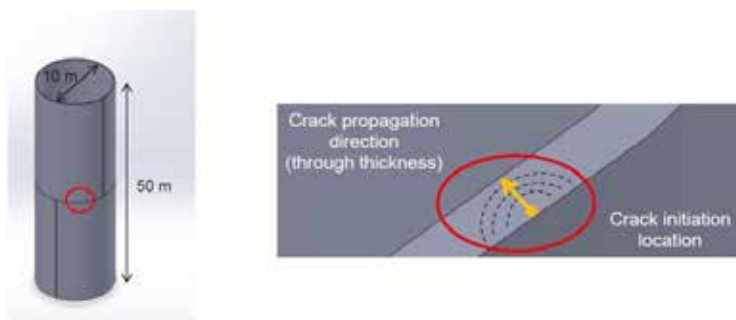
ENGIN-X has helped tackle one of the most pressing concerns facing the offshore wind turbine industry – the assessment of the structural integrity of turbine foundations. Offshore wind farms are developing quickly and, by 2030, they could be providing up to a third of the UK’s electricity. Wind turbines require resilient foundations that must cope with both high stresses during installation and a harsh offshore environment during operation. The assessment of the structural integrity of wind turbine foundations is, therefore, a critical issue for the energy industry.

The most widespread type of wind turbine foundation, the monopile, is constructed by welding a series of steel “cans” together. Once assembled, the full-sized structure can span up to 10 metres in diameter and 70 metres in length. The monopiles are then hammered deep into the seabed, anchoring the wind turbine to the ground and supporting its structure.

Researchers from Cranfield University, the Open University and the Norwegian University of Science and Technology used ENGIN-X to investigate the influence of the welding process on steel used in offshore monopile structures. They conducted neutron diffraction measurements on a welded component often used in offshore wind monopiles. Their findings will help to improve the design of future offshore wind monopile structures.



Left: The monopile, installation into the seabed. Monopile is typically 50-70 m in length and 3-10 m in diameter. Right: Monopiles are made of thick hot-rolled structural steel plates subjected to cold-rolling and bending followed by welding in the longitudinal direction to form “cans”. Image reproduced from: A. Jacob et al. *Theoretical and Applied Fracture Mechanics* 96 (2018) 418–427 DOI:10.1016/j.tafmec.2018.06.001



Left: A schematic representation of a circumferential weld in an offshore wind turbine monopile. Right: Representation of the crack initiation and propagation within a circumferential weld of a monopile. Cracks are often first created in the circumferential weld region. Image reproduced from: A. Jacob et al. *Theoretical and Applied Fracture Mechanics* 96 (2018) 418–427 DOI:10.1016/j.tafmec.2018.06.001

### Investigating marine aerosols at night

**Related publication:** “Night-Time Oxidation of a Monolayer Model for the Air–Water Interface of Marine Aerosols—A Study by Simultaneous Neutron Reflectometry and in Situ Infra-Red Reflection Absorption Spectroscopy (IRRAS)” *Atmosphere* 2018, 9(12), 47

DOI: 10.3390/atmos9120471

**Instrument:** INTER

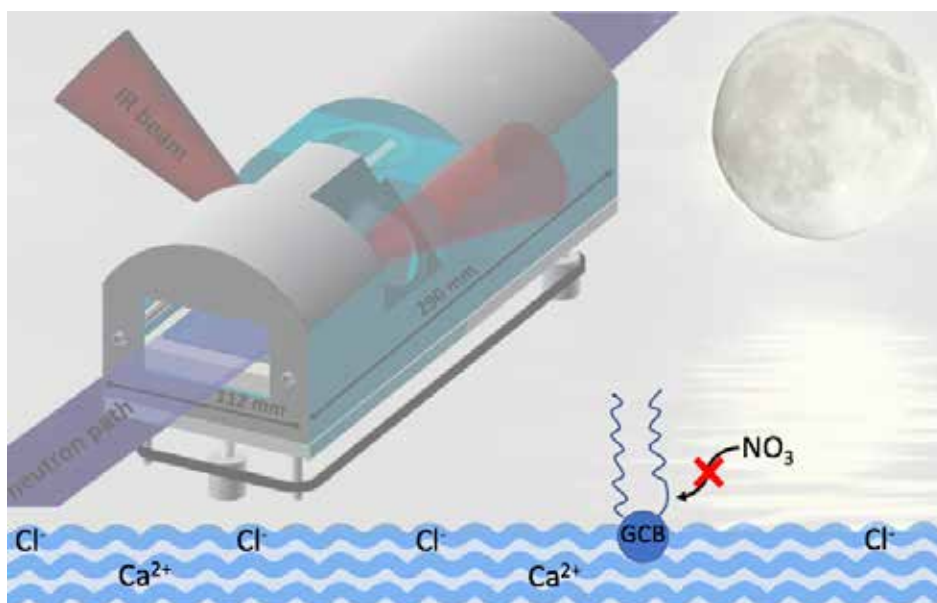
**Funding:** NERC and STFC

 Ben Woden (University of Reading), Maximilian W. A. Skoda (ISIS), Matthew Haggren (University of Reading) and Christian Pfrang (University of Birmingham).

The role of atmospheric aerosols in cloud formation is a topic of crucial importance for climate science. The difference between the sunlight absorbed by the Earth and the energy radiated back into space is called radiative forcing. How aerosol concentrations affect this radiative forcing is exceptionally complex, poorly understood, and challenging to measure.

Lipopolysaccharides (LPS) are large molecules, made up of a lipid and a polysaccharide, which have been observed in marine aerosols. Researchers from the universities of Birmingham and Reading used the neutron reflectometry instrument INTER to investigate a typical glycolipid, galactocerebroside (GCB), as a proxy for these more complex lipopolysaccharides. Their pioneering experiment was explicitly designed to study mixed organic monolayers at the air-water interface. Using neutron reflectometry simultaneously with Fourier transform infrared reflection absorption spectroscopy allowed for more sophisticated observations than were previously possible. They investigated the structure at the air–water interface using complementary Brewster angle microscopy.

Their work, published in *Atmosphere*, looked specifically at the oxidation of organic films by nitrate radicals ( $\text{NO}_3^\cdot$ ), the key atmospheric oxidant present at night. Their results suggest that aerosols produced from the sea-surface microlayer at night remain covered in surfactant molecules on timescales that are atmospherically relevant. Most surprisingly, the presence of salt ( $\text{CaCl}_2$ ) was found to substantially extend the lifetime of the, usually reactive, tails of the surfactants that cover the aerosols, offering a new explanation for their longer lifetimes in the atmosphere. The extended atmospheric lifetimes of the surfactants may reduce the surface tension of droplets and could affect transport across the air-water interface.



*Applying a novel experimental set-up that combines simultaneous interrogation of floating one-molecule thin films by infra-red (IR) spectroscopy and neutron reflectometry demonstrated that night-time oxidation by  $\text{NO}_3^\cdot$  cannot fully remove a galactocerebroside (GCB) monolayer from the sea surface on atmospherically relevant timescales, leaving its saturated tail at the interface.*


## Developing efficient organic solar cells

**Related publication:** "Efficient non-fullerene organic solar cells employing sequentially deposited donor-acceptor layers" *J. Mater. Chem. A*, 2018,6, 18225-18233

DOI: 10.1039/C8TA06860G

**Instrument:** Offspec

**Funding:** EPSRC, China Scholarship Council, NSFC and MOST of China, Marie Skłodowska Curie Fellowship scheme, Wallenberg Academy Fellow, Royal Society University Research Fellow.

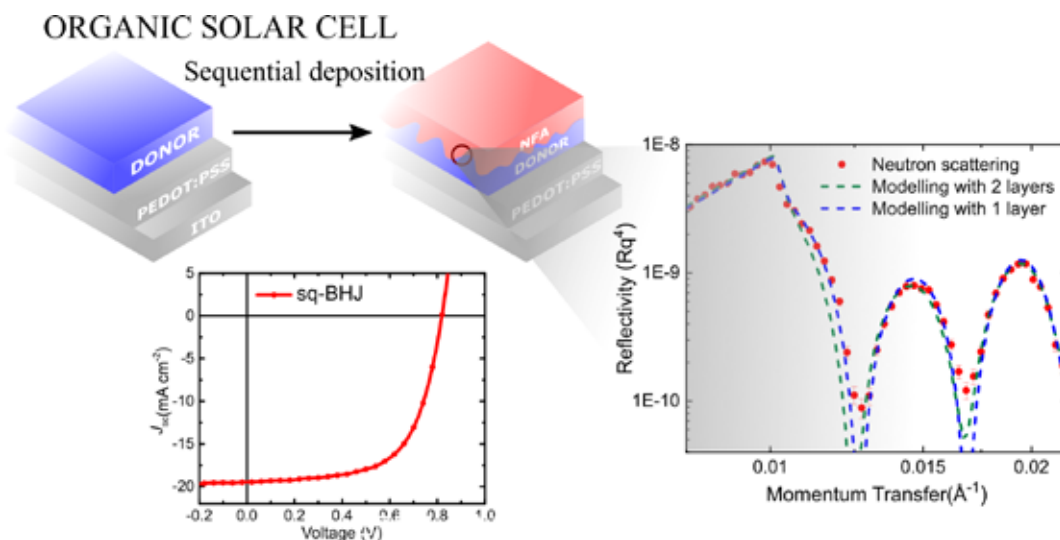
 Jiangbin Zhang (University of Cambridge, Imperial College London), Bin Kan (Nankai University), Andrew J. Pearson (University of Cambridge), Andrew J. Parnell (The University of Sheffield), Joshaniel F. K. Cooper (ISIS), Xiao-Ke Liu (University of Cambridge, Linköping University), Patrick J. Conaghan (University of Cambridge), Thomas R. Hopper (Imperial College London), Yutian Wu (University of Cambridge), Xiangjian Wan (Nankai University), Feng Gao (Linköping University), Neil C. Greenham (University of Cambridge), Artem A. Bakulin (Imperial College London), Yongsheng Chen (Nankai University) and Richard H. Friend (University of Cambridge)

The mechanical flexibility and relatively low cost of organic solar cells (OSCs) enables their use as an integrated power-generating source in niche applications, such as wearable electronics, and in building-integrated photovoltaics that could revolutionise infrastructure design.

Current OSCs use fullerene-based semiconductors as electron acceptors, but the recent development of high-performance non-fullerene acceptors (NFAs) has transformed the research into OSCs. NFAs have recently outperformed their fullerene counterparts in bulk-heterojunction (BHJ) organic solar cells.

In research published in the *Journal of Materials Chemistry A*, an international team of researchers used neutron reflectivity measurements on the Offspec beamline to investigate the potential of a sequentially deposited BHJ (sq-BHJ) layout using an NFA as the acceptor component. This sq-BHJ layout occurs when the NFA is deposited onto the electron donor layer (usually a polymer), rather than using a co-deposition technique.

Their results show that this layout can offer comparable performance to that measured when co-depositing BHJ, without the need for solvent additives, or post-treating the deposited sample. Their two-step process may have other relevant advantages, including higher stability, large-scale production and green processing. It could therefore be possible, after further investigation, to produce a sq-BHJ system that can be used in practical applications.



Left: the device layout via sequential deposition, and the device photovoltaic performance; Right: Modelling of neutron scattering data using one or two layers.




### New mechanism observed for CO<sub>2</sub> transfer in flexible MOFs

**Related publication:** “Night-Time Oxidation of a Monolayer Model for the Air–Water Interface of Marine Aerosols—A Study by Simultaneous Neutron Reflectometry and in Situ Infra-Red Reflection Absorption Spectroscopy (IRRAS)” *Atmosphere* 2018, 9(12), 47

DOI: 10.1038/s41467-019-08939-y

**Instrument:** IRIS and TOSCA

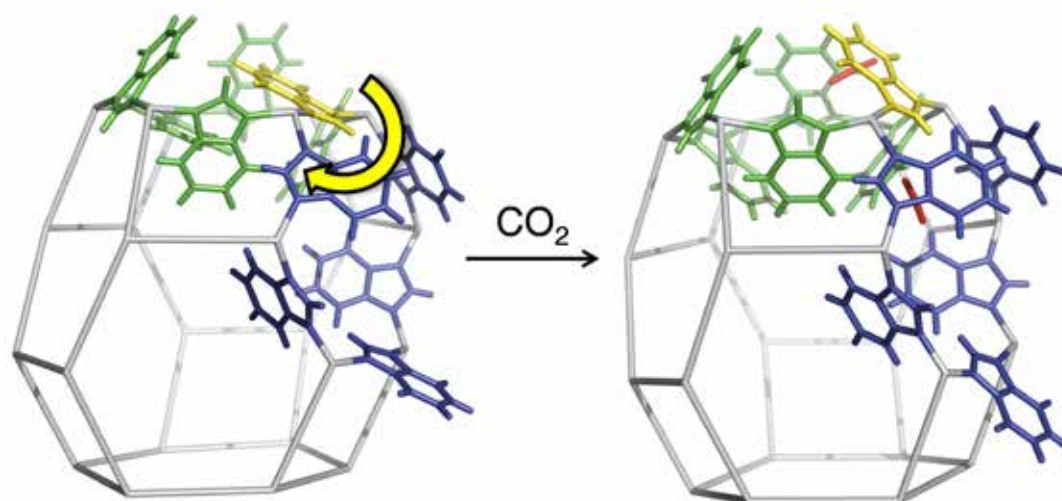
**Funding:** Cambridge Commonwealth, European and International Trust, and STFC.

 Pu Zhao (University of Cambridge; University of Oxford), Hong Fang (Virginia Commonwealth University), Sanghamitra Mukhopadhyay (ISIS), Aurelia Li (University of Cambridge), Svemir Rudić (ISIS), Ian J. McPherson (University of Oxford), Chiu C. Tang (Diamond Light Source), David Fairen-Jimenez (University of Cambridge), S. C. Edman Tsang (University of Oxford) and Simon A. T. Redfern (University of Cambridge).

Flexible Metal-Organic Frameworks (MOFs) show promise in a wide variety of applications such as gas separation, drug delivery and molecular sensing, because of their stimuli-responsive behaviours. Considerable research has been dedicated to improving our understanding of the structural changes of flexible MOFs in response to external stimuli. However, the general model used has been one of uniform pore deformation, and advances have been made in synthesising MOFs with pores that vary in size, shape, and environment.

In work published in *Nature Communications*, a team of researchers from the universities of Oxford and Cambridge, and Virginia Commonwealth University in the USA, used quasielastic neutron scattering on IRIS and inelastic neutron scattering on TOSCA to investigate the structural change seen in the flexible MOF ZIF-7 on CO<sub>2</sub> adsorption. They demonstrated that the change occurs because of CO<sub>2</sub> migration in its non-uniform porous structure, and not by its guest-hosting pores opening. This mechanism is distinct from the majority of guest-host interactions reported for other MOFs and extremely uncommon.

This work provides new insights into MOF flexibility and offers new methods for analysing adsorption mechanisms in flexible MOFs, which could help design new materials.



Linker rotation and phase transition caused by CO<sub>2</sub> migration.


## Neutrons offer insights into proton conduction in crystalline MOFs

**Related publication:** “Modulating proton diffusion and conductivity in metal–organic frameworks by incorporation of accessible free carboxylic acid groups” *Chem. Sci.*, 2019, 10, 1492-1499

DOI: 10.1039/C8SC03022G

Instrument: IRIS

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

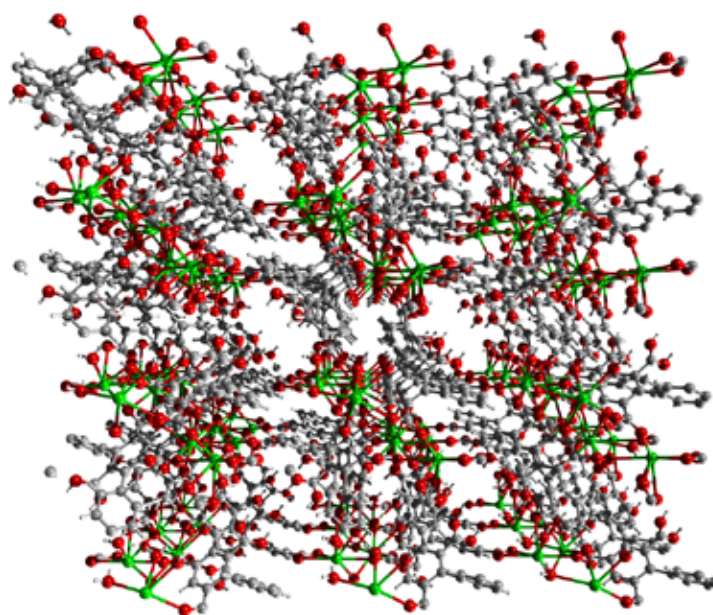
 Peter Rought, Christopher Marsh, Simona Pili (University of Manchester), Ian P. Silverwood, Victoria García Sakai (ISIS), Ming Li (University of Nottingham), Martyn S. Brown (University of Manchester), Stephen P. Argent (University of Warwick), Inigo Vitorica-Yrezabal, George Whitehead (University of Manchester), Mark R. Warren (Diamond Light Source), Sihai Yang and Martin Schröder (University of Manchester)

Proton exchange membrane fuel cells (PEMFCs) are a promising technology for powering hydrogen-based vehicles. Their delivery will require the development of materials that can move protons efficiently across the membrane.

The polymer Nafion is the most commonly used membrane material in PEMFCs, but the lack of long-range order in polymers makes them poor candidates for new materials with higher conductivity and a wider temperature range for operation.

Hybrid MOF (Metal-Organic Framework) materials are emerging as a potential new class of proton conductors. Including acidic groups such as  $-\text{COOH}$ ,  $-\text{PO}_3\text{H}_2$  and  $-\text{SO}_3\text{H}$  can facilitate efficient proton transfer pathways. However, it is very challenging to synthesise MOFs with these acidic groups.

Recent research has shown quasi-elastic neutron scattering (QENS) to be a powerful technique for gaining insights into proton conduction in crystalline MOFs. In work published in *Chemical Science*, a team of researchers used QENS on IRIS to investigate new barium-based MOFs. They designed and synthesised three new MOFs (MFM-510, -511 and -512) from a family of organic ligands containing multiple carboxylic acid groups. Their results showed that MFM-512 (see image below) is a promising candidate compared to other low-temperature proton-conducting MOFs.



Structural model of MFM-512


## Using neutrons to determine the diffusion mechanism for Na-ion battery materials

**Related publication:** "Diffusion mechanism in the sodium-ion battery material sodium cobaltate" *Scientific Reports* (2018) 8:3210

DOI: 10.1038/s41467-019-08939-y

**Instrument:** IRIS and TOSCA

**Funding:** Cambridge Commonwealth, European and International Trust, and STFC.

 T. J. Willis (Royal Holloway, ISIS), D. G. Porter (Diamond Light Source), D. J. Voneshen (ISIS), S. Uthayakumar (Royal Holloway), F. Demmel, M. J. Gutmann (ISIS), M. Roger (Service de Physique de l'Etat Condensé), K. Refson (Royal Holloway, ISIS) & J. P. Goff (Royal Holloway)

The revolution in mobile electronic technology has been made possible by high-performance batteries based on the movement of lithium ions in materials of the form  $\text{Li}_x\text{CoO}_2$ . Increasing demand for energy storage for renewable energy sources and the scarcity of lithium have led to intense interest in sodium-ion batteries, including the structurally-related  $\text{Na}_x\text{CoO}_2$ .

In work published in *Scientific Reports*, an international team of researchers used diffuse X-ray scattering, quasi-elastic neutron scattering (QENS) and ab-initio molecular dynamics simulations to determine the diffusion mechanism for  $\text{Na}_{0.8}\text{CoO}_2$ . The group performed QENS measurements of Na-ion diffusion on single-crystal and high-purity-powder samples using the OSIRIS spectrometer. Beforehand, they measured their samples using diffraction on SXD to determine which crystal to use in their experiment.

Using an approach that could also be used to understand the diffusion mechanism in other Na-ion, and Li-ion, battery materials, they found that the ordering of the sodium ions in the material structure is what determines the diffusion pathways and governs the diffusion rate. Their work uncovered factors that enhance the ionic conductivity for layered Na-ion cathode materials, and those which suppress diffusion. Their results are a step towards designing electrodes and solid electrolytes with better ionic conductivity.



Toby Willis, David Bowman, and Jon Goff, Royal Holloway, on the SXD instrument

## Chemistry


### Neutron scattering reveals the orientational structure of liquid benzene under confinement

**Related publication:** "Confinement Effects on the Benzene Orientational Structure" *Angew. Chem. Int. Ed.* 2018, 57, 4565-4570

DOI: 10.1002/anie.201713115

**Instrument:** NIMROD

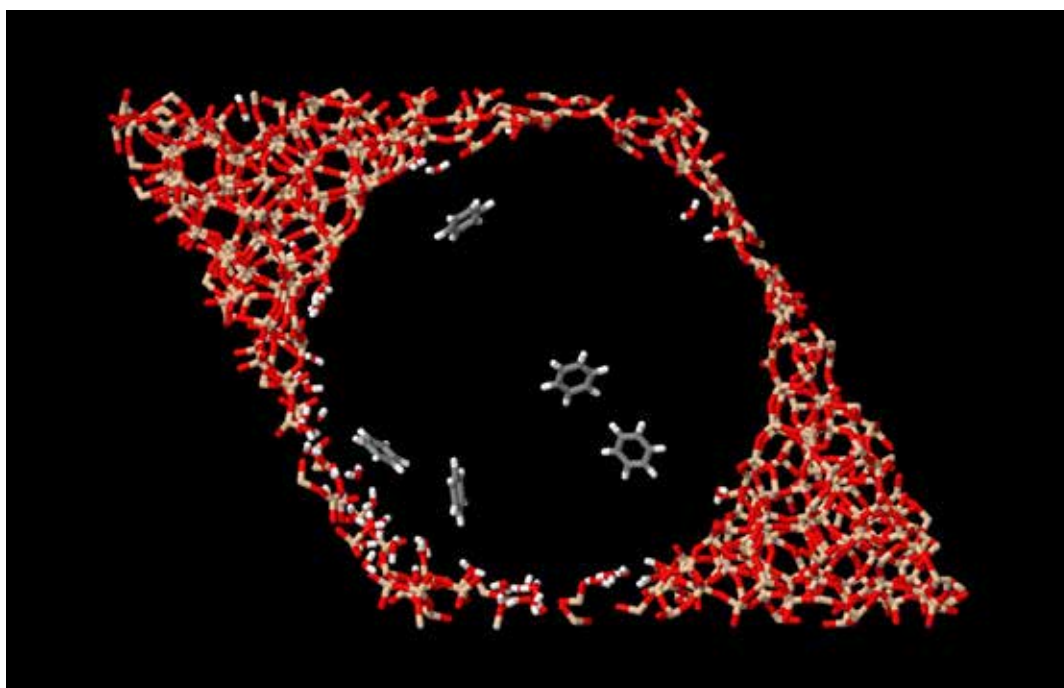
**Funding:** EPSRC, the UK Catalysis Hub, STFC Scientific Computing Department.

 Marta Falkowska (The University of Manchester), Daniel T. Bowron (ISIS), Haresh Manyar (Queen's University Belfast), Tristan G. A. Youngs (ISIS), and Christopher Hardacre (The University of Manchester).

Liquids often behave differently when confined inside a restricted space. Water, for example, can remain liquid at significantly lower temperatures (rather than freezing and becoming a solid) when it is confined. Confined liquids are being studied in many different areas of science including geology, biology, food, catalysis and drug preservation.

Researchers from the University of Manchester and Queen's University Belfast used neutron scattering at ISIS to obtain the structural properties of liquid benzene (the archetypical example of an aromatic compound) in confinement. Their results, published in *Angewandte Chemie*, show that the structure of liquid benzene is very different when it is confined. Confinement tends to change the local ordering between benzene molecules, which may change their reactivity, although more research is needed to confirm this.

Future experiments could explore how the behaviour depends on different parameters, by changing the size and shape of the confining pores, for example. The authors also hope to use complementary in situ techniques such as nuclear magnetic resonance (NMR) to extract more information.



Structural properties of benzene in pores of MCM-41 were probed using NIMROD




## First observation of the elusive encounter complex in Frustrated Lewis Pairs

**Related publication:** "Frustrated Lewis pairs in ionic liquids and molecular solvents – a neutron scattering and NMR study of encounter complexes" *Chem. Commun.*, 2018, 54, 8689

DOI: 10.1039/c8cc03794a

**Instrument:** SANDALS

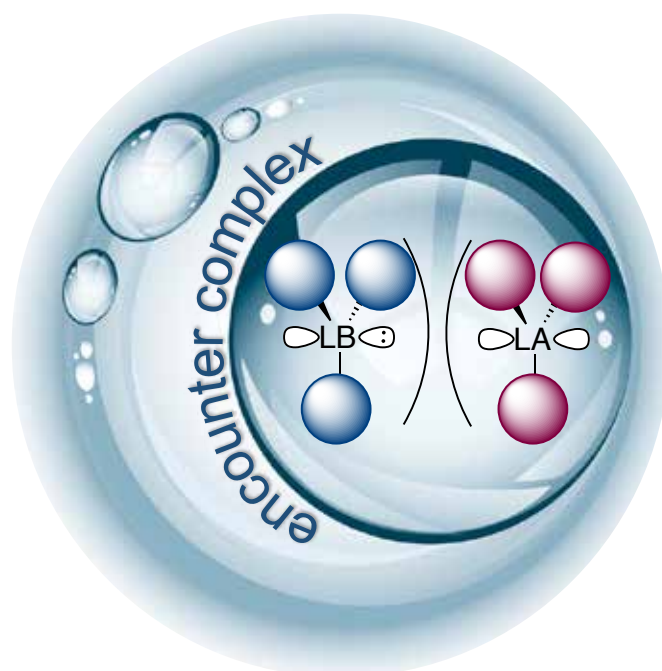
**Funding:** EPSRC, QUILL and the European Union's Horizon 2020 research and innovation programme.

 Lucy C. Brown, James M. Hogg, Mark Gilmore (Queen's University of Belfast), Leila Moura (Queen's University of Belfast), Silvia Imberti, Sabrina Gärtner (ISIS), H. Q. Nimal Gunaratne, Ruairi J. O'Donnell, Nancy Artioli, John D. Holbrey and Małgorzata Swadźba-Kwaśny (Queen's University of Belfast).

Frustrated Lewis Pairs (FLPs) integrate Lewis acidic and basic sites (that can either accept or donate a pair of electrons), which then act in partnership to activate small molecules. They are often based on abundant elements and are notable as metal-free catalysts for hydrogen activation, a characteristic that can be extended to other small molecules, such as nitrogen. As hydrogen activation catalysts, they offer an inexpensive alternative to platinum-group metal catalysts, avoiding the risk of heavy metal pollution.

In work published in *Chemical Communications*, chemists from Queen's University Belfast teamed up with members of the ISIS Disordered Materials Group to study the liquid structure of a FLP solution using the instrument SANDALS. Their findings agree with predictions made via density functional theory structural modelling, enabling the determination of catalytically active sites and offering the first direct observational evidence for the formation of weakly associated Lewis acid-base 'encounter complexes' in solution.

The researchers then carried out the first study of FLPs in ionic liquids, showing that the formation of an encounter complex could be enhanced by use of an ionic liquid solvent. Significantly higher concentrations of long-lived associated FLPs were reported which, it is anticipated, will enhance catalytic activity compared to conventional solvents.



*Illustration of a Frustrated Lewis Pair encounter complex solution on the SXD beamline*


## Developing a transferable theoretical framework for magnetic exchange in asymmetric lanthanide dimetallics

**Related publication:** "Measurement of Magnetic Exchange in Asymmetric Lanthanide Dimetallics: Toward a Transferable Theoretical Framework" *J. Am. Chem. Soc.* 2018, 140, 7, 2504-2513

DOI: 10.1021/jacs.7b10714

**Instrument:** LET, IRIS and MARI

**Funding:** EPSRC, the Ramsay Memorial Trust, The University of Manchester, The Italian Ministry of Education, Universities and Research (MIUR) and DFG.

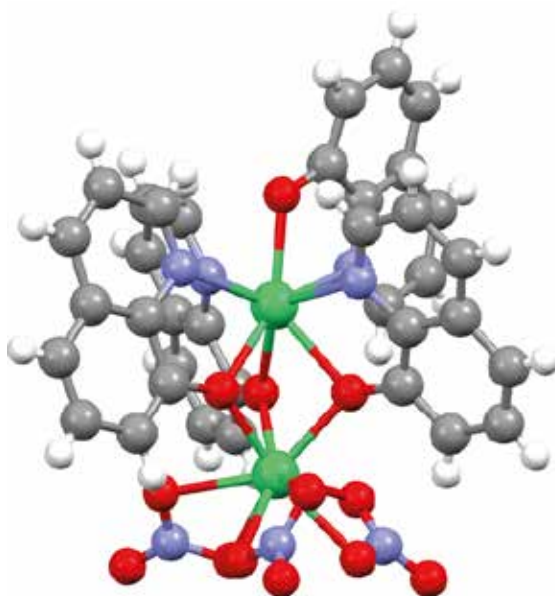
 Marcus J. Giansiracusa, Eufemio Moreno-Pineda (The University of Manchester), Riaz Hussain (Università di Parma), Raphael Marx, María Martínez Prada, Petr Neugebauer (Universität Stuttgart), Susan Al-Badran, David Collison, Floriana Tuna (The University of Manchester), Joris van Slageren (Universität Stuttgart), Stefano Carretta (Università di Parma), Tatiana Guidi, (ISIS) Eric J. L. McInnes, Richard E. P. Winpenny, and Nicholas F. Chilton (The University of Manchester).

There is increasing interest in the use of lanthanide ions for quantum information processing and in single-molecule magnets. Because of this, researchers are seeking to understand the nature of magnetic interactions in lanthanide compounds.

An international team of researchers studied the magnetic interactions within Ln dimetallic compounds; compounds which contain atoms of two metallic elements. They aimed to define a series of detailed benchmark measurements on which to build a transferable theoretical framework and used electron paramagnetic resonance (EPR) spectroscopy to directly probe the lowest-lying exchange states.

In work published in the *Journal of the American Chemical Society*, the team directly probed the magnetic exchange interactions within two asymmetric dimetallic compounds using EPR spectroscopy, which they were then able to accurately model. They collected inelastic neutron scattering (INS) spectra on the LET, IRIS, and MARI spectrometers, and used them alongside far-infra-red measurements to support calculations for identifying the origin of the magnetic signals for each site in the molecule.

Their results will contribute to the development of theoretical models of magnetic exchange. Future theoretical studies may be able to demonstrate the feasibility of tailoring lanthanide compounds for technological use.



*Asymmetric dimetallic lanthanide molecules were studied with EPR and INS spectroscopies to unravel the fine magnetic structure due to the exchange interaction*

## Advanced Materials

### Muons shed light on the unusual behaviour of high-temperature superconductors

**Related publication:** "Discovery of slow magnetic fluctuations and critical slowing down in the pseudogap phase of  $\text{YBa}_2\text{Cu}_3\text{O}_y$ ", *Sci. Adv.*, 2018, 4, 1, eaao5235

DOI: 10.1126/sciadv.aao5235

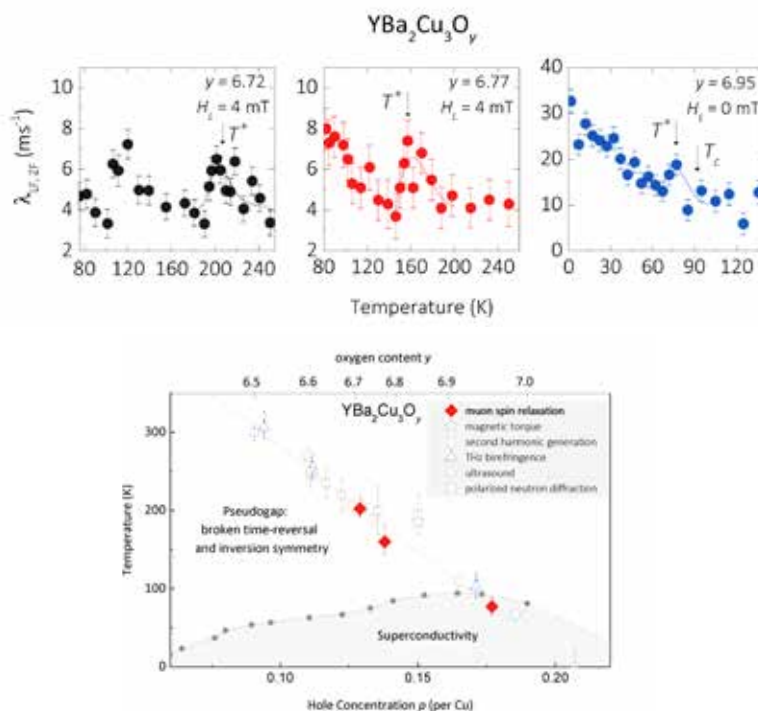
Instrument: MuSR, EMU

**Funding:** National Key Research and Development Program of China, National Natural Science Foundation of China, Science and Technology Commission of Shanghai Municipality of China, University of California Riverside Academic Senate, National Science Foundation Division of Materials Science, USA.

**Jian Zhang**, Zhaofeng Ding, Cheng Tan, Kevin Huang (Fudan University), Oscar O. Bernal (California State University), Pei-Chun Ho (California State University), Gerald D. Morris (TRIUMF), Adrian D. Hillier, Pabitra K. Biswas, Stephen P. Cottrell (ISIS), Hui Xiang (Shanghai Jiao Tong University), Xin Yao (Shanghai Jiao Tong University; Collaborative Innovation Center of Advanced Microstructures), Douglas E. MacLaughlin (University of California) and Lei Shu (Fudan University; Collaborative Innovation Center of Advanced Microstructures).

One of the most puzzling features of high-temperature superconductors is the pseudogap phase, in which unusual properties such as broken-time reversal and inversion symmetry are observed. Although the pseudogap phase has been the subject of considerable research, there is not yet a consensus on either its origin, or its role in high-temperature superconductivity.

An international team of researchers used muon spin relaxation experiments on MuSR and EMU to measure dynamic muon spin relaxation rates in single crystals of the material  $\text{YBa}_2\text{Cu}_3\text{O}_y$ . Their discovery of slow magnetic fluctuations, reported in *Science Advances*, provides an understanding of the absence of static magnetic fields due to intra-unit-cell (IUC) magnetic order. Their results are strong evidence for IUC order and its excitations, and establish them as important for understanding the unusual behaviour of these materials.



Dependence of the LF exponential relaxation rate  $\lambda_{LF}(HL)$  on LF HL in  $\text{YBa}_2\text{Cu}_3\text{O}_y$  (top) and Phase diagram of pseudogap and charge-density-wave/charge inhomogeneity onset temperatures in  $\text{YBa}_2\text{Cu}_3\text{O}_y$  (bottom).


## A simple 'one pot' synthesis produces silica nanoparticles with great potential

**Related publication:** "Structure and characterisation of hydroxyethylcellulose–silica nanoparticles" *RSC Adv.*, 2018, 8, 6471-6478

**DOI:** 10.1039/C7RA08716K

**Instrument:** SANS2D

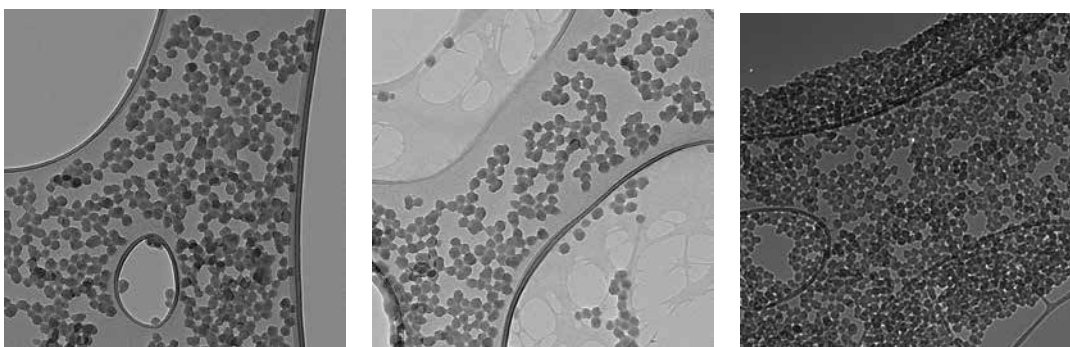
**Funding:** University of Reading

 Edward D. H. Mansfield, Yash Pandya, Ellina A. Mun (University of Reading), Sarah E. Rogers (ISIS), Inbal Abutbul-Ionita, Dganit Danino (Technion – Israel Institute of Technology), Adrian C. Williams and Vitaliy V. Khutoryanskiy (University of Reading).

Silica nanoparticles are used in applications as wide-ranging as drug delivery and engineering, water treatment and detergents, and cosmetics. These tiny particles are between 1 and 100 nanometres in diameter. For comparison, a sheet of paper is around 100,000 nanometres thick.

In recent years, there has been considerable interest in tailoring nanoparticles for specific applications using polymers, with thiol-functionalised silica nanoparticles attracting particular attention. A team of researchers from the University of Reading synthesised polymer-coated thiolated silica nanoparticles in a "one-pot" reaction, publishing their results in *RSC Advances*.

They analysed the size and functionality of the synthesised nanoparticles using a variety of techniques, including small-angle neutron scattering (SANS) on the SANS2D instrument, dynamic light scattering, transmission electron microscopy and cryo-transmission electron microscopy. By comparing the results from the different techniques, they observed a clustering effect of the nanoparticles, with increasing numbers of particles aggregating as a function of hydroxyethylcellulose concentration in the reaction. As hydroxyethylcellulose is cheaper and easier to produce than other polymers, this method may allow the mass production of thiolated silica nanoparticles tailored to a wide range of applications.



*Transmission electron microscopy images of thiolated silica nanoparticles coated with hydroxyethylcellulose*




## High-pressure neutron study changes our understanding of an important synthetic oxide

**Related publication:** "Magnetic and structural changes in  $\text{LaCo}_{0.9}\text{Mn}_{0.1}\text{O}_3$  at high pressure" *Journal of Physics: Condensed Matter*, 2018, Volume 30, Number 3

DOI: 10.1088/1361-648X/aaa042

**Instrument:** PEARL and Materials Characterisation Lab

**Funding:** STFC

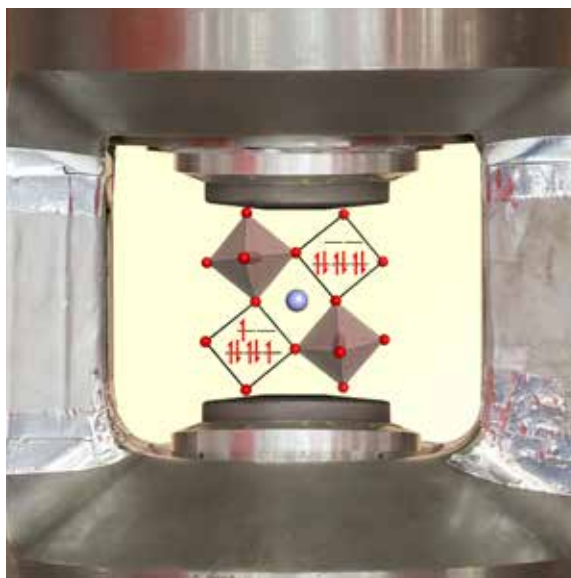
 M Capone (ISIS, ESS, University of Edinburgh), C J Ridley, N P Funnell, G B G Stenning (ISIS), J S Loveday (University of Edinburgh), M Guthrie (ESS) and C L Bull (ISIS).

It is possible to alter the atomic arrangement of materials under extremely high pressures, altering the structure of matter and tuning important technological properties. The PEARL diffractometer at the ISIS Neutron Facility was explicitly designed to measure these changes under pressure. Mara Capone is a PhD student at the University of Edinburgh, co-funded by the European Spallation Source and ISIS through an ISIS Facility Development Studentship grant. The group performed neutron-diffraction measurements up to 6 GPa on PEARL, and high-pressure temperature-dependent magnetisation measurements in the ISIS Materials Characterisation Laboratory to study the structural and magnetic properties of the perovskite structured  $\text{LaCo}_{0.9}\text{Mn}_{0.1}\text{O}_3$ .

Oxides with the perovskite structure are an important class of materials, and the  $\text{LaCo}_x\text{Mn}_{1-x}\text{O}_3$  series is an appealing ferroic material with potential solid-state technological applications. It has been shown, for example, that low-level doping of  $\text{LaCoO}_3$  with manganese (Mn) cations forms an effective catalyst for the oxidation of substances in vehicle exhausts. The electronic properties of the material are governed by subtle distortions of the atomic octahedra that build up its structure, and this study measured these distortions with unprecedented precision. The results, published in the *Journal of Physics: Condensed Matter*, revealed different behaviour than earlier X-ray studies.



*Left: PhD student Mara Capone with the high-pressure cell currently being developed for use on the PEARL diffractometer.*



*Right: The Paris-Edinburgh press has been used to compress perovskite related materials tuning the octahedral tilting and electronic properties at high pressure.*


## Investigating SnIP, the first atomic-scale double helical semiconductor

**Related publication:** "Flexible and ultrasoft inorganic 1D semiconductor and heterostructure systems based on SnIP" *Advanced Functional Materials*, 2019, Volume 29, Issue 18, 1900233

DOI: 10.1002/adfm.201900233

**Instrument:** TOSCA

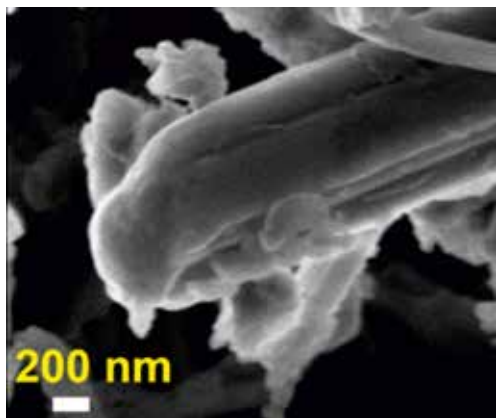
**Funding:** German Science Foundation and Natural Sciences and Engineering Research Council of Canada within the International Graduate School ATUMS IRTG 2020 and German Science Foundation Grant NI1095/8-1; CALIPSO plus Grant 730872 from the EU Framework Program HORIZON 2020; Germany's Excellence Strategy-EXC2089/1-390776260

 Claudia Ott, Felix Reiter, Maximilian Baumgartner, Markus Pielmeier, Anna Vogel, Patrick Walke, Stefan Burger, Michael Ehrenreich, Gregor Kieslich, Dominik Daisenberger (Technical University of Munich), Jeff Armstrong (ISIS), Ujwal Kumar Thakur, Pawan Kumar (Donadeo Innovation Centre For Engineering, Edmonton), Shunda Chen, Davide Donadio (University of California), Lisa S. Walter, R. Thomas Weitz (Ludwig-Maximilians-University Munich), Karthik Shankar (Donadeo Innovation Centre For Engineering, Edmonton) and Tom Nilges (Technical University of Munich).

Electronic devices demand ever-increasing efficiency, flexibility, and stability, driving the development of new semiconductors. The first atomic-scale double helical semiconductor, SnIP, offers exceptional electronic properties, with potential applications in energy conversion and water splitting that could revolutionise the hydrogen economy.

In work published in *Advanced Functional Materials*, an international team of researchers performed high-resolution inelastic neutron scattering measurements on TOSCA to investigate the physical properties of pure SnIP, and SnIP-like systems with differing chemical composition.

They formed core-shell particles of SnIP and  $C_3N_4$ , which might be used in energy conversion applications. The SnIP@ $C_3N_4$  system showed both polymer-like behaviour, and the semiconducting behaviour of SnIP. Their results demonstrate the potential of a double helical SnIP as a defined one-dimensional material for semiconductor applications, and that tube-like or 1D semiconductors could offer considerable promise as a new class of flexible semiconductors.



*SnIP needles after synthesis. Length up to 10 nm and diameter several hundred micrometers.*




*He-ion microscope picture of a SnIP needle enwrapped in a  $C_3N_4$  shell.*

## Our people



### PhD to Beamline Scientist

 Dr Genoveva Burca

#### Beamline scientist on IMAT

Genoveva's PhD work at The Open University focused on detailed modelling calculations crucial to the design and building of the IMAT instrument, and developing a tomography driven diffraction technique that combined neutron imaging and diffraction. Since completing her PhD in 2012, she has worked as a post-doc on the IMAT instrument, and is now a beamline scientist.

#### Background

After ten years of teaching applied mathematics to engineering students and researching pure mathematics, Genoveva decided it was time for a new challenge: to use her knowledge and experience in cutting edge interdisciplinary research.

Having a background in mathematics and physics, she came across an opportunity with the Open University and ISIS to be involved in the development of the first instrument in the world that would use neutrons for both imaging and diffraction.

Performing the modelling calculations for IMAT (Imaging and Materials Science & Engineering) was a very exciting time for Genoveva and provided her with a wider perspective on neutron science and its applications. This is how she began her interesting and productive collaboration with ISIS, which entered a new phase when she was offered a position as a post-doctoral scientist working on IMAT. The experience she gained proved to be very useful when she became an instrument scientist.

#### Innovative, interdisciplinary, research

Determined to fully exploit the capability of the new IMAT instrument, Genoveva initiated and developed several projects from different research fields: soil-plants systems, palaeontology, medical sciences, textile fibres and materials engineering. These involved collaboration with universities, museums and companies from UK and abroad including the Oxford University Museum of Natural History, the Royal Botanic Gardens - Kew, SLU-Sweden, Rolls Royce and the Indian Institute of Technology Kharagpur, investing a lot of effort and energy in scientific community outreach. Through the STFC Food network, Genoveva had the opportunity to connect with researchers from agriculture and the food industry.

#### Future

Being passionate about her research has led Genoveva to initiate the building of a research greenhouse - first of its kind at a neutron facility. This will be integral part of the future Interdisciplinary Research Centre for Imaging in Life Sciences at ISIS. She is also in charge of the implementation and development of the future diffraction capabilities on IMAT, which will certainly widen the neutron applications by exploiting the dedicated technique she developed during her PhD: tomography-driven diffraction. Encouraged by the preliminary results obtained, Genoveva will continue her joint projects with Diamond Light Source to employ the advantages of the complementarity between X-ray and neutron imaging.



# ISIS Support Laboratories





# ISIS Materials Characterisation Laboratory

The Materials Characterisation Laboratory (MCL) boasts a wide range of instrumentation for studying a variety of material properties including determining sample structure, composition, purity and magnetic and electronic or electrical properties.

During 2018, the lab hosted 720 separate user visits supporting experiments across the range of instrumentation. The data collected were used to screen samples for neutron and muon experiments as well as collecting data to support publications, significantly contributing to over 30. The MCL team are involved in a number of collaborative projects with ISIS users, producing publications from the MCL in their own right.



Marek Jura (ISIS) in the Materials Characterisation Laboratory

## MCL highlights:

### Novel method of creating a semiconducting thin film

Germanium telluride (GeTe) is a promising candidate for a number of technologically important applications including incorporation into thermoelectric, ferroelectric and spintronic materials. One of the techniques used to deposit GeTe thin films, chemical vapour deposition (CVD), has previously been carried out with two source chemicals. A group from the University of Southampton developed and characterised a single source precursor:  $\text{Ge}(\text{TenBu})_4$ . Use of a single reagent could offer more control over both the stoichiometry and the precise deposition location of the GeTe. The MCL has played a crucial role in determining the composition and properties of these films.

**DOI: 10.1039/c8dt03263g**

### Spin-glass behaviour in hollandite materials

A team from Kent University (led by Donna Arnold) and MCL have studied the hollandite material  $\text{K}_x\text{Ru}_{4-y}\text{Ni}_y\text{O}_8$ . The samples synthesised at Kent were extensively studied within the MCL, looking at physical and structural properties using X-ray diffraction, magnetometry and X-ray fluorescence, and were found to exhibit novel magnetic behaviour. Given the interest in 4d (and 5d) magnetic systems, spin glasses, and frustrated magnetism, this work could revitalize the study of magnetism in hollandite materials.

**DOI: 10.1103/PhysRevB.98.174429**

“The Materials Characterisation Laboratory (MCL) provides pivotal support and training for the metrology aspects of our research program which develops thin-film electrodes for solar cells. The MCL staff are always on hand to help and provide the flexibility that we need for ground-up developments that lead into results that sure up our complementary neutron experiments.”

Professor Jacqui Cole, ISIS and Cambridge University

## ISIS Deuteration Facility

The ISIS Deuteration Facility (D-lab) is now in its sixth year of operation, supporting a growing user community across wide-ranging science areas. In 2018, the facility received 115 proposals, and delivered deuterated materials for experiments on 20 of the ISIS neutron instruments. The capability of the lab has grown considerably in the last few years and it now offers materials in the areas of surfactants, lipids, ionic liquids, peptides, oligomers and ligands for metal complexes.

The Deuteration Facility staff have been involved in many collaborative projects with ISIS users from academia and industry, and now host visiting researchers. Many of these projects have led to high impact publications:

### Multilayers formed by polyelectrolyte-surfactant and related mixtures at the air-water interface

The D-lab staff collaborated with a group from the University of Oxford to produce the first complete review of the spontaneous formation of multilayer structures at the air-water interface. The paper highlights multilayer formation strongly associated with unusual wetting characteristics.

**DOI: 10.1016/j.cis.2019.04.002**

### Liquid phase blending of metal-organic frameworks

The Deuteration Facility staff worked with researchers from the University of Cambridge on Metal Organic Framework (MOF) materials. The deuterated materials produced for this study in the D-lab were critical to the neutron measurements carried out on the NIMROD instrument.

**DOI: 10.1038/s41467-018-04553-6**




ISIS Deuteration Facility

## Our people



### From industrial placement to deuteration scientist

 Jasmine Hind

#### Deuteration Lab Sandwich Student

After finishing her placement year in the Deuteration Lab in the support laboratories, Jasmine Hind will go straight into a full time role within the facility.

#### Background

I chose to do the final year of my Chemistry degree as a placement in industry, rather than completing a research project at the University of Southampton, to see what working in a non-academic environment would be like.

There are strong links between the University of Southampton and the staff in the support laboratories at ISIS, so the STFC sandwich student positions were well advertised.

#### Projects

During my placement year, I worked on a project that aimed to develop a procedure for deuterating carbohydrates, driven by a demand from ISIS users. This has been successful and, thanks to my work, the group can now offer this service to support beamtime applications in the future.

In addition to gaining lab skills that I wouldn't have got from a university project, I have really enjoyed the support from the rest of the team, giving me space to try out my own ideas, whilst also being there to answer questions when needed.

Alongside my work at ISIS, while I was here I also had to complete coursework and exams for my university course. This involved watching recorded lectures and completing online workshops once I got home from work in the lab.

Whilst based at ISIS, I lived with other sandwich students, and took part in public engagement activities both at ISIS and back at the University of Southampton. This is in addition to joining one of the many Harwell rounders teams!

#### Future

Just as my year with ISIS was coming to an end, a position became available in the group for maternity cover. I was keen to stay on and, having developed the key skills and experience needed, I got the job and I am joining the group full time.

My focus will now be on supporting the ISIS users, as the deuteration lab work towards the synthesis of their 500th compound for the user programme! I will also be supporting the new summer and work experience students about to join the group.



# International Collaborations

## ISIS and Japan

ISIS has had very long-standing collaborations with Japan for neutron science and, in particular, for the RIKEN-RAL Muon Facility based at ISIS. The muon science collaboration is now over 30 years old, and continues to see an active Japanese user programme on the ISIS muon instruments, governed by the fourth in a long line of agreements between ISIS and RIKEN.

*It is a great honour for me to visit this Laboratory. Thank you very much for your hospitality. I hope that the collaboration between the UK and Japan will be enhanced further.*

*Akira Aohet*  
Shuichi Akamatsu  
Minister for Economy  
Embassy of Japan the UK  
27 February 2019.



Mr Shuichi Akamatsu, Minister for economic affairs at the Embassy of Japan in London, signing the ISIS visitor book with Dr Philip King (ISIS)



## ISIS and Italy

One of ISIS' longest collaborations, since 1984, is with the Consiglio Nazionale delle Ricerche (CNR) in Italy. The agreement was renewed in 2014 for 6 years. This partnership has included development of many ISIS instruments including Prisma, Tosca, Vesuvio, INES (which is operated by CNR), Sandals, and, most recently, Nimrod, IMAT and ChiPr on TS2. The collaboration also now includes working with CNR to deliver in-kind contributions to ESS instruments.

Francesco Cugini and Simone Chicco (University of Parma, Italy) studying the magnetic properties of Heuser alloys on Wish.



## Celebrating 30 years of collaboration with Sweden

ISIS has benefitted from a collaboration with Sweden lasting over 30 years. The first agreement with the Swedish Research Council (VR) was signed in 1988. Recent agreements include contributions to Polaris and IMAT instruments coordinated through Chalmers Technical University. In 2014 the partnership was significantly expanded to assist Sweden in developing its user community in preparation for future ESS operation through a combination of facility access and joint projects. The result is a big increase in proposals to use ISIS from Swedish researchers – a four-fold increase over the past few years.

On 5 September 2018 ISIS Neutron and Muon Source welcomed a group from Sweden's Council for Research Infrastructures to mark the 30-year anniversary of ISIS-Sweden agreements. Prof Björn Halleröd, VR Secretary General, and Prof Jan-Eric Sundgren (Chair, Council for Research Infrastructures) unveiled a plaque on IMAT to mark the event.



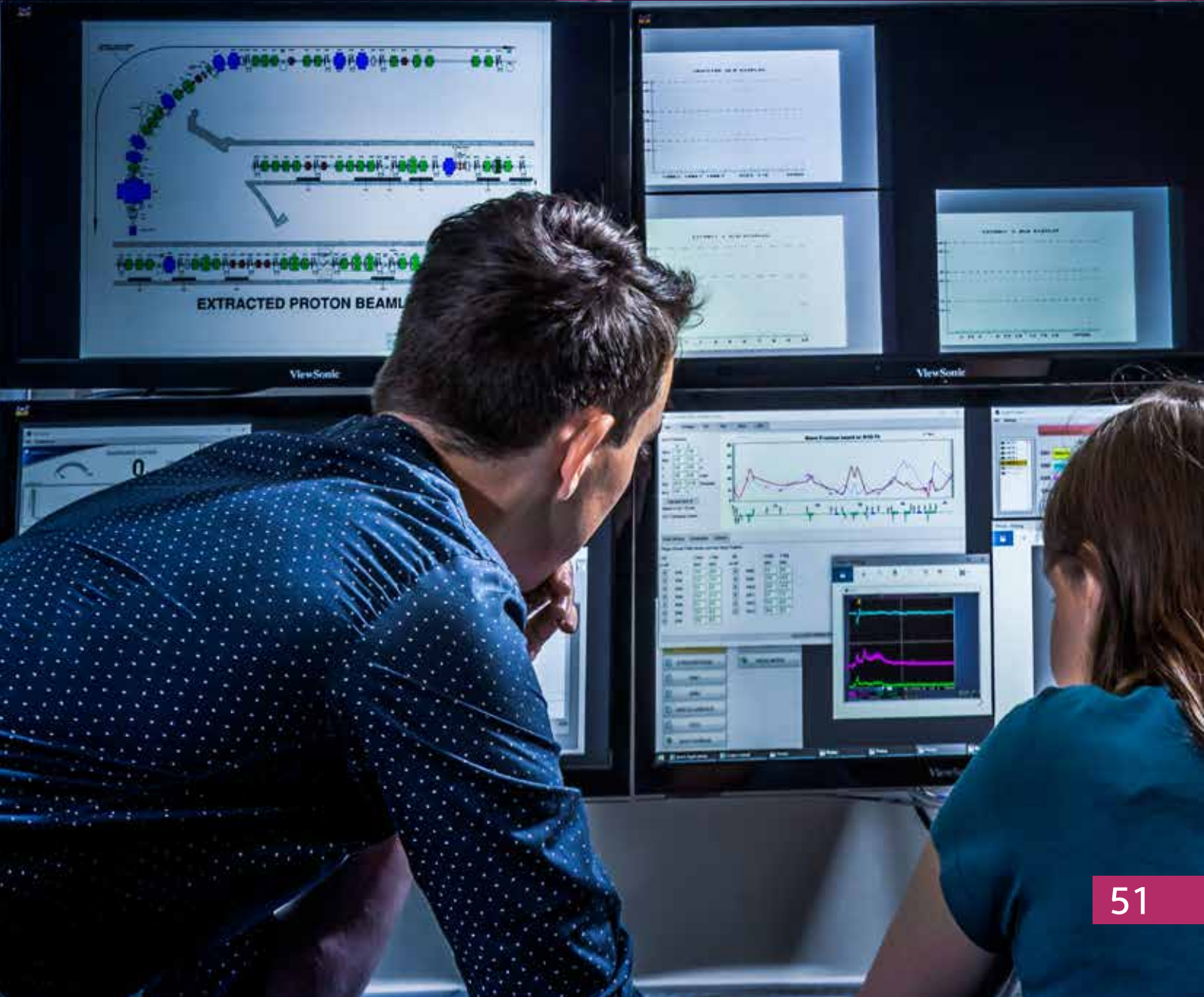
## ISIS and India

In 2016 ISIS signed a new agreement with the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), through the NanoMission of the Department of Science and Technology, for collaboration between UK and Indian scientists in neutron scattering and muon spectroscopy. This includes contributions to the Zoom instrument on the ISIS Second Target Station.

Amitava Bhattachayya (Vivekaranda University, India) loading a sample onto MuSR for muon studies of an unconventional superconductor.



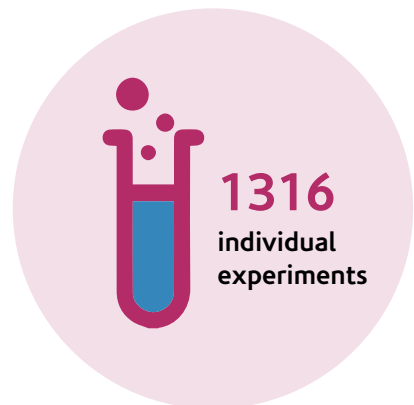
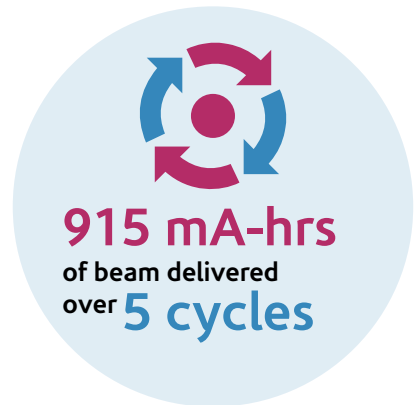
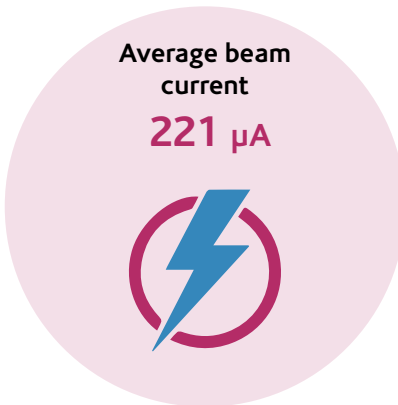
# Technology





# Technology

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



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

Table 1.1: Performance in 2018 Cycle by Cycle

Cycle	2018-1A	2018-1	2018-2	2018-3	2018-4
	17 Apr-18 May	5 Jun-13 Jul	11 Sep-26 Oct	13 Nov-18 Dec	5 Feb-29 Mar
Beam on time (h)	643	791	951	689	1078
Availability (%)	90	92	90.8	85	89.9
Total Beam (mAh)	141	180	207	150	237
Mean current when beam on Synchrotron (uA)	219	228	219	218	219
TS1 (uA)	179	188	178	176	180
TS2 (uA)	40	40	41	41	39

# Major Projects

## Preparing for the long shutdown

ISIS will have an extended shutdown during 2021 for significant refurbishment work on the first target station and installation of a new linear accelerator tank, in order to extend the life of the facility for many years to come.

### TS1 project

The Target Station 1 (TS1) Project will enable the continued operation of TS1 for many years into the future – the target station has run for over 30 years without significant maintenance or development work. The project will see new designs of the target and its cooling systems, the moderators, the reflector and all their associated services. This includes the target station instrumentation and controls; the trolley that the target, moderator and reflectors sit on; and the large area of plant which deals with the TS1 services, which sits behind the target station.

#### Target

This year has seen many milestones for the project, including the first time the new target was assembled. Its modular design with ten individual plates of tantalum-clad tungsten took over a year to design and another year to build.

#### Water Circuits

The design of the new water circuits was completed in July 2018 based on four modules (skids) that can be individually assembled to form the basis of the new services trolley. The water plant and equipment was delivered over the following months, along with the skid bases. During 2019 the skid structures were assembled and water plant was mounted ready for the pipework build.

#### Pre moderators

The pre moderators are currently in manufacturing. The first prototypes are almost ready and, once tested, will be ready for assembly. Both the methane and hydrogen pre moderators are made using the specialist technique of Electron Beam Welding to ensure a minimal distortion of the assembly. This ensures a good fit of the pre moderators inside the reflector due to the tight tolerances of the assembly.

#### Reflector Assembly

The next TS1 project milestone will be the delivery of the reflector assembly. The £3.4M reflector is being manufactured from solid beryllium blocks similar to the one used on TS2. It has been developed to improve neutronic performance and to access to the moderators. It is being manufactured by Leading Metal Mechanic Solutions in their specialist beryllium manufacturing facility based just outside Santander in northern Spain.



Dan Blanco Lopez working on the pre-moderators on the ISIS Target Station One Target upgrade project.



## Linac Tank 4

Linac tank 4 is due to be replaced in the 2021 long shutdown of ISIS. While the present tank has served us well for over 30 years, it does not have the enhancements and serviceability which have been designed into the replacement. Should an unpredictable but likely failure occur, it would prove extremely challenging from both a mechanical and radiological perspective to deal with. Looking ahead, the new and spotlessly clean vessel will consume less RF power, present fewer beam losses and remove significant risk to future operation.

All six sections of the new tank have been assembled in our Linac Test Area, and accurately aligned on mounting rails. Vacuum pressure tests have demonstrated good section to section seals. Drift tubes, post couplers, tuning mechanisms and cooling parts will be attached next, before RF tuning and setup can be performed. Lastly, conditioning of the tank with a high power amplifier will be carried out ahead of its planned move on to ISIS next year.



Members of the ISIS Mechanical, RF, Design and Vacuum sections have all been working hard to get the replacement tank ready.

## Muon Ionization and Cooling Experiment (MICE)

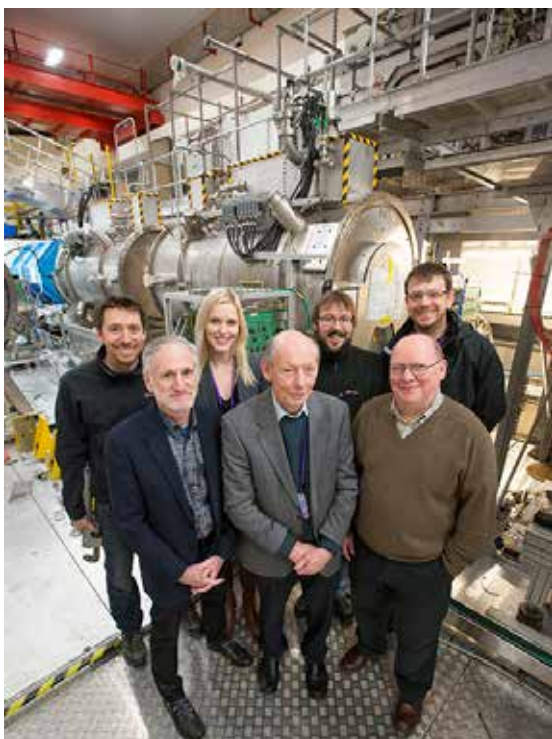
The MICE demonstration experiment has been run at ISIS over recent years. The collaboration, which is composed of scientists and engineers from the UK, Europe, Asia and the USA, has analysed data to demonstrate muon ionization cooling, a key technology in the design of a particle accelerator that can accelerate muons.

In ionization cooling, a muon beam is passed through liquid hydrogen or lithium hydride while being focussed extremely tightly by the large magnetic field produced by a super-conducting solenoid. This process, referred to as 'cooling', reduces the transverse size of the beam, which allows the beam to be accelerated to high energy. The muons in the beam oscillate about the beam centre and the amplitude of the oscillations determines the size of the beam. Muons with a small oscillation amplitude are said to be 'cold'.

Ionization cooling was the main technical hurdle in constructing a muon accelerator. Using the MICE muon beam on ISIS, the collaboration has measured the amplitude of the muon oscillations before and after a cooling system using state-of-the-art detector systems. The data analysis, led by Chris Rogers from ISIS, shows that the number of cold muons is increased by their passage through the cooling system. This is the first time that the ionization-cooling of muons has been observed.

As it has now been shown that ionization cooling works, muon colliders could be the successor to the Large Hadron Collider. The results have impact beyond the high-energy physics community as well, as accelerator physicists have proposed using ionization cooling in 'internal target' systems for nuclear waste transmutation, medical radioisotope production and cancer treatment.

The result was a real cross-campus success, with contributions from across STFC including ISIS, ASTeC, PPD, CCD and Technology. The expertise from staff based at both Rutherford and Daresbury was crucial to the successful delivery of the MICE programme.



The MICE tracker group, following successful installation of the MICE diagnostic trackers.



MICE employed a 12-coil superconducting solenoid assembly combining large apertures with strong magnetic fields to contain and focus the highly divergent muons.

## European Spallation Source (ESS)

As part of the UK's contribution to the ESS, which is currently under construction in Sweden, ISIS staff are engaged in delivering two instruments: Loki and Freia. Furthermore, staff are supporting colleagues in Italy (CNR) to deliver the Vespa spectrometer.

Loki is a versatile small angle neutron scattering instrument and will be amongst the few tranche of instruments operational at ESS. Many areas of the detailed design are complete and major component orders have been placed. Interestingly, to deliver the ESS instruments we are prebuilding sections of the beamlines at ISIS to ensure efficient construction in Sweden and to test some of the operational demands placed by the nature of the ESS.

Freia is a liquid reflectometer for the ESS. Freia has moved from its concept phase into detailed design. ESS instruments offer interesting technical challenges and

we have recently made significant progress on verifying the feasibility of several critical components required to implement the Freia concept.

Working with our colleagues from the CNR, Italy this year has seen significant progress in the conceptual design of the Vespa spectrometer and has also resulted in the first tender being placed.

ISIS hosts the Programme Management Office for the whole of the UK's £165m contribution to ESS. Our three staff are working to ensure that the UK gets the most possible value from this investment. This includes carrying out the projects above and others within STFC, and others at UKAEA and Huddersfield University. ISIS staff are also playing an important advisory role sitting on various ESS committees and hosting "show and tell" visits from ESS staff.



Engineering representation of the Loki instrument.

# Instrument Updates

## RIKEN-RAL refurbishment

The RIKEN-RAL muon beamlines were constructed by the Japanese RIKEN institute, but ownership and operation have now passed to ISIS under a new 5-year agreement signed with RIKEN last year. As part of this agreement, the beamlines are being refurbished to enable them to continue to operate for many years to come – including replacement of beamline cabling, water circuits, power supplies, and vacuum and control systems, as well as refurbishment of detects and sample environment equipment. Detailed planning for this work has been ongoing this year, with the major part due to take place during the 2021 long shutdown.

## Polarised neutrons on LET

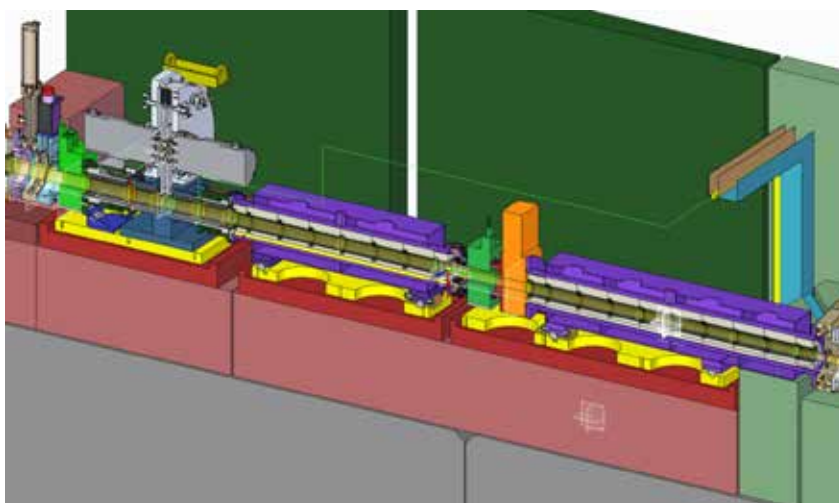
The new polarised neutrons option on LET was commissioned in the summer of 2018, with the first external user group conducting an experiment in March 2019. The uniaxial polarisation option allows the coherent and incoherent part of the neutron scattering cross section to be separated, with particular application for the study of diffusion in a range of hydrogenous materials. With further improvements to the helium-3 polarisation analyser in the pipeline, the system may also soon be used for separating magnetic and non-magnetic scattering in a range of magnetic materials.

## SANDALS Interim Upgrade Project

A major upgrade of the SANDALS instrument is currently in progress. This project will modernise the primary flight line of the instrument to allow SANDALS to take better advantage of the enhanced performance of Target Station 1 following its refurbishment. There are three primary components to this project:

- (i) The installation of a double disk chopper to reduce the long-wavelength frame-overlap neutron background in the instrument detector array.
- (ii) An upgrade of the primary flight line collimation, converting this from circular to square cross-section to improve neutron flux delivery to the sample point.
- (iii) The installation of a modern set of motorized beam defining apertures that will allow improved control of the size and position of the beam footprint incident on the sample.

Collectively these developments should significantly enhance the performance of the instrument for measuring the small isotopic-difference scattering signals that underpin its science programme.



Engineering model of the SANDALS incident flight line showing the beamline components that will be installed or upgraded as part of its upgrade project: Double disk frame overlap chopper (Grey), incident-beam collimation units (Purple) and motorized beam-defining apertures (Green). The neutron beam from the Target Station travels from left to right.



## Completion of the MARI detector upgrade

The second phase of the upgrade of the MARI instrument, the installation of new detector electronics, was completed in March 2019. This followed the installation of a neutron guide and new choppers in 2017. The guide increased the flux on MARI by an order of magnitude in its low energy mode of operation, opening up new opportunities to study smaller samples or weaker signals in ever finer detail. The new detector electronics replace equipment that was nearly 30 years old, and will be much more reliable and easy to maintain. The occasion of the MARI upgrade being completed was marked in April by an opening ceremony at which Andrew Taylor (former ISIS Director, Executive Director of STFC National Labs, and former MARI instrument scientist!) cut the ribbon on the new instrument.

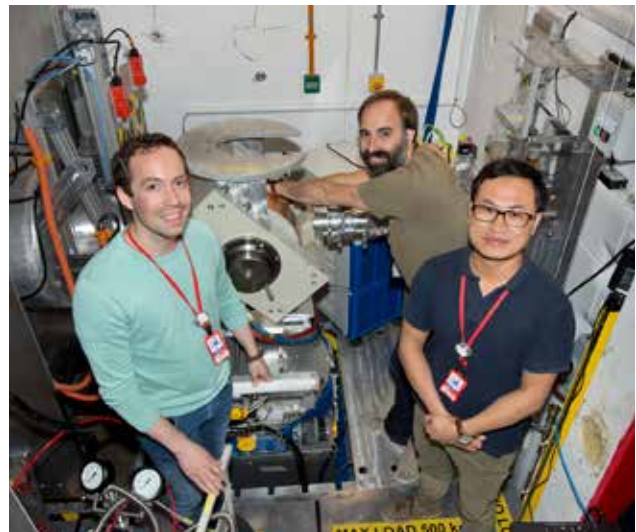


Dr Andrew Taylor performs the ribbon cutting at the MARI instrument upgrade celebration.

## First users on Zoom

ZOOM is a new small-angle neutron scattering (SANS) instrument on TS2. SANS allows users to probe structural details on the nanometre scale, allowing a variety of systems from biology and chemistry through to magnetic and engineering systems to be structurally characterised. The new Zoom SANS instrument will complement the existing SANS2d beamline and will offer polarised neutron beams, which will allow us to extend our structural understanding of magnetic systems. Future upgrade projects also include neutron beam focussing, allowing us to probe much longer length scales, including food science systems and virus particles.

Saturday 2 March saw the first users on the Zoom beamline. The group of materials scientists, from Imperial College London, used SANS to investigate the nanoscale properties of their thermoexpansive gels. The first group to use the capability for polarised neutron beams visited in June, investigating magnetic thin-film silicon.



ISIS users left to right; Philipp Bender, University of Luxembourg, Diego Albavener, ISIS, and Tai Nguyen, Luxembourg Institute of Science and Technology, loading a sample on the ZOOM instrument for experiment RB1910376.

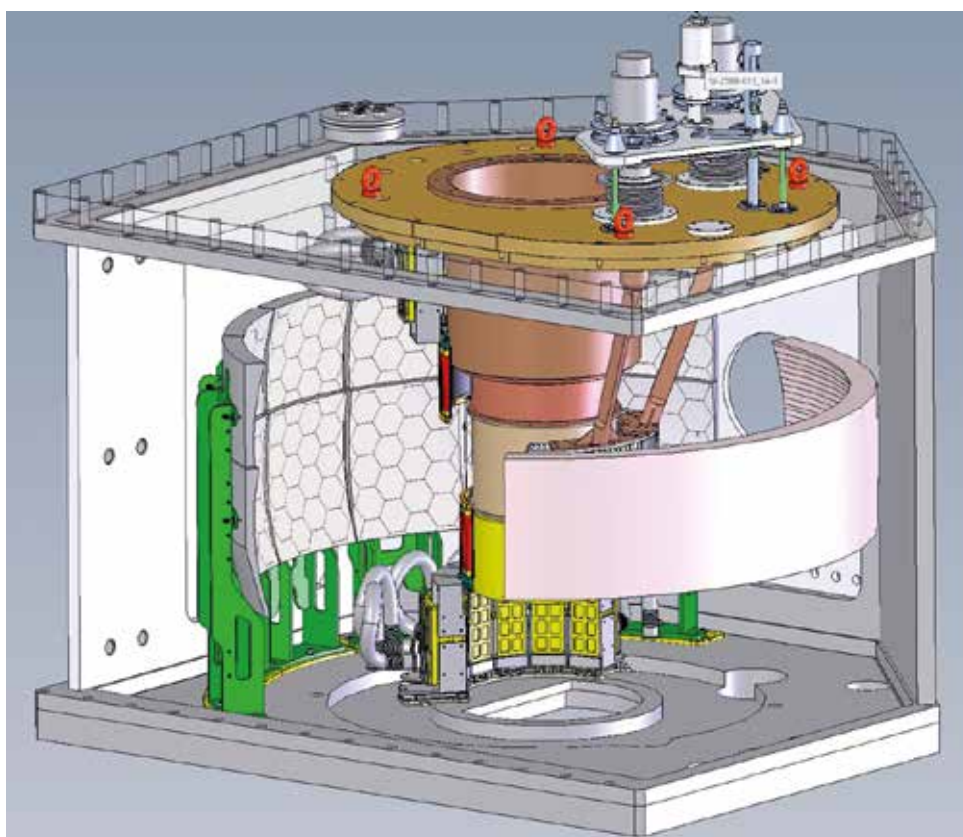
## HRPD

A recent refurbishment to HRPD has seen the addition of a new user cabin outside the current brick building, with a high-level doorway cut through to a new extended mezzanine platform. The motivation for doing this was to replace ageing and failing electronic components, which had been subjected to decades of humidity, dust and substantial temperature variations. Replacing the electronics meant providing them with an air-conditioned room, and this, in turn, necessitated moving users out into a new space. Users will benefit from a clean, quiet and comfortable space to work in. Once the lift is installed, it also makes HRPD completely accessible with step-free access from parking outside to the cabin and to the instrument for users with different levels of mobility.



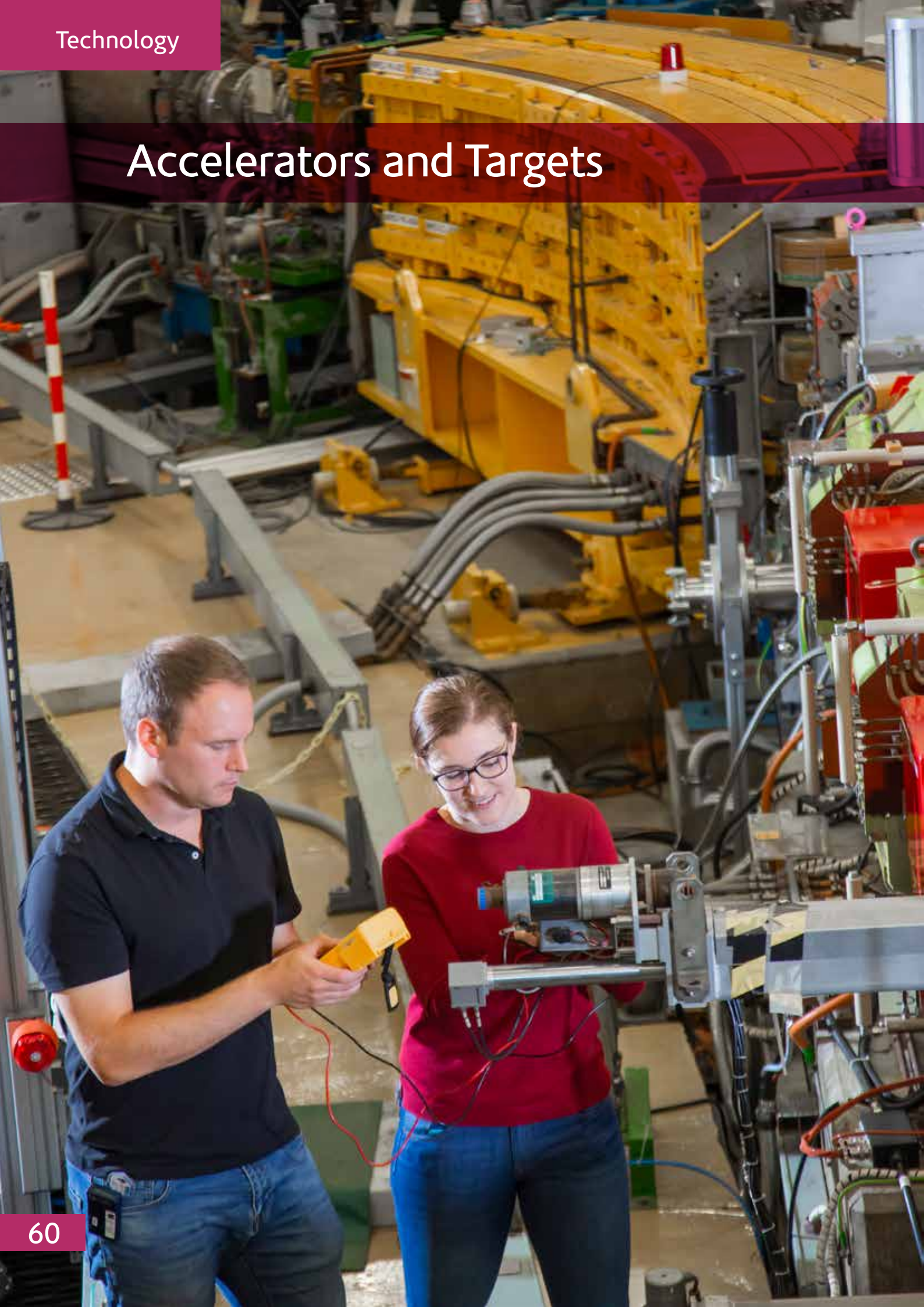
## OSIRIS Si analyser project

The indirect time-of-flight backscattering spectrometer OSIRIS is currently being upgraded with the addition of a silicon analyser, positioned on the vacant side inside the vacuum tank of the secondary spectrometer. The new analyser bank will increase the dynamic range towards three orders of magnitude and provide a further dimension in momentum transfer detection with the help of position-sensitive detectors. The silicon analyser can be operated simultaneously with the existing pyrolytic graphite analyser bench.





# Accelerators and Targets



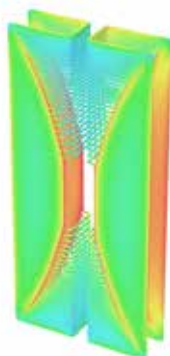


## Accelerators and Targets

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.

### Development of a vFFA Accelerator Design for ISIS-II

Shinji Machida and the Intense Beams Group have been hard at work developing a vertical Fixed Field Alternating Gradient accelerator (vFFA) for potential use as the main accelerator on ISIS-II. The vFFA combines the DC and variable pulse benefits of a cyclotron with the smaller magnets and beam pipe of a synchrotron to achieve the required proton energies for spallation. A prototype accelerator is being designed to prove the concept and would fit on the end of the FETS (Front End Test Stand) project. If built (tentatively scheduled for between 2022-24), it would be the first accelerator of its kind in the world.

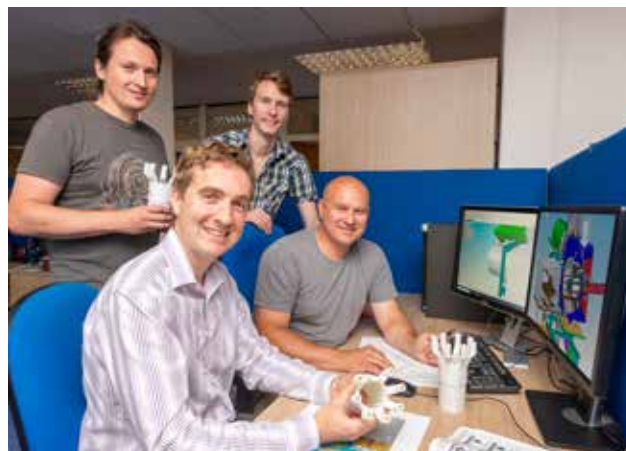


Finite Element Analysis modelling of the complex magnetic coil design needed to realise a vFFA accelerator.

### Upgraded Ion Source Design

The ISIS accelerator chain begins with a negative hydrogen ion source. The present design of ion source has been in use for over 35 years, but its short lifetime of two or three weeks affects the time it takes the facility to come online. A new type of ion source is being developed, which will survive several months without maintenance. A critical challenge for the new ion source is thermal management. ISIS engineers and physicists Jon Speed, Scott Lawrie, Dan Zacek and Olli Tarvainen have been working on detailed CAD models and 3D-printed prototypes to ensure the cooling system is suitable. The ion source will begin

commissioning on an off-line test stand in 2020, with an aim to install on ISIS a couple of years later.



Technical staff from the ion source project: Jon Speed, Scott Lawrie, Dan Zacek and Olli Tarvainen (left to right).

### Fast Feedback Damping System Tests

A method of countering the major head-tail beam instability in the ISIS synchrotron is under development, showing promising results in testing throughout the year. By repurposing the Q-kicker, a device normally used to excite the beam and allow measurement of its properties, staff from the ISIS diagnostics section have built a prototype fast-feedback system, working with colleagues from SNS and CERN. The system uses a beam position monitor to measure the offset of the beam from its ideal position during each orbit of the synchrotron. Each measurement is used to calculate the electrical field required to push the beam back towards its ideal position, which is then generated by the Q-kicker and applied to the beam within roughly  $1\mu\text{s}$ . In this way, instabilities are prevented from growing over multiple orbits of the synchrotron ring. Tests at 50Hz operation are being planned and, if successful, will reduce beam loss levels and allow higher beam intensities to be reached as a result.



Alex Pertica (left) and David Posthuma de Boer (right) testing the feedback system.



## Beam Delivery Record Broken

On 19 June 2019, ISIS delivered a record-breaking 5.64 mAh of beam to its target stations. This equates to an average beam current of 245  $\mu\text{A}$  at 50Hz, with 99.4% availability. Average beam intensity has steadily increased by around 10% over the last 3 years, while at the same time average beam loss levels in the synchrotron have been halved. This progress is the result of various upgrades to accelerator hardware, including the new trim quadrupole filtering system (see below) and scintillating beam loss monitors within each dipole, which have given accelerator physicists improved beam diagnostic and control capabilities.



Machine operators Ben Pine, Peter Griffin-Hicks and Bryan Jones (left-right) studying beam data in the MCR.

## High Power Trim Quadrupole Filters


The Magnet Power Supplies Group have designed new high power filters, which have been installed on the outputs of the trim quadrupole and steering magnet power supplies. These filters remove specific frequency content from the power supply outputs that can interfere with the beam, which oscillates at similar frequencies midway through its acceleration cycle. As a result, the synchrotron can be set up and operated at higher intensities, while also reducing beam loss levels.



Magnet power supplies group staff Jaysen Tydeman, Michael Julian and Noel McNamee, installing a trim quad filter unit.

## Our people



 Tristan Canfer

### ISIS Diagnostics Technician

After finishing his apprenticeship with STFC, based at ISIS, Tristan has recently joined the beam diagnostics team as a technician.

#### Background

I studied A-level electronics, although was always more into arts and crafts than engineering. I knew I wanted to be an engineer and looked into apprenticeships. Most were in the manufacturing industry, but the placements at RAL give the opportunity for lots of variety.

My advice for potential apprentices is to do lots of research: there are loads of apprenticeships out there but there is no central place to find them, so keep looking. Once you start, every scheme is what you make of it: ask questions, branch out and make your own path.

It's a bit daunting at first but everyone has been so welcoming; I've never felt looked down on as an apprentice.

#### Projects

During the three years that I was based at RAL as an apprentice, I worked across eight different groups, including going to CERN for seven weeks to work on a project with some fellow apprentices. It's hard to pick a favourite project, but any project where I use skills that are really fiddly and take time and practice to develop make me most proud, and give me most satisfaction. I really like going into the inner synchrotron. It's a concrete vault of electronics with so much heritage: it's great being part of something so huge.

#### Future

I've recently started a job as a diagnostics technician, which is an extension of the work I began as an apprentice. I will be developing, testing and repairing electronic systems that keep track of the beam. Our busiest times are when it's quiet for everyone else and the beam is off.

After doing the apprenticeship placements, all I knew was that I wanted to work at ISIS. I felt inspired by the sheer scale of the machine and the effort that keeps it running. The combination of the work I'm doing and its variety, the people I'm working with and the environment here means my only worry is that I'll never work anywhere else!

#### LGBT in STEM network

While I was at CERN for my placement, I discovered their LGBT network and that gave me the inspiration to start one at RAL. We recently celebrated LGBT STEM day for the second year in a row, and the next step will be to build connections between us and other organisations, to see how we can improve life on campus.

Whilst running the network takes up some of my time, I've had lots of support from my managers and HR, and it gives me that extra nugget of purpose. My goal is to be a good colleague and friend, not just a great engineer.

On Thursdays, I can be spotted dancing with the RAL-based Lepton Morris side – we perform in lab coats, with yellow and black hazard hankies!

# 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



**31**  
on Graduate  
training  
programme



**23**  
vacation  
students



**work experience  
placements**



**Apprentice  
placements**



**23**  
undergraduate  
sandwich  
students



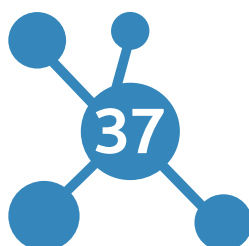
**825 PhD students**  
used our instruments  
gaining valuable skills  
and knowledge of  
neutron and muon  
techniques



**42**  
co-sponsored  
PhD students



**3604 total visitors,**  
including 2088  
school students,  
teachers and  
members of  
the public



**scientific  
seminars**



**at meetings,  
conferences and  
workshops**



# Inspiring the next generation



## Inspiring the next generation

2018/19 has been another successful year for public engagement at ISIS, with the facility welcoming over 2000 school students, teachers and members of the public for talks, workshops and tours of the experimental halls. We have also doubled our reach at off-site events, with an estimated 5000 members of the public engaging with ISIS science and engineering during festivals and fairs, and local school and community visits.

ISIS opens its doors to the general public and schools for several large events every year, seeing hundreds of visitors pouring into the facility to experience the scale of our science and engineering, meet our staff and hear our stories, and explore the cutting edge research that goes on, from superconductors and soaps to beetle wings and polar bear fur.

Our school events continue to be very popular, with tours of ISIS reported to be a highlight of visits to RAL. School activities including RAL Education Access Days, the Particle Physics Masterclass, Chemistry@Work, Atomic Afternoons, Science in your Future and Science in the Park have inspired hundreds of pupils from across the country with ISIS science and engineering.

From Chemistry@Work, the percentage of students interested in chemistry went up from 60% before to 80% after the event; 90% said that they had learnt new things and 75% said that as a result of the event, they would now consider a career in science in the future.

Over the summer of 2018, ISIS staff hosted 62 work experience students.

*"My work experience at ISIS was incredible and the supervisors were all incredibly friendly. This was such a fantastic opportunity that I would recommend to anyone wanting to learn more about scientists. It was an amazing opportunity and I have definitely learnt much more about what their daily routine consists of."*

**Sofia Lambert, Work Experience Student in the Impact Team**

*"This has been an amazing experience for me, and it has made me actively excited to pursue a career in STEM. Thank you to everyone here"*

**Jack Dixon, Work Experience Student in ISIS Design Division**

Our public events have spanned a wide range of activities and themes, to reach and inspire new audiences. With our on-site public access days, Stargazing at RAL, and the RAL and Harwell Campus summer festivals combined with our off-site events such as the Family Science Day in Didcot, Wantage Museum STEM day, Oxford Science and Ideas Festival, and Cowley Road Carnival, we have been able to reach new and diverse audiences. This year has also seen ISIS at large international public events including New Scientist Live in London and the American Association for the Advancement of Science Exhibition in Washington.

*"I found the work experience incredibly fun, useful and engaging, and I was able to make some new friends from other departments along the way. I loved the camaraderie of the experience, as there were others our age that we could chat to."*

**Ukendar Kumar Vadivel, Work Experience Student in ISIS Design Division**

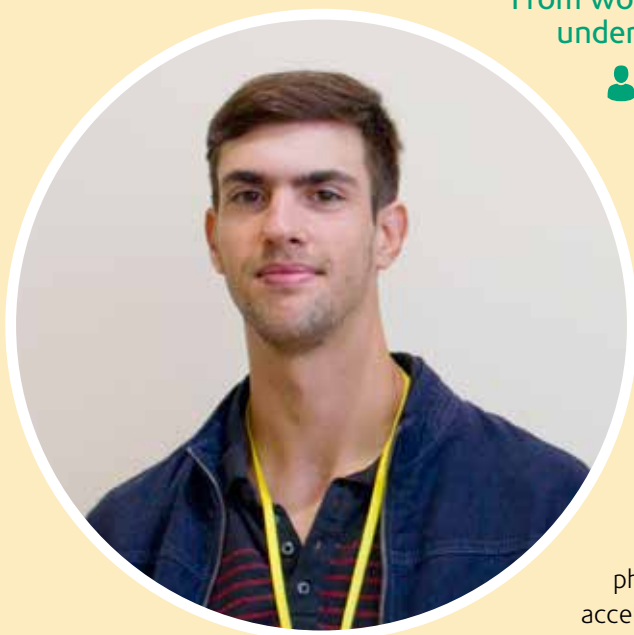
## 2018 – The Year of Engineering

2018 – The Year of Engineering – saw a step-up in our engineering-focused activities. Events including Exploring Engineering days, the ISIS Schools Accelerator Day, Apprentice Open Days and Engineering your Future have excited secondary school pupils about engineering at ISIS and STFC. For the second year running 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. Students were tasked with the ambitious project of designing a mechanism for a halo neutron beam monitor for the Loki instrument at the ESS.

**ENGINEERING**  
TAKE A CLOSER LOOK



## Developing our people



### From work experience placement to undergraduate degree

 Leo Rozanov

#### Undergraduate Physics student at the University of Chicago

While studying for his A-levels at Westminster school, Leo did a week of work experience at ISIS that confirmed his decision to study physics at university, and strengthened his applications for universities in the United States.

#### Background

I was interested in Physics at A-level, but had absolutely no idea what a physicist did, and had only heard of particle accelerators in science fiction. After my school visited the Diamond Light Source, and through a recommendation from a family friend, I discovered the RAL work experience scheme.

Before my placement, I was thinking about doing physics at university, but only because I wasn't sure what else to do. My placement allowed me to see the varied projects and real world applications of working in physics. Not everyone is making spaceships, but they are using physics to help researchers in other subjects from all over the world.

#### Projects

While I was at ISIS, I worked to develop a python script for a new experiment. Although the experiment was not up and running during my placement, I have been able to come back and visit the group this year to see it working. I wanted to come back to ISIS once again, to be part of the great working environment and to catch up with the team.

The application process for US universities is much more detailed than in the UK, and focusses a lot on your activities outside the curriculum. Writing about my work experience at ISIS, and how it influenced my journey towards studying physics, made my applications much stronger.

#### Future

I can't wait to start at the University of Chicago, and hope to play tennis for the university while I'm out there. As for beyond that – I don't believe a future in physics is ever really based in one country! The work I have seen at ISIS has shown me that physics is all about collaboration.



## Developing the student community

**The student community continues to lie at the heart of ISIS Neutron and Muon Source. More than 85 co-sponsored PhD students, vacation and sandwich students worked at the facility in 2018/2019. In addition, there were visits from over 800 PhD students to ISIS for experiments. The facility seeks to encourage and grow the student community through training courses, direct supervision and on the job training.**

### Students at Harwell

At any one time, ISIS hosts many co-supervised PhD students in addition to sandwich students, apprentices and graduates. While they are here, they all have the opportunity to join the growing community on the Harwell Campus. Many have joined sports teams and been on tours and training courses organised by the new Harwell Campus Nxt Gen group, which supports early career stage professionals on the campus. There is also a new student section on our external website, providing information for new starters and potential PhD and placement students.

### PhD student training and events

2018/19 saw a range of training events aimed at students, including the ISIS Neutron Training Course. These courses are always extremely popular and enable students to get a hands-on experience of work at the facility, gaining skills to help them when they come back as users and when they take the data back to their institution.

Each year ISIS organises two 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 other students who also spend significant time at large scale facilities. 2018/19 saw increased attendance at both events and excellent presentations showcasing the diverse research with the ISIS student community.

ISIS also supported some PhD students to attend the European Conference in Neutron Scattering (ECNS) conference in St Petersburg. Thanks to this funding, the students were able to present findings resulting from experiments at ISIS. Students wrote an ISIS 'Science Highlight' to accompany their presentation, which was published on the ISIS website during the conference.

## Facility Development Studentships

ISIS has an annual call for Facility Development and Utilisation Studentships. These are co-funded studentships, normally 50% funded by ISIS and 50% by a university, which contain an element of facility development - for example development of equipment, software or experimental processes. Studentships have an ISIS supervisor and a university supervisor who work in partnership throughout the student's project. Over recent years, ISIS has funded around 50 of these studentships across a wide range of topics and university partners.

### Visits to ISIS

In addition to beamtime allocation, many groups of students at both undergraduate and postgraduate level visit ISIS through the year.

"The students really enjoyed their visit and found that the visit in ISIS was definitely the highlight of the whole industrial tour week. Several of them are really interested in the fields of neutron and muon technologies so found it very helpful to be given an overview of the incredible work being carried out at the ISIS Neutron and Muon Source facilities. They were quite amazed by the huge experimental areas and facilities. Your talk gave an excellent insight into a series of diffractometer and spectroscopy, and other neutron and muon instruments, appreciating your valuable knowledge across a wide range of science areas and facilities. Thank you for making them feel so welcome and let them have such an amazing and valuable experience. I hope that we may be able to visit the ISIS again at some point in the future."

**Alison Martin, Centre for Doctoral Training in Ultra Precision Engineering, Centre for Industrial Photonics, University of Cambridge.**

### Sandwich student scheme

In 2018, ISIS hosted 23 undergraduate students for twelve-month placements as part of their degree. The students are a crucial resource to the facility, offering new ideas and perspectives. It also gives them an introduction to work outside of academia and to the range of careers available at ISIS and STFC more widely.

"It's reinvigorated my drive for my studies because I can now see where it will lead me one day. It's the clarity of purpose that comes with the experience of doing a placement year that is going to help me the most in my final year."

**Liam, 2018/19 Sandwich student**

# Events





## UK Neutron & Muon Science and User Meeting

Over 300 people attending; over 110 students at the student day; over 46 universities or institutions represented; 70 talks; 75 student posters – just a few of the facts and figures for the UK Neutron & Muon Science and User Meeting (NMSUM) that was held in Warwick in April 2019. NMSUM is organised jointly by ISIS and ILL, and provides an opportunity for UK scientists who use neutrons or muons to hear about the latest science results, instrument developments and other facility news. This year saw the highest number of attendees to-date, with the science day in particular being very appreciated.



Student day



All delegates



Student delegates



Presenter



### PARI III (April 2019)

The first workshop on Public Awareness of Research Infrastructures took place in 2015. This international conference brought together science communication and public engagement professionals and practitioners from across Europe. Given its success and very positive feedback from the participants, a second event took place in 2017 and was equally well received. In 2019, the ISIS Neutron and Muon Source hosted the conference at the Rutherford Appleton Laboratory, collaborating with colleagues from across the other STFC facilities including Diamond Light Source and the Central Laser Facility.

Over three days, the conference saw 87 paid attendees from 65 different companies/institutions in 14 different countries attend talks and workshops on topics including Equality and Diversity communications, and Building and Maintaining Trust.



PARI III delegates



Prof Anu Ojha OBE, Director of the UK National Space Centre, speaking on "The Secret Rulers of the World" at PARI 2019.



Dr Alfredo Carpineti, IFL Science, speaking on being LGBTQ+ in STEM.



Prof Sheila Rowan, Director, Institute of Gravitational Research at the University of Glasgow, gave the after dinner speech at the Williams F1 Centre.

### UK TEMM (July 2018)

July saw the 16th annual Theoretical and Experimental Magnetism Meeting (TEMM), organised by the indefatigable Adroja. As in previous years the meeting was supported by the IoP magnetism group and the theory of condensed matter group from Cambridge. Over three days scientists from all over the world gathered together at Cosener's house to hear about the latest developments in the field of magnetism, with a particular focus on bringing together experimentalists and theorists. The subject matter of talks ranged from the sounds made by moving monopoles in spin ice, to the latest developments in the search for a quantum spin liquid, to technical developments on ISIS instruments that will allow researchers to probe ever finer details of the structure and dynamics of magnetic materials.

### Crystallography User meeting at Milton Hill House (November 2018):

On 13-14 May, a meeting organised by ISIS, the Physical Crystallography Group of the British Crystallographic Association and the Crystallography Group at Diamond brought together UK, European and US researchers with a joint interest in performing neutron scattering experiments at extreme pressure and temperature conditions.

Technical talks were provided by instrument scientists from ISIS in the UK, SNS in the United States, ILL in France and ESS in Sweden (currently under construction), giving an overview of their

### PNCMI (July 2018)

ISIS hosted the Polarised Neutrons for Condensed Matter Investigations (PNCMI) conference in July 2018. This meeting allowed scientific and technical specialists in the field of polarised neutrons an opportunity to share knowledge and experience at a dedicated conference. As well as talks about the latest instrumentation at neutron sources around the world, talks were given on a wide range of scientific topics, including magnetic structures, frustrated magnetism, soft matter and biology. ISIS also hosted a specialist training school over two days before the meeting, at which early career researchers were given in-depth tutorials and hands-on experience of polarised neutron scattering methods.

current capabilities. A further ten science talks were provided by a cross-section of the user community and presented science from diverse areas such as the study of halogen bonding at extreme conditions, new phases of co-ordination frameworks, and formation of planetary ices. In addition, on the first evening, a lively poster session was held, where work presented by PhD students and postdocs was discussed.

It is expected that the meeting will open up new and exciting areas of research at high pressure using neutron scattering techniques and develop further international collaborations within the user community.



PNCMI delegates at Milton Hill House in July 2018



# Publications 2018

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