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ISIS Neutron and Muon Source Annual Review 2017

Science and Technology Facilities Council

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ISIS Neutron and Muon Source Annual Review 2017

The ISIS Neutron and Muon Source

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UK Astronomy Centre, Edinburgh; Chilbolton Observatory, Hampshire; Boulby Underground Science Facility
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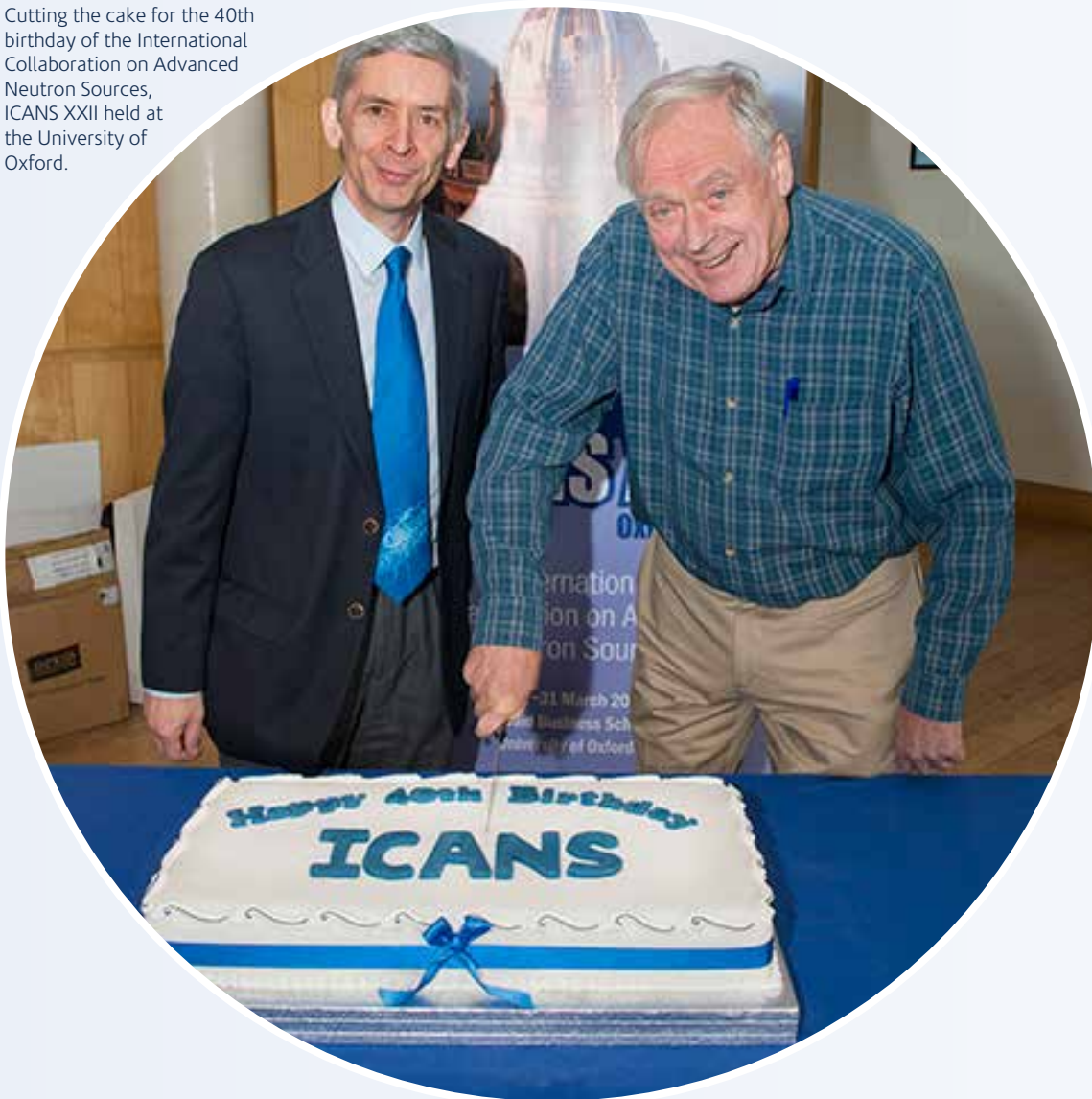


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Cutting the cake for the 40th birthday of the International Collaboration on Advanced Neutron Sources, ICANS XXII held at the University of Oxford.



Members of the Thai Embassy & SLRI Thailand visited ISIS in September 2017.

Dr Shigeo Koyasu, Executive Director of RIKEN visited the ISIS facility in November 2016.

Foreword

Welcome to the ISIS Neutron and Muon Source Review for 2017!

There have been two assessments published in the past year that send very positive messages both about the past and present performance of ISIS, but also about the future. The Strategic Review of Neutron and Muon Science and Facilities confirms that neutron and muon facilities will continue to be needed for at least ten years from a scientific perspective and that ISIS is the core of this provision for the UK research community. The Independent Review of National Large Facilities at Harwell examined the fundamental 'free at the point of access' model on which these facilities operate, and came to the conclusion that this is definitely the right model. Few people are aware that the model of user facilities, which is now common worldwide, was pioneered by Peter Egelstaff at Harwell in the 1960's. ILL was the first neutron user facility completely based on this paradigm, and Daresbury hosted the first synchrotron.

The strength of science at the UK large facilities is fundamentally based on our external user community. ISIS has many first class scientists on its staff, as our users are well aware, but it is not a research department. Our success is achieved through collaboration with our colleagues in universities, research institutions and industry. To drive both science and technology forward our staff need to be experts in their own right, but the relationship with external users is symbiotic – we succeed or fail together. While reviews always concentrate on the facility itself, they should in future also consider the skills base in the community, built up over 50 years of the user facility model. Just like the UK National Health Service, this model is something to be proud of. Long may both continue.

Robert McGreevy, ISIS Director



In January 2017 John Wix, 90, visited ISIS – back in the 1950s John led the design of a tank for the Nimrod accelerator, which was later installed in the ISIS linac and is still in use today!



Chris Lawson's liquid nitrogen show took place during the ISIS summer Open Day.



Dr James Lord, Dr Philip King, Dr Adrian Hillier, Professor Steve Cox and Dr Francies Pratt can be seen celebrating 30 years of muons.



Dr Manuel Heitor, Portuguese Minister of Science, Technology and Higher Education is pictured with his party and ISIS's Dr Philip King and Portuguese scientist Maria Paula Marques, University of Coimbra in the Target Station 2 foyer.

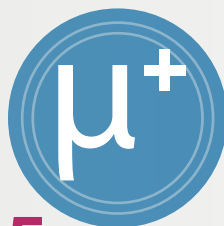
The ISIS Neutron and Muon Source

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.

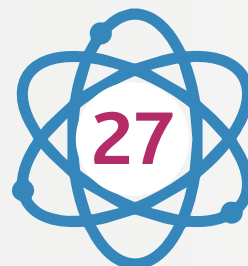
We are part of the global research structure, providing tools for over 2,000 scientists a year to use our suite of 32 instruments.

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

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



5 Muon instruments



Neutron instruments



including 1907 school pupils and public



607 PhD students visited as users



1156 proposals
received from
35 countries

2278 user visits



Companies

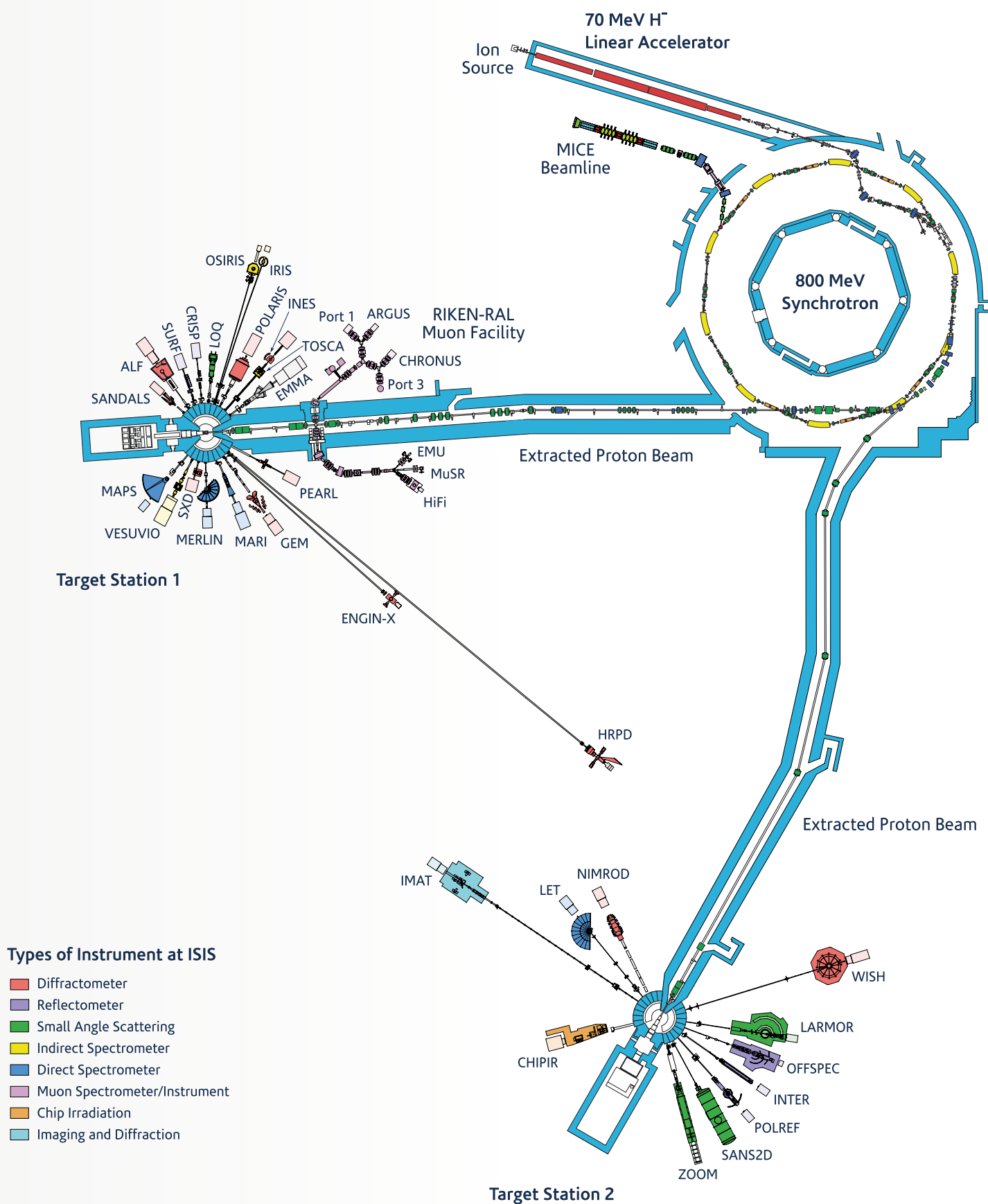
involved in experiments including healthcare, energy, automotive and chemical engineering



Journal publications



284 Xpress proposals

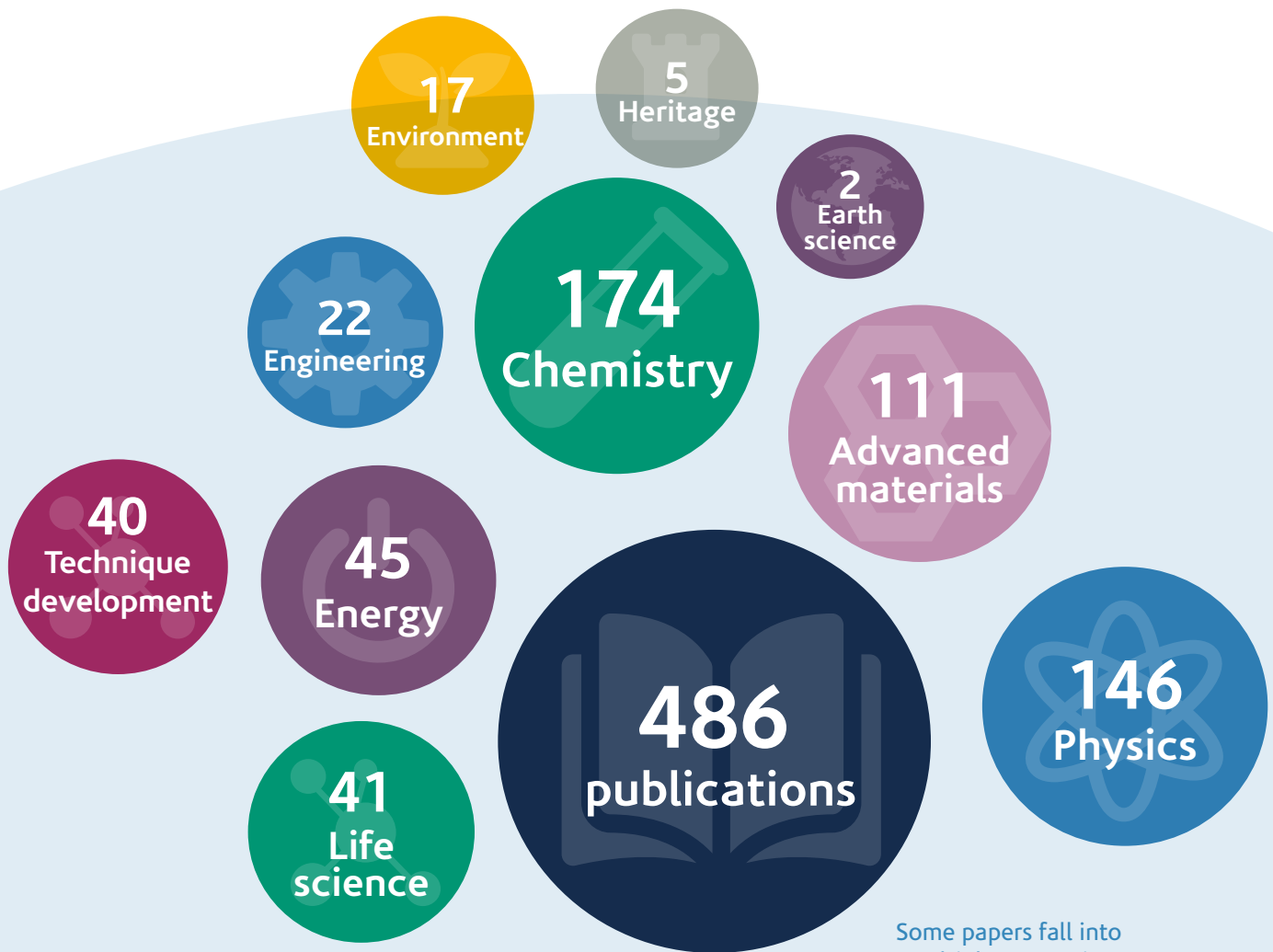


Science at ISIS

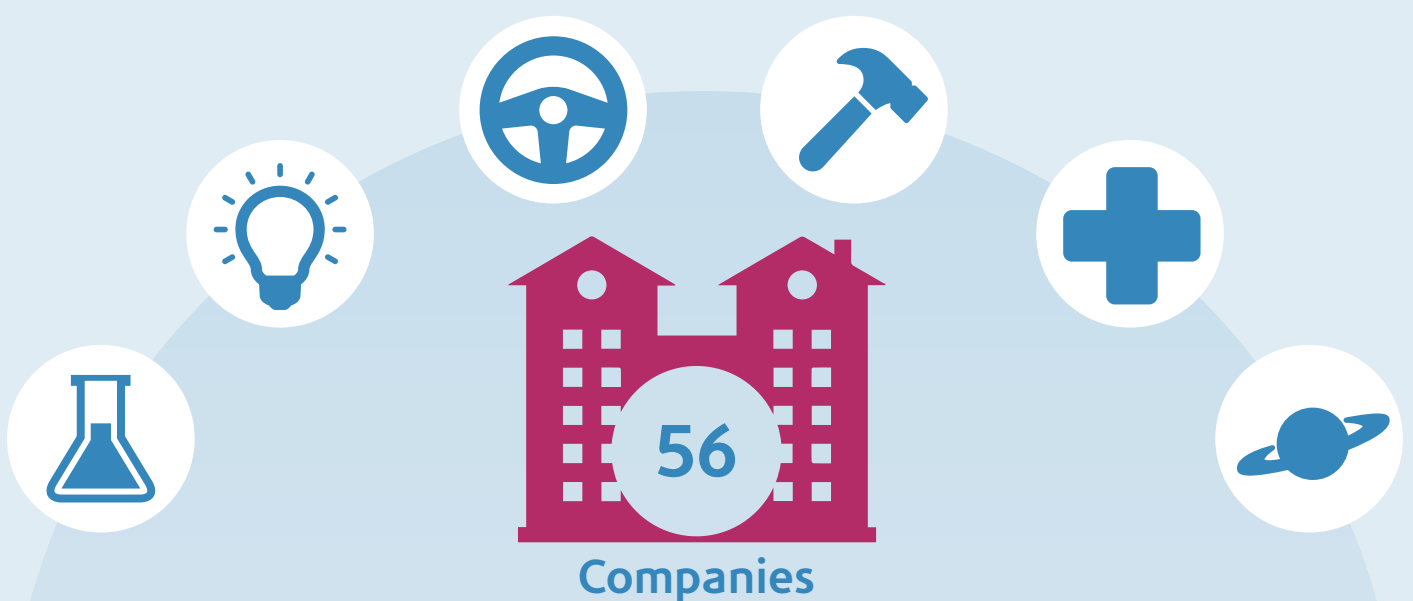


Science at ISIS

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 2,000 scientists every year from both academia and industry. This section gives a snapshot of ISIS research over the past year.



Some papers fall into multiple categories



used ISIS in 2016/7 including chemicals, healthcare, automotive, manufacturing, energy and aerospace.



Industrial Science

Industrial science

ISIS has long established industrial links with more than 100 companies, including household names such as Rolls Royce, Unilever and BP.

Companies can come in through three routes: partnerships with academia, direct payment, or the ISIS Collaborative R&D (ICRD) programme. 56 companies used ISIS through one of these routes in 2016.

Rolls Royce

Nickel based superalloys are a class of material designed for high-temperature applications, such as turbine blades for jet engines. During the manufacturing process single crystal turbine blades are subject to a series of heat treatments. Scientists at Rolls Royce identified a mechanism they believed led to the formation of surface defects in the blades, potentially limiting their performance and leading to costly reworking of the blades.

The Rolls Royce team used the Engin-X instrument through the ICRD scheme to study test samples produced in their precision casting facility and heat treated. They then subjected the samples to further *in situ* heat treatment on Engin-X using neutron diffraction to follow the phase transformation throughout this process. This enabled the team to conclusively prove this mechanism and allowed them to implement a new manufacturing process that prevented surface defects from occurring.

See also, *Neutrons illuminate stress/strain in high-temperature superalloys* on p30.

“The experiments on Engin-X provided the evidence we needed to support an existing patent. We’ve now been able to use this patent in the foundry, and also read the technique across to other turbine components, leading to significant cost savings.”

Neil D’Souza, Rolls Royce.

Infineum - Using neutron scattering to address complex additive challenges

Understanding the mechanism by which detergent particles are formed is crucial for their improved development and design. Infineum, a world-class formulator, manufacturer and marketer of petroleum additives, has used small angle neutron scattering (SANS) at the ISIS Neutron and Muon Source to build a picture of detergent components and formulations to a level of detail that has not previously been possible. By studying additives at a scale much smaller than ever before, scientists at Infineum are hoping to gain a better understanding of the mechanisms between the components within formulations, with the aim of improving the efficiency of the manufacturing process for an extensive range of commercial applications.

Small-Angle Neutron Scattering (SANS) is a technique that allows scientists to explore materials at the nano-scale by probing structures at length scales from around 1 nanometre to more than 100 nanometres with a beam of neutrons. Scientists at Infineum UK Ltd have used cutting-edge neutron scattering technology the (SANS2D instrument) at ISIS to identify the key parts of the detergent synthesis process which affect the properties and performance of the final formulation and more imperatively, have revealed how these attributes can be influenced.

“The data obtained using SANS has improved our understanding of the mechanism by which detergent particles are formed, paving the way for future research into the valuable contribution that detergents make to petroleum additives, such as those used to control rust and prevent deposits forming on engine components.”

Pete Dowding, Infineum

Pharmacology and Biology

Optimising the formulation of monoclonal antibodies

Related publication: C. Smith et al. "Antibody adsorption on the surface of water studied by neutron reflection" *MAbs*. 9 (2017): 466-475.

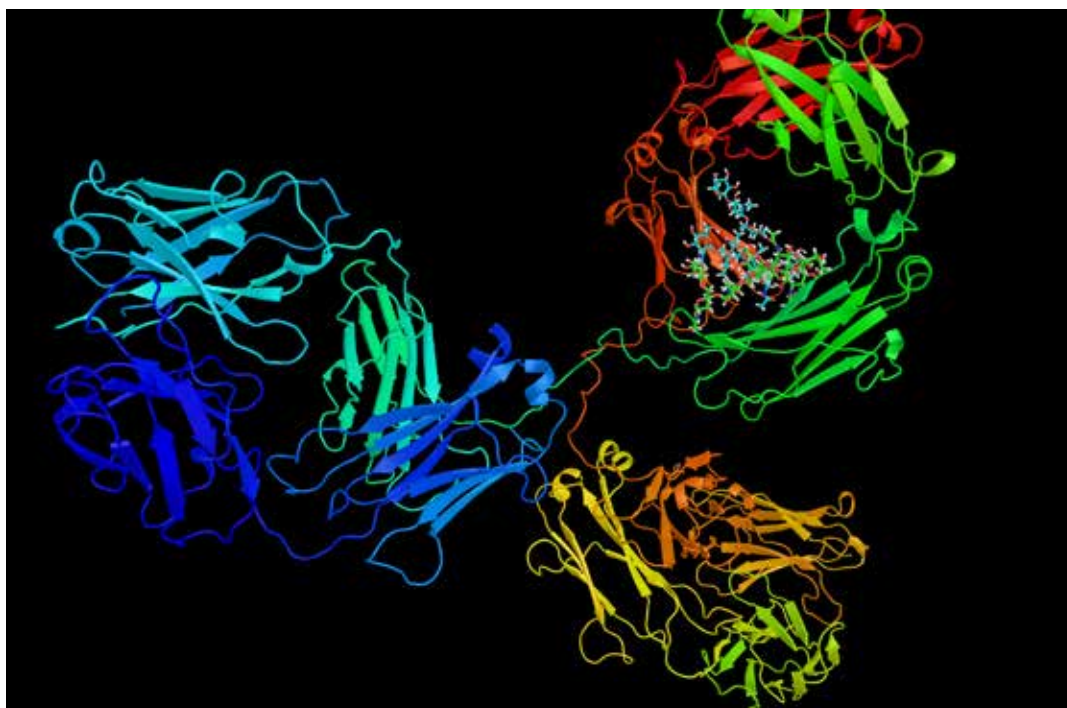
DOI: 10.1080/19420862.2016.1276141

Instrument: SURF

Funding: EPSRC

 Jian Lu (University of Manchester).

Monoclonal antibodies (mAbs) are an increasingly important class of medical drugs. High concentration liquid formulations are needed in order to give a clinically-effective dose in a low volume subcutaneous injection. During the optimization of these formulations it is necessary to limit the formation of aggregates and particulates. These can arise via a number of processes, including surface adsorption-desorption effects, and characterizing the precise molecular nature of adsorbed mAbs at an interface requires state-of-the-art analytical techniques and data interpretation. In a recent paper, researchers demonstrate the power of neutron reflection to unravel the amount and structural conformation of the adsorbed antibody layers at the air/water interface with and without surfactant.



Monoclonal antibody © ibreakstock | Dreamstime.com

Intracellular water: a new target for breast cancer drugs

Related publication: 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

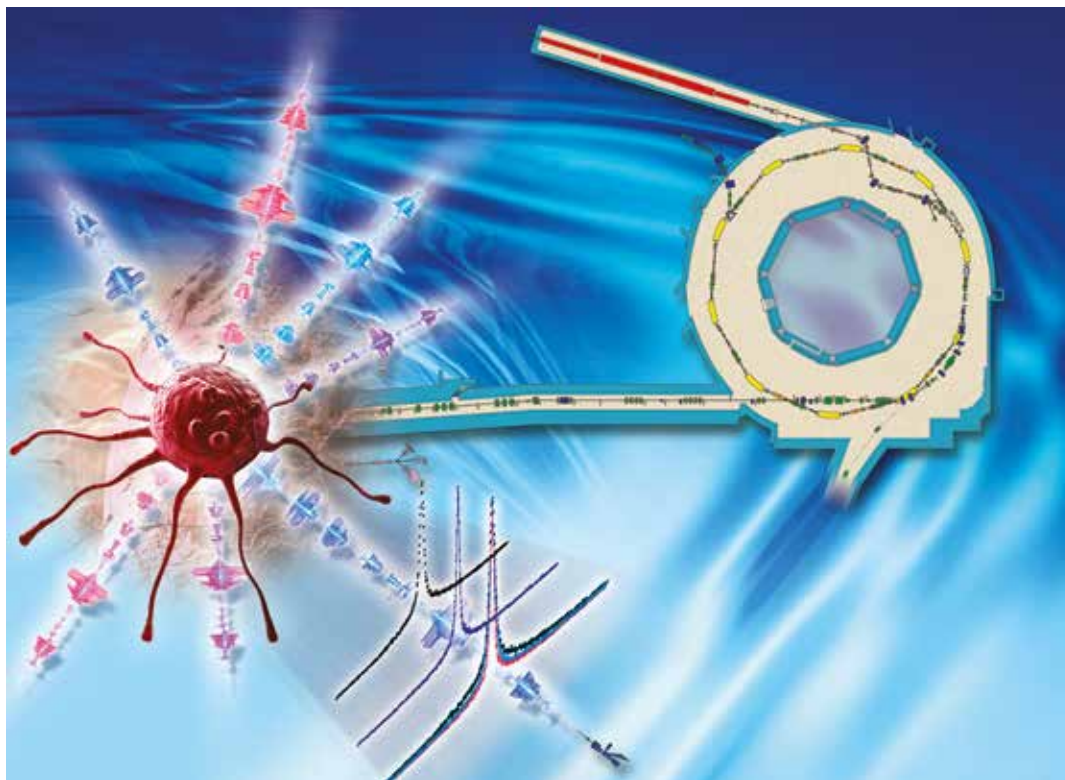
Instrument: OSIRIS and TOSCA

Funding: Portuguese Foundation for Science and Technology, EC Framework 7

 Maria Paula Marques (University of Coimbra) and Victoria Garcia Sakai (ISIS Neutron and Muon Source).

Breast cancer is the third most common cause of cancer death in the UK. Chemotherapy is one treatment, and cisplatin – a platinum-based drug in clinical use since the 1970s – stops cancer cells from multiplying by damaging their DNA. However, cisplatin has very limited success for this particular type of cancer, as it can affect healthy cells (like other chemotherapy drugs) leading to severe side effects, and is often associated with acquired resistance.

The development of targeted anticancer drugs aims to improve efficiency and reduce resistance mechanisms and deleterious side effects. Despite 80% of a cell's mass being water and this intracellular water playing a vital role in the cell's mechanisms, it has been overlooked as a potential drug target. Collaborative research efforts between the University of Coimbra and ISIS, using a combination of neutron vibrational spectroscopy on TOSCA and quasi-elastic neutron scattering on OSIRIS, have demonstrated that intracellular water may be a viable secondary target for anticancer agents, particularly towards low prognosis triple negative breast cancer. Their work paves the way for new drugs that are more efficient, lead to fewer cases of acquired resistance and have less damaging side effects for patients.



*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.*

Natural World

Meridianiite and planetary modelling

Related publication: D. Fortes et al. "Isothermal equation of state and high-pressure phase transitions of synthetic meridianiite ($\text{MgSO}_4 \cdot 11\text{D}_2\text{O}$) determined by neutron powder diffraction and quasielastic neutron spectroscopy", *Acta Cryst. B* 73 (2017): 33-46.

DOI: 10.1107/S2052520616018254

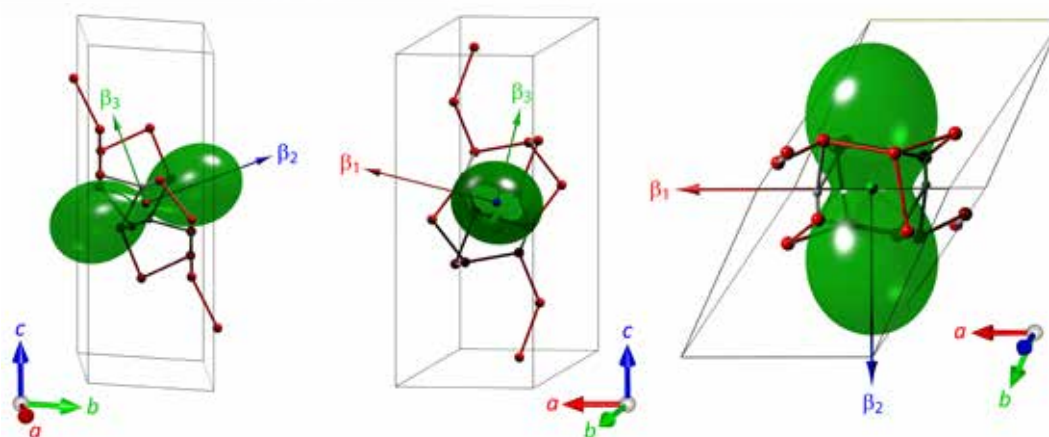
Additional reference D. Fortes et al. "Structure, thermal expansion and incompressibility of $\text{MgSO}_4 \cdot 9\text{H}_2\text{O}$, its relationship to meridianiite ($\text{MgSO}_4 \cdot 11\text{H}_2\text{O}$) and possible natural occurrences" *Acta Cryst. B* 73(2017), 47-64 (DOI:10.1107/S2052520616018266)

Instrument: PEARL/HiPr and OSIRIS

Funding: ADF acknowledges an Advanced Fellowship from the UK Science and Technology Facilities Council (STFC), grant number PP/E006515/1 and STFC standard grant number ST/K000934/1.

 Dominic Fortes (ISIS Neutron and Muon Source).

Meridianiite is a naturally-occurring mineral, found in a variety of cold very salty environments on Earth and very likely on Mars as well. It is also believed to be a major rock-forming mineral in some of the solar system's icy satellites (e.g. Ganymede). Researchers have carried out the first high-pressure experimental study of synthetic meridianiite on PEARL/HiPr and OSIRIS, using medium- and high-resolution neutron powder diffraction, to determine its elastic properties and phase behaviour as a function of pressure, knowledge that is fundamental to accurate planetary modelling. The work reveals in detail how the hydrogen-bonded structure compresses (as can be seen in the figure) and also the pressure-induced decomposition of meridianiite to a new hydrate containing nine water molecules per formula unit. This result has important implications for the distribution of salts and ices inside icy planetary bodies.



*Image reproduced from A. D. Fortes et al. "Isothermal equation of state and high-pressure phase transitions of synthetic meridianiite ($\text{MgSO}_4 \cdot 11\text{D}_2\text{O}$) determined by neutron powder diffraction and quasielastic neutron spectroscopy", *Acta Cryst. B* 73 (2017): 33-46. DOI: 10.1107/S2052520616018254*

Energy

Detection of lithium diffusion using muon spin relaxation

Related publication: I. Umegaki, et. al. "Li-ion diffusion in Li intercalated graphite C_6Li and $C_{12}Li$ probed by μ^+SR " *Phys. Chem. Chem. Phys.*, 19 (2017), 19058-19066

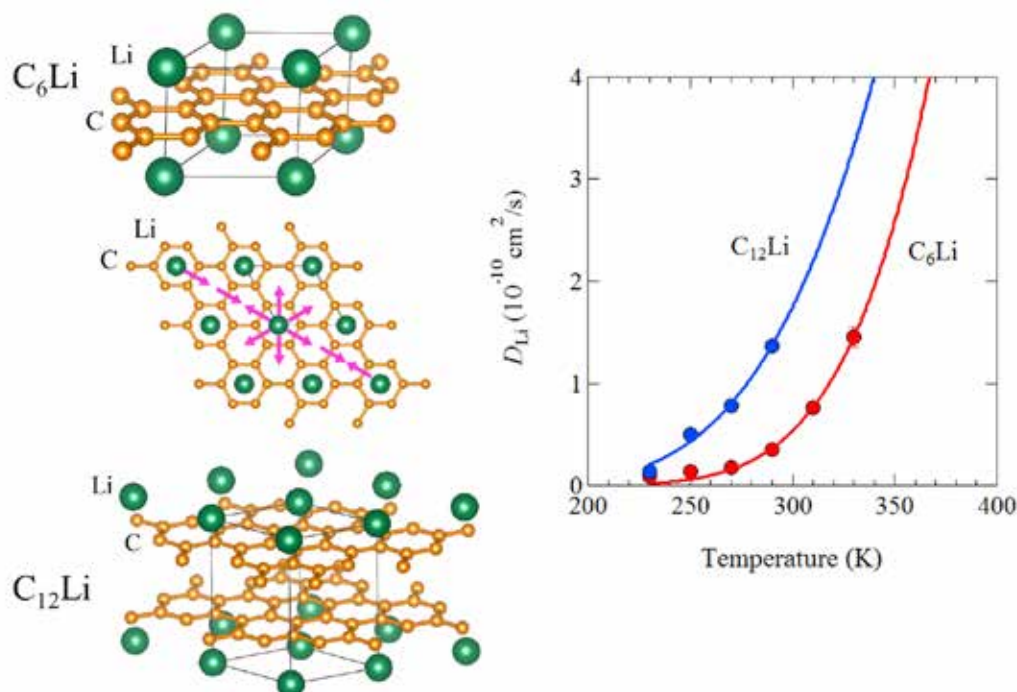
DOI: 10.1039/C7CP02047C

Instrument: EMU

Funding: Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan, and Japan Society for the Promotion Science (JSPS)

 Izumi Umegaki (Toyota Central Research & Development Laboratories Inc), Mark Telling (ISIS Neutron and Muon Source) and Stephen Cottrell (ISIS Neutron and Muon Source).

Many of the Li-ion batteries that power our mobile phones, tablets and other electronic devices use graphite as an anode, due to its high rechargeable capacity, low voltage, high cycle performance, and relatively low cost. During charging and discharging, Li^+ ions are intercalated into (or deintercalated from) the graphite. Li diffusion in solids is one of the main parameters determining the charge and discharge rate, and a study published in *Physical Chemistry Chemical Physics* used muon spin relaxation spectra to investigate diffusive behaviour of Li^+ in lithium intercalated graphites. The detection of Li diffusion using muon spin relaxation is an important precursor to in operando studies of Li diffusion in Li-ion batteries, allowing observations of the diffusive behaviour both in the cathode and anode as a function of the state of charge (SOC).



I. Umegaki, S. Kawauchi, H. Sawada, H. Nozaki, Y. Higuchi, K. Miwa, Y. Kondo, M. Månsson, M. Telling, F. C. Coomer, S. P. Cottrell, T. Sasaki, T. Kobayashi and J. Sugiyama, *Phys. Chem. Chem. Phys.*, 2017, 19, 19058 DOI: 10.1039/C7CP02047C
Published by the PCCP Owner Societies.

Doping: a better approach to producing thermoelectric materials?

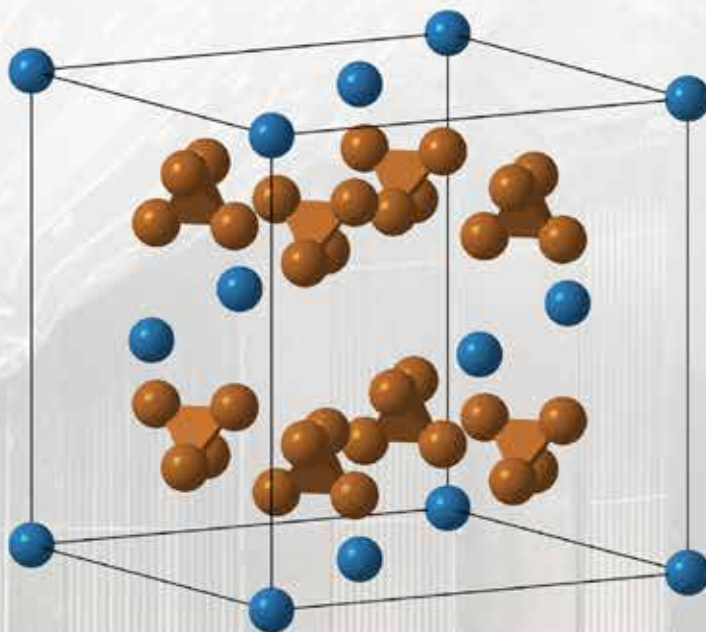
Related publication: D. J. Voneshen, et. al. "Hopping Time Scales and the Phonon-Liquid Electron-Crystal Picture in Thermoelectric Copper Selenide" *Phys. Rev. Lett.* 118 (2017) 145901-145905

DOI: 10.1103/PhysRevLett.118.145901

Instruments: LET and Merlin

 David Voneshen (ISIS Neutron and Muon Source)

With energy efficiency a hot topic, there is considerable interest in making use of the thermoelectric effect to turn waste heat into electricity. Thermoelectric devices could be used in many places, including power stations, cars and computers, and their lack of moving parts means they would be ideal for generating power in spacecraft. To develop better thermoelectric materials, we need to increase our understanding of their structure and properties, and recent research on LET and MERLIN used neutron spectroscopy to investigate Cu_2Se , one of the best thermoelectric materials at present. The experiments disproved the Phonon-Liquid Electron-Crystal (PLEC) approach to producing thermoelectric materials, and suggest that these materials can be improved further through doping.



*Reprinted figure with permission from D. J. Voneshen, H. C. Walker, K. Refson, and J. P. Goff *Phys. Rev. Lett.* 118, 145901 (2017) DOI: 10.1103/PhysRevLett.118.145901. Copyright 2017 by the American Physical Society.*

Investigating the effect of counterions on selective catalytic reduction

Related publication: A. J. O'Malley et al. "Ammonia mobility in chabazite: insight into the diffusion component of the NH_3 -SCR process" *Phys. Chem. Chem. Phys.*, 18 (2016), 17159-17168

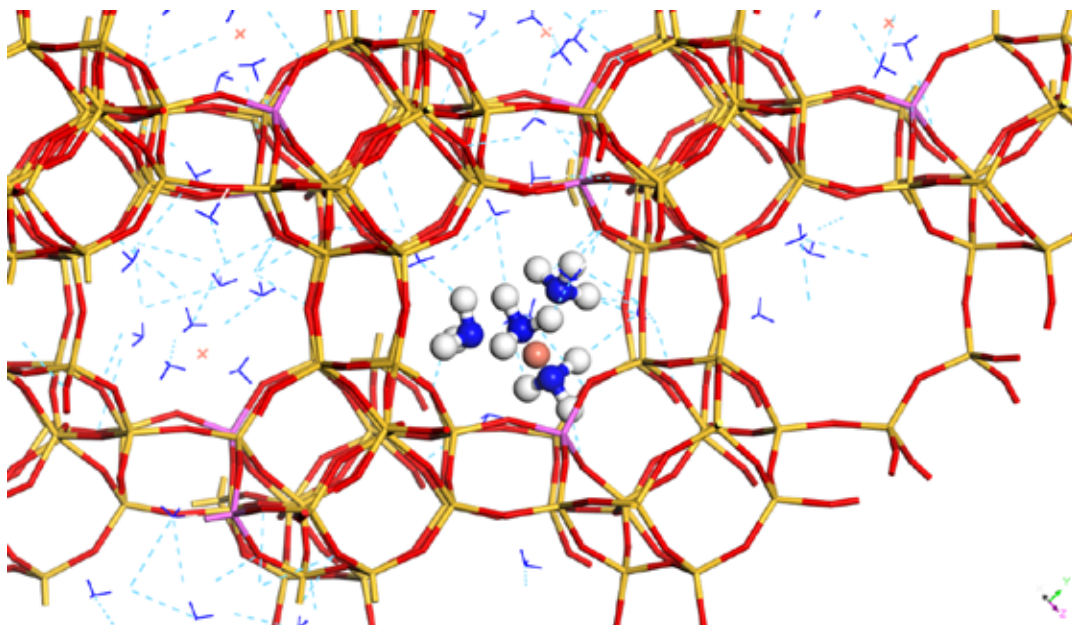
DOI: 10.1039/C6CP01160H

Instrument: OSIRIS

Funding: Engineering and Physical Sciences Research Council (EPSRC): grant no. EP/G036675/1, EP/K014706/1, EP/K014668/1, EP/K014854/1 EP/K014714/1 and EP/M013219/1)

 Alexander O'Malley (University College London and UK Catalysis Hub) and Paul Collier (Johnson Matthey Technology Centre).

Air pollution from road vehicles has damaging health and environmental effects. The Selective Catalytic Reduction (SCR) reaction can convert harmful NO_x gases to nitrogen gas and water, and often uses ammonia with metal exchanged zeolite catalysts. Researchers measured the diffusion of ammonia across a commercial copper-chabazite (Cu-CHA) zeolite catalyst, and compared it with measurements in H-CHA. They used quasielastic neutron scattering (QENS) on OSIRIS to look at the effect of counterion presence. Their results, published in *Physical Chemistry Chemical Physics*, showed similar rates and activation energies of diffusion for both systems, suggesting that the presence of counterions has little impact on the diffusion of ammonia. Molecular dynamics simulations showed that strong coordination of NH_3 with Cu^{2+} counterions in the centre of the chabazite cage shielded other molecules from interaction with the ion, allowing diffusion through the windows of the chabazite structure to continue freely.



Reproduced from A. J. O'Malley et al. "Ammonia mobility in chabazite: insight into the diffusion component of the NH_3 -SCR process" *Phys. Chem. Chem. Phys.*, 18 (2016), 17159-17168 DOI: 10.1039/C6CP01160H with permission of the PCCP Owner Societies.

Advanced Materials

The magnetic phases of thin-film erbium

Related publication: J. D. S. Witt et al. "Magnetic Phases of Sputter Deposited Thin-Film Erbium" Scientific Reports 6(2016) 39021

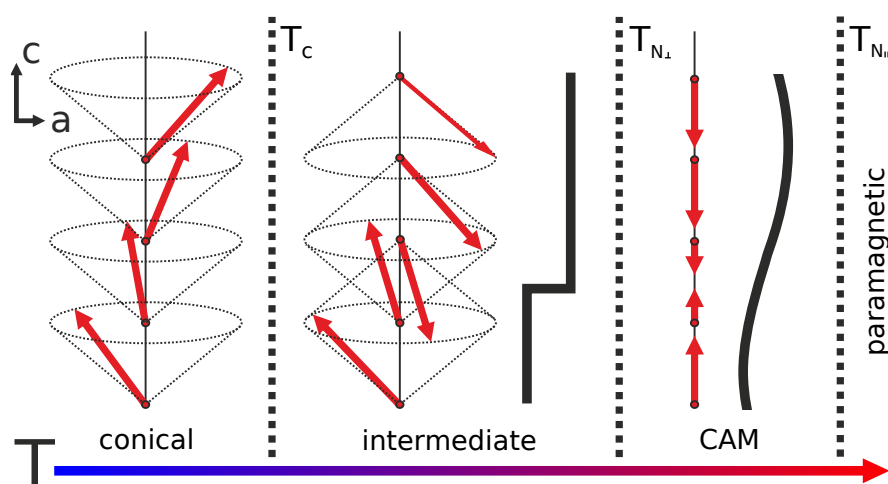
DOI: 10.1038/srep39021

Instrument: POLREF

Funding: EPSRC grant numbers: EP/J010634/1, EP/J010650/1, EP/J010626/1R532. JEOL Europe and ISIS neutron and muon source for PhD funding.

 Gavin Burnell (University of Leeds).

Erbium is an interesting example of a magnetic system with a very rich magnetic phase diagram. Understanding the complex nature of erbium, and other rare earth metals and their alloys, has led to many breakthroughs in magnet technology. In a paper published in Scientific Reports, Witt et al., detail their investigations into sputter-deposited thin-film erbium, which included neutron diffraction using the POLREF reflectometer. An understanding of the magnetic and crystal structure of sputter-deposited erbium, and the ways in which different parameters (such as strain) can modify it, is necessary to understand its magnetic phases. This work will aid the realisation of applications requiring complex magnetic thin films, such as the lowering of current densities needed in switching spin-transfer-torque (STT) devices and the nascent fields of spin-triplet superconductivity and superconducting spintronics.



Schematic showing the magnetic structure as a function of temperature for bulk Er.

Credit: STFC/John Willoughby

A magnetoelectric design strategy

Related publication: K. Kimura et al. "Magnetodielectric detection of magnetic quadrupole order in $\text{Ba}(\text{TiO})\text{Cu}_4(\text{PO}_4)_4$ with Cu_4O_{12} square cupolas" *Nature Communications* 7 (2016) 13039

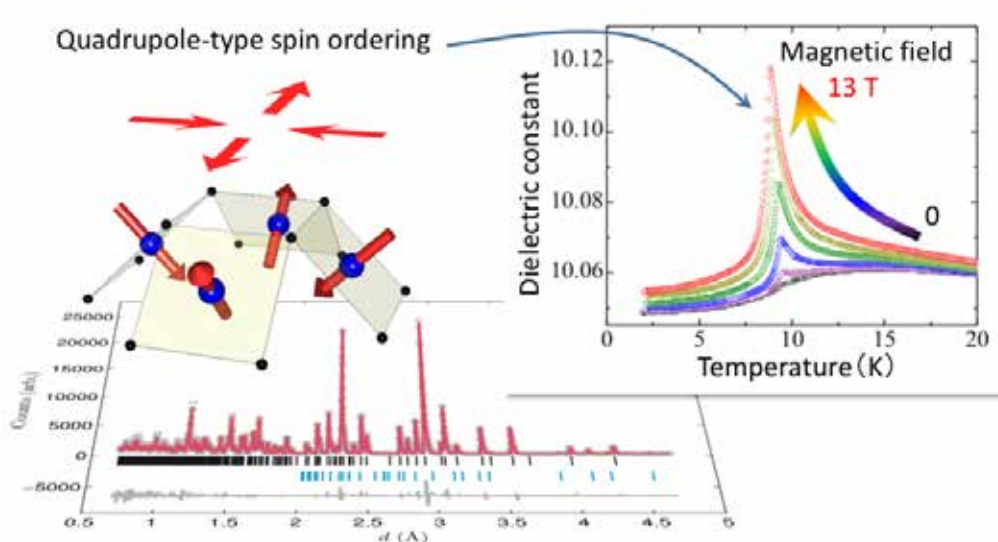
DOI: 10.1038/ncomms13039

Instrument: WISH

Funding: Partially supported by JSPS KAKENHI Grants 26610103, 16K05449, 26800186 and 24244058, by European Research Council grant CONQUEST, and by the Swiss National Science Foundation and its Sinergia network MPBH.

 Kenta Kimura (Osaka University)

The magnetoelectric (ME) effect is a coupling between the magnetic and electric properties of a material, so that magnetization is induced by an electric field, or electric polarization is induced by a magnetic field. Linear ME activity can arise in geometrically frustrated lattices, where multiple spins combine into emergent multipole moments that have broken space-inversion and time-reversal symmetries. Researchers proposed a magnetic square cupola cluster as a promising design to produce ME activity, then used neutron diffraction measurements on WISH to experimentally verify that it was present. Their findings, published in *Nature Communications*, are an important contribution to exploring new states of matter. Promising applications of ME include ME sensitive detection of magnetic fields and advanced logic devices.



Kimura, K. et al. Magnetodielectric detection of magnetic quadrupole order in $\text{Ba}(\text{TiO})\text{Cu}_4(\text{PO}_4)_4$ with Cu_4O_{12} square cupolas. *Nat. Commun.* 7, 13039 doi: 10.1038/ncomms13039 (2016)

A promising candidate for a quantum spin liquid

Related publication: Yuesheng Li et al. "Muon Spin Relaxation Evidence for the U(1) Quantum Spin-Liquid Ground State in the Triangular Antiferromagnet YbMgGaO_4 " *Phys. Rev. Lett.* 117 (2016) : 097201.

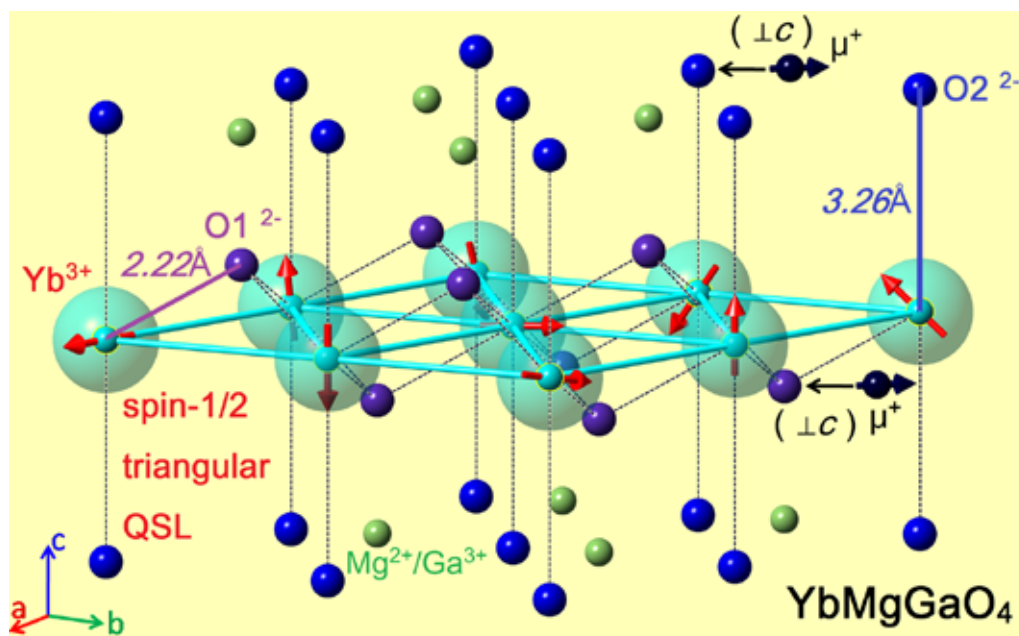
DOI: 10.1103/PhysRevLett.117.097201

Instrument: MuSR

Funding: This work was supported by the NSF of China and the Ministry of Science and Technology of China (973 Project No. 2016YFA0300504). Y. S. L. was supported by the start-up funds of Renmin University of China. The work in Augsburg was supported by German Federal Ministry for Education and Research through the Sofja Kovalevskaya Award of the Alexander von Humboldt Foundation. Q. M. Z. was supported by the Fundamental Research Funds for the Central Universities, and by the Research Funds of Renmin University of China.

 Yuesheng Li (Renmin University of China and University of Augsburg) and Qingming Zhang (Renmin University of China and Collaborative Innovation Center of Advanced Microstructures)

Ytterbium-magnesium-gallium-tetraoxide (YbMgGaO_4) is a newly discovered material and a promising candidate for a quantum spin liquid (QSL) - an exotic state of matter with magnet moments that exhibit unusual behaviour. QSLs have potential applications in high temperature superconductivity and quantum computing. Muon spin relaxation and rotation (μSR) is an ideal technique for experimentally probing the ground state, and can be performed in a true zero field. A paper in *Physical Review Letters* presents a comprehensive μSR investigation of the ground state spin dynamics of single crystals of YbMgGaO_4 , and provides compelling evidence for the formation of a gapless U(1) QSL ground state in this structurally perfect rare-earth triangular antiferromagnetic.



Reprinted figure with permission from Yuesheng Li, Devashibhai Adroja, Pabitra K. Biswas, Peter J. Baker, Qian Zhang, Juanjuan Liu, Alexander A. Tsirlin, Philipp Gegenwart, and Qingming Zhang, *Phys. Rev. Lett.* 117, 097201 (2016). Copyright 2016 by the American Physical Society. DOI: 10.1103/PhysRevLett.117.097201

Solitary magnons: a new discovery that could provide next generation data storage

Related publication: C.Stock et al. "Solitary Magnons in the S=5/2 Antiferromagnet CaFe_2O_4 " Phys. Rev. Lett. 117 (2016) 017201

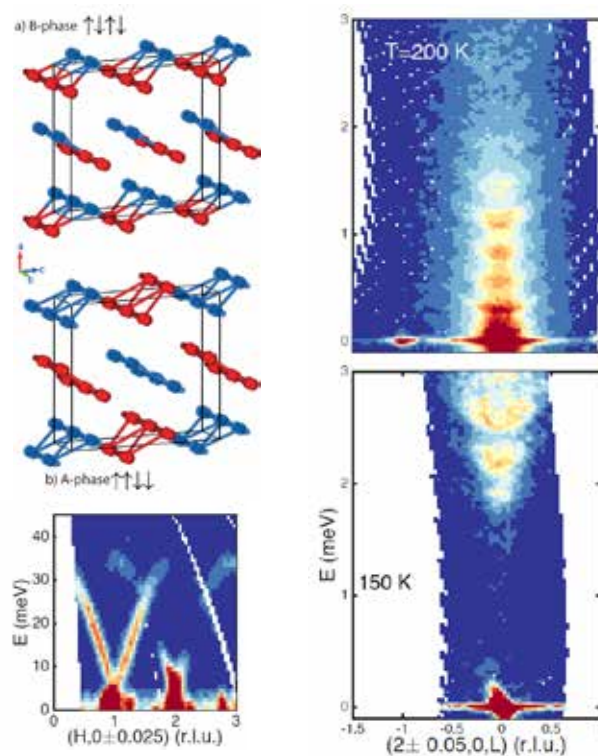
DOI: 10.1103/PhysRevLett.117.017201

Instrument: MAPS and OSIRIS

Funding: This work was supported by the EPSRC, Carnegie Trust for the Universities of Scotland, Royal Society of London, Royal Society of Edinburgh, STFC, EU-NMI3, NSF (No. DMR-1508249), and the Swiss spallation neutron source (SINQ) (Paul Scherrer Institute, Villigen, Switzerland). The work at Rutgers University was supported by the DOE under Grant No. DE-FG02-07ER46382.

 Russell Ewings (ISIS Neutron and Muon Source) Franz Demmel (ISIS Neutron and Muon Source)

Materials in which waves do not propagate, but are trapped in localised regions, give us the opportunity to study unusual quantum behaviour. One example is photonic crystals, in which light becomes trapped and can be used to enable processing of laser light on microchips. Researchers using a variety of neutron scattering techniques in different facilities, including MAPS and OSIRIS at ISIS, discovered behaviour in calcium ferrate that could lead to the use of magnetic materials in a similar way to photonic crystals. Their results, published in Physical Review Letters, showed two different ways of arranging the iron magnetic moments, with boundaries between these two phases just a few nanometres across. Inside these tiny regions, the team found localised waves of magnetic excitations, which they named "solitary magnons". Their discoveries could lead to new magnetic logic or data storage devices.



Left above: A & B phase arrangements of the iron magnetic moment in calcium ferrate. Left below: MAPS data that allowed the team to confirm the 2-dimensional magnetic structure and the strength of the magnetic interactions between the iron atoms. Right: OSIRIS data showing how the energy levels of the solitary magnons are affected by changes in temperature.

Finding the elusive Majorana fermion

Related publication: S.H. Do et al. "Majorana fermions in the Kitaev quantum spin system α -RuCl₃" Nature Physics (2017)

DOI:10.1038/nphys4264

Instrument: MERLIN and LET

 Sungdae Ji (Pohang University of Science and Technology)

The development of quantum computers is still in its early stages, but offers significant promise for national security purposes (e.g. cryptography). Majorana fermions are a promising choice for qubits (the quantum equivalent of computer bits). Hypothesised by Ettore Majorana in 1937, Majorana fermions have not yet been found as elementary particles, but were detected as quasiparticle excitations in 2014. Inelastic neutron scattering is the perfect tool for probing magnetism, and recent work on the LET instrument found two distinct Majorana fermions in the magnetic insulator α -RuCl₃, with experimental results that corresponded surprisingly well to the theoretical model. The next step will be to examine the behaviour of these Majorana fermions within a magnetic field.

Realising 3D data transfer in nanomagnetic logic

Related publication: A. Fernández-Pacheco, et al. "Magnetic State of Multilayered Synthetic Antiferromagnets during Soliton Nucleation and Propagation for Vertical Data Transfer" *Adv. Mater. Interfaces*, 3 (2016): 1600097.

DOI: 10.1002/admi.201600097

Instruments: OFFSPEC

Funding: EPSRC EP/M008517/1, the Winton Foundation, and by the European Community under the Seventh Framework Programme Contract No. 247368, 3SPIN.

 Amalio Fernandez-Pacheco (University of Cambridge) and Nina-Juliane Steinke (ISIS Neutron and Muon Source).

Nanomagnetic logic (NML) is an area of spintronics which could lead to future ultra-low power computing technologies. The transport of data in NML is carried out by means of topological solitons, via strongly-coupled neighboring nanomagnets. Until now, studies in this field have been performed in two-dimensional nanomagnets coupled by dipolar interactions, allowing for the transport of information and logic operation along the substrate plane. One of the main unresolved challenges in NML is how to perform vertical data transfer, a necessary step towards three-dimensional spintronic systems.

In work published in *Advanced Materials Interfaces*, researchers from the University of Cambridge and ISIS Neutron Source have investigated the nucleation and propagation of solitons in multilayered synthetic antiferromagnets, where data is vertically transferred via RKKY interactions. By employing magneto-optical Kerr effect, magnetoresistance and polarized neutron reflectivity measurements (collected on OFFSPEC), a detailed picture of the complex soliton nucleation process in these systems has been obtained. The work shows the paramount importance of employing a multiple, complementary characterization techniques for the investigation of 3D nanomagnetic systems.

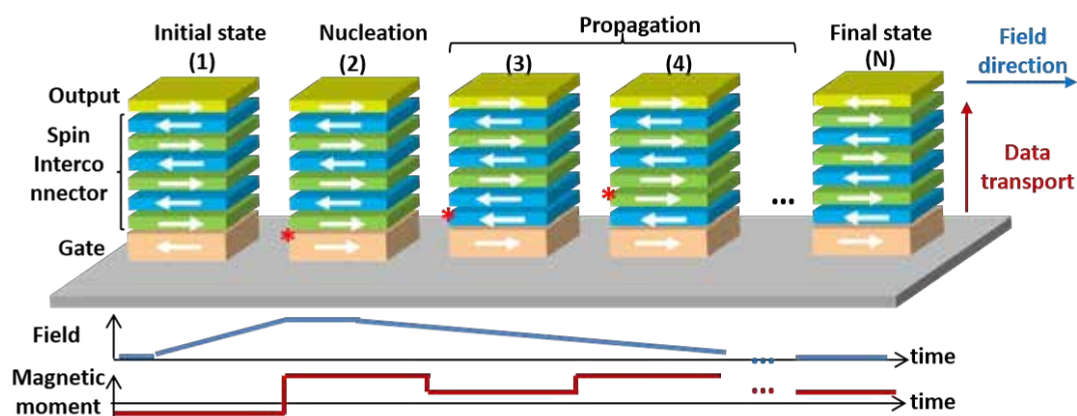


Image reproduced from Fernández-Pacheco A., Steinke Nina-Juliane, Mahendru D., Welbourne A., Mansell R., Chin S. L., Petit D., Lee J., Dalgliesh R., Langridge S., Cowburn R. P. (2016). Magnetic State of Multilayered Synthetic Antiferromagnets during Soliton Nucleation and Propagation for Vertical Data Transfer. *Adv. Mater. Interfaces*, 3: 1600097. doi: 10.1002/admi.201600097

Topological numbers could be the key to novel materials

Related publication: P. A. McClarty et al. "Topological triplon modes and bound states in a Shastry–Sutherland magnet" *Nature Physics* 13 (2017): 736–741.

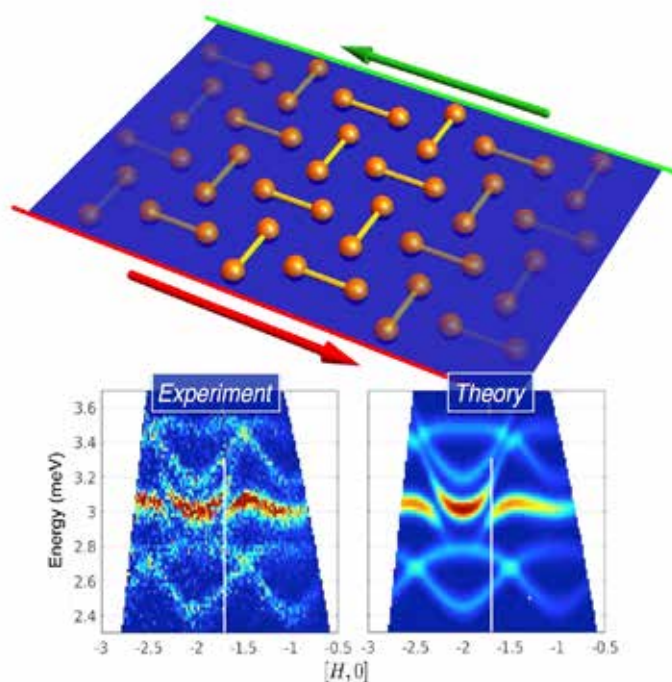
DOI:10.1038/nphys4117

Instruments: ALF and LET

Funding: P.A.M. acknowledges financial support from a Keeley-Rutherford fellowship. EPSRC Grants EP/K028960/1 (D.P.) and EP/M020517/1 (D.P. and R.C.).

 Frank Kruger (ISIS Neutron and Muon Source and UCL) Paul Alexander McClarty (ISIS Neutron and Muon Source and Max Planck Institute for the Physics of Complex Systems)

The realisation that there are states of matter that cannot be distinguished by examining the material at a local level has revolutionised our understanding of matter. The differences between these states are encoded in topological numbers, and determine the properties of a material. Researchers used inelastic neutron scattering on LET to study a quantum magnet system, and their results – published in *Nature Physics* – could pave the way for a new class of materials. They found that topology plays an important role in the quantum magnet they examined and that the signatures of topology live in the excitations about a very simple ground state. This could lead to an entirely new set of topological insulating materials with novel properties, and to new technologies.



The top panel shows the orthogonal arrangement of “dimers” in SCBO. The dimers are formed of pairs of magnetic copper ions which are in a quantum mechanical superposition with zero total magnetic moment. It requires a finite energy to break-up this superposition and induce a net moment. These excitations are called “triplons”, in order to express that they behave as quantum mechanical particles. The coupling between spins of adjacent dimers is responsible for the peculiar motion of triplons as well as for the strong interactions between them. In a small magnetic field perpendicular to the dimer planes, the magnetic excitation acquire a topological character. This goes hand-in-hand with the appearance of excitations that circulate around the edges of the sample. The bottom panel shows the comparison between the excitations measured by inelastic neutron scattering using the LET spectrometer at ISIS and theoretical calculations based on a model of interacting triplons.

Catalysis and Chemistry

A new class of economic, eco-friendly solvents

Related publication: O. S. Hammond et al. "Deep eutectic-solvothermal synthesis of nanostructured ceria" *Nature Communications*, 8 (2017): 14150

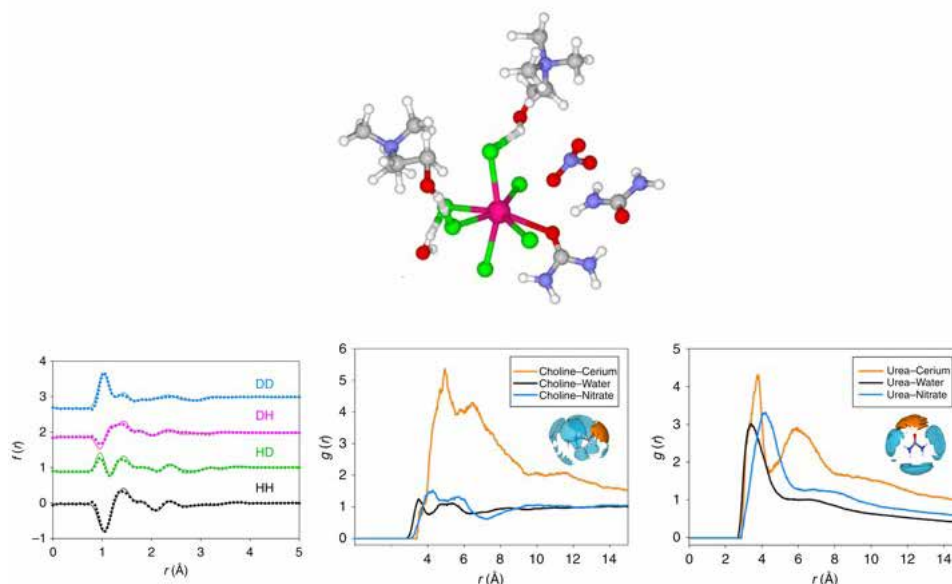
DOI: 10.1038/ncomms14150

Instruments: SANDALS

Funding: ISIS Pulsed Neutron and Muon source and EPSRC co-funding a PhD studentship for O.S.H. in the Centre for Doctoral Training in Sustainable Chemical Technologies at the University of Bath (EP/L016354/1; STFC Studentship Agreement 3578) and LTM EPSRC's Fellowship EP/L020432/2.

 Karen Edler (University of Bath) and Laura Torrente-Murciano (University of Cambridge)

Deep Eutectic Solvents (DESs) are part of an extended class of ionic liquids. Often made from cheap and safe components, they have the potential to be used as designer solvents, with none of the inherent toxicity of many room temperature ionic solvents. A paper published in *Nature Communications* details work carried out on SANDALS, using wide Q-range liquid-phase neutron diffraction to investigate the synthesis of nanostructured ceria using a DES. Ceria is a technologically-important material, used in catalysis, emissions control and solid-oxide fuel cells. The new understanding this work has given us of deep eutectic-solvothermal methodology will enable future developments in low-temperature synthesis of nanostructured ceria and other oxides, facilitating their manufacture with economic, eco-friendly and non-toxic solvents.



Solvent-driven pre-organisation of Ceria ions. Ce^{3+} integrated by ligation; Ce_2O_3 , Ce-Cl and ligand-ligand H-bonding. Strong close-range correlation between reactive components urea, H_2O , Ce^{3+} . DES effectively acting as a supramolecular catalyst.

Using muonium radicals as surrogates for hydrogen radicals

Related publication: J. A. Wright et al. "Muonium Chemistry at Diiron Subsite Analogues of [FeFe]-Hydrogenase" *Angew. Chem. Int. Ed.* 55 (2016):14580.

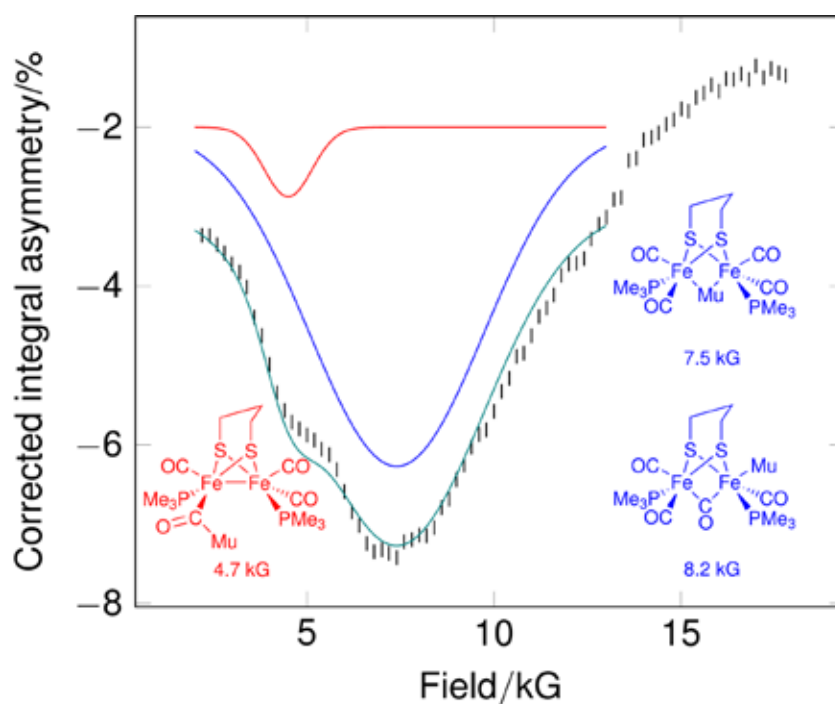
DOI: 10.1002/anie.201607109.

Instruments: MuSR

Funding: EPSRC grant EP/M011879/1 and the University of East Anglia.

 Joseph Wright (University of East Anglia)

Muonium is an exotic atom, consisting of an electron and an antimuon, discovered in 1960. A paper published in *Angewandte Chemie* explores the potential of using muonium radicals as surrogates for hydrogen radicals in the study of catalytic and electrocatalytic reactivity at metal centres, using the active site of [FeFe]-hydrogenase. When a beam of energetic muons is implanted into a solid sample, some sub-atomic muons capture an electron to form muonium radicals. As a low isotopic mass analogue of hydrogen, the muonium radical can be used to probe the early stages of hydride formation at metal centres. This first example of the application of muon spin rotation/relaxation/resonance spectroscopy to electrocatalytic systems is likely to herald a wider application of muon chemistry.



J. A. Wright et al. "Muonium Chemistry at Diiron Subsite Analogues of [FeFe]-Hydrogenase" *Angew. Chem. Int. Ed.* 55 (2016):14580. DOI 10.1002/anie.201607109

Probing the mysteries of molecular self-assembly

Related publication: M. J. Hollamby et al. "Simultaneous SAXS and SANS Analysis for the Detection of Toroidal Supramolecular Polymers Composed of Noncovalent Supramacrocycles in Solution" *Angew. Chem. Int. Ed.* 55 (2016): 9890.

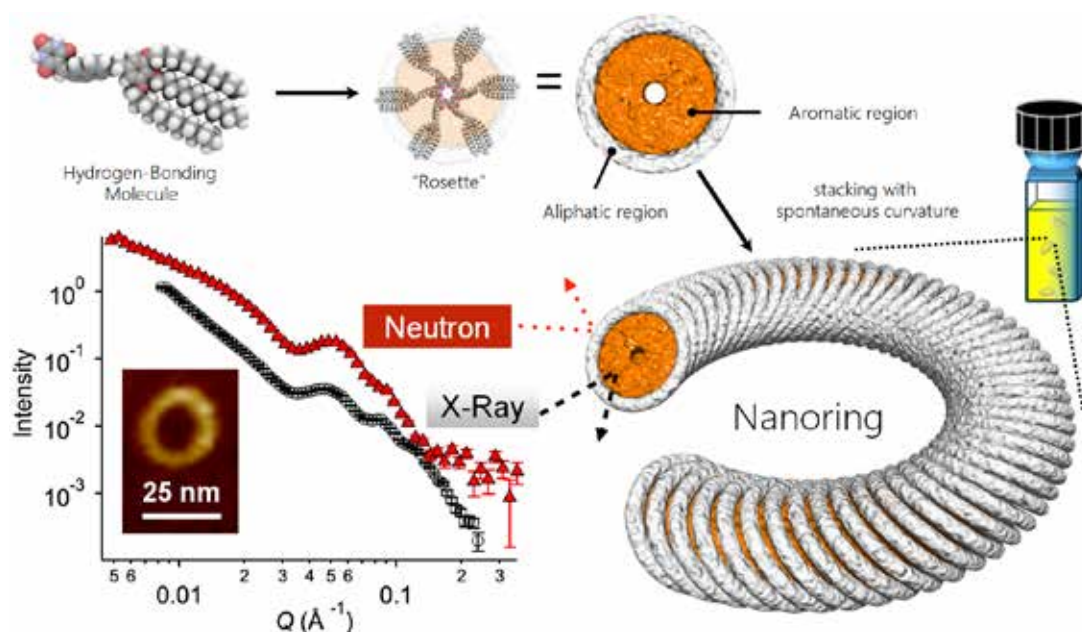
DOI: 10.1002/anie.201603370

Instruments: SANS2D

Funding: The authors acknowledge Diamond Light Source and the STFC for beam time on I22 and SANS2D, and consumables funding. This work was supported by KAKENHI (no. 26102010); a Grant-in-Aid for Scientific Research on Innovative Areas "π-Figuration" (no. 26102001) of the Ministry of Education, Culture, Sports, Science, and Technology, Japan.

 Martin J. Hollamby (Keele University)

Molecular self-assembly primarily occurs in solution and is key to many natural and industrial processes, including cell membrane formation, protein folding, foaming and detergency. To build accurate assembly models so that we might better understand these processes, we need techniques that can probe the structure of complex solutions. In work published in *Angewandte Chemie*, researchers used a combination of small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) to detect the formation of unusual ring-like (toroidal) assemblies in solution. Details concerning the internal structure of the toroids established links between molecular design and assembly morphology. Their work adds to the growing evidence of the power of combining SANS and SAXS analysis and in particular shows the applicability of such measurements to unusual or complex solution-based self-assembled structures.



M. J. Hollamby et al. "Simultaneous SAXS and SANS Analysis for the Detection of Toroidal Supramolecular Polymers Composed of Noncovalent Supramacrocycles in Solution" *Angew. Chem. Int. Ed.* 55 (2016): 9890.

A step closer to a metal-amine high-temperature superconductor

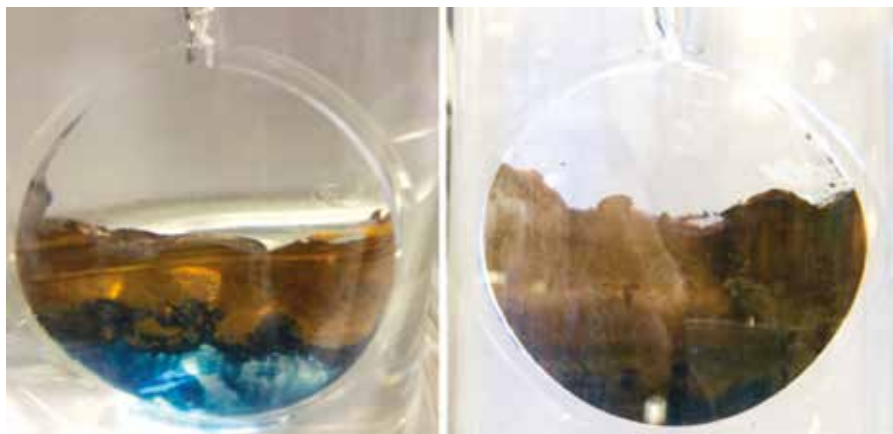
Related publication: A. G. Seel et al. "Electron Solvation and the Unique Liquid Structure of a Mixed-Amine Expanded Metal: The Saturated Li-NH₃-MeNH₂ System" *Angew. Chem. Int. Ed.* 56 (2017): 1561.

DOI: 10.1002/anie.201609192

Instruments: SANDALS

 Neal Skipper (University College London)

Since the late 1990s, neutron diffraction experiments at ISIS have been adding to our understanding of metal-amine solutions, an unusual class of liquids that contain solvated electrons and allow us to study fundamental physical phenomena. By varying the electron density, a metal-amine solution can be continuously changed from an electrolyte to a liquid demonstrating genuine metallic behaviour. Varying the amine and metal used adds to this 'tunability'. New work carried out on SANDALS, and published in *Angewandte Chemie*, adds another level of tunability, by using a mixed amine solvent. Researchers created an unusual liquid which is truly homogeneous, with strong longer-range order in which the solvated electron acts as a structural template. Their discoveries open up new avenues for fundamental research, and may bring us one step closer to a metal-amine high-temperature superconductor.



*Phase separation of solutions. A. G. Seel et al. "Electron Solvation and the Unique Liquid Structure of a Mixed-Amine Expanded Metal: The Saturated Li-NH₃-MeNH₂ System" *Angew. Chem. Int. Ed.* 56 (2017): 1561.*

The kinetics of oil exchange in nanoemulsions

Related publication: I. Hoffmann et al. "Kinetics of Oil Exchange in Nanoemulsions Prepared with the Phase Inversion Concentration Method" *Langmuir* 32 (46) (2016): 12084-12090.

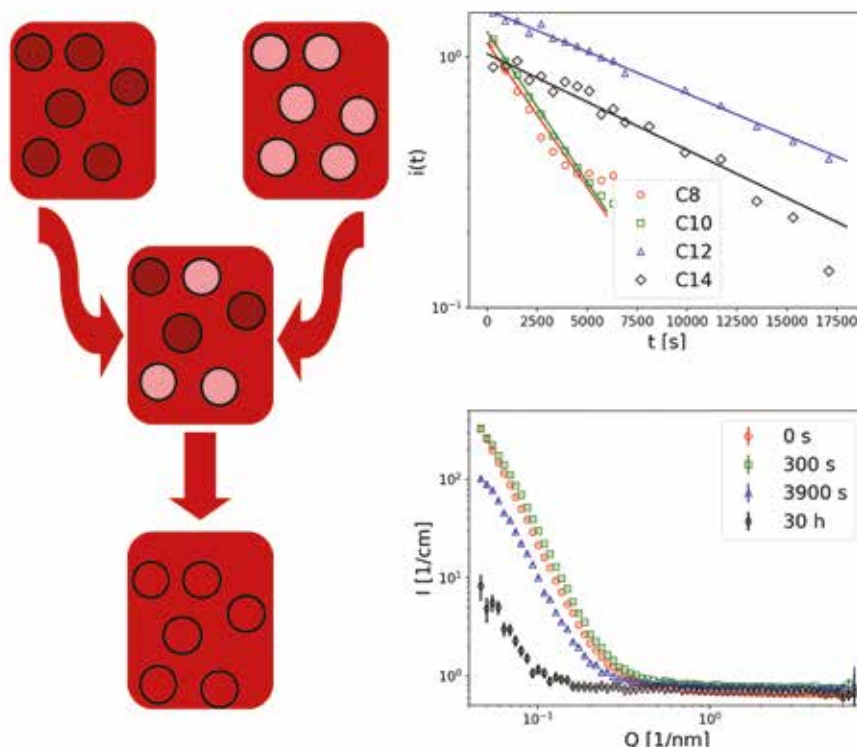
DOI: 10.1021/acs.langmuir.6b03009

Instrument: SANS2D

Funding: Financial support from the BMBF via the project 03GR7TUB PT-J.

 Michael Gradzielski (Technische Universität Berlin) and Ingo Hoffmann (Institut Max von Laue-Paul Langevin and Technische Universität Berlin)

Nanoemulsions (NEs), metastable emulsions with droplet sizes between 20 and 100nm, have a wide range of applications. These self-assembled, highly-dynamic systems can be used in polymerization and pharmaceutical and cosmetic formulations, and as drug delivery systems. Compared to microemulsions, NEs require less surfactant to emulsify a given amount of oil, and unlike emulsions they can be formed through low energy input methods such as phase inversion temperature or the phase inversion concentration (PIC) method. In a paper published in *Langmuir*, researchers detail their investigation of the kinetics of the oil exchange process in NEs formed via the PIC method. They used small-angle neutron scattering (SANS) on SANS2D to make the first direct observations of the exchange rate of a single type of oil molecule. This was only possible due to the ability of neutron scattering to differentiate between different isotopes, and the results have important implications for the optimization of NE formulations.



*I. Hoffmann et al. "Kinetics of Oil Exchange in Nanoemulsions Prepared with the Phase Inversion Concentration Method" *Langmuir* 32 (46) (2016): 12084-12090.*

Improving our understanding of metal-organic frameworks

Related publication: T. L. Easun et al. "Structural and dynamic studies of substrate binding in porous metal–organic frameworks" *Chem. Soc. Rev.*, 46 (2017): 239.

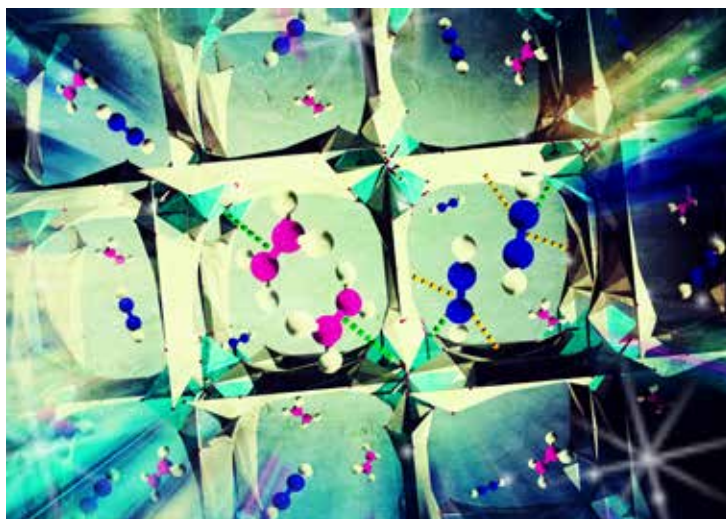
DOI: 10.1039/C6CS00603E

Instrument: TOSCA

Funding: Universities of Manchester, Nottingham, EPSRC and ERC for funding. MS acknowledges receipt of a Russian Megagrant from the Russian Ministry of Education and Science. TLE gratefully acknowledges the Royal Society for the award of a University Research Fellowship.

 Sihai Yang (University of Manchester) and Martin Schröder (Siberian Branch of the Russian Academy of Sciences and University of Manchester)

Work carried out on the Tosca instrument at ISIS has been included in a review of recent progress in the field of porous metal-organic frameworks (MOFs). With their high porosity and capability of binding small molecules, MOFs underpin a wide range of materials functions, including gas adsorption, separation, drug delivery, catalysis and sensing. The review, published in *Chemical Society Reviews*, examines recent investigations into the crystallographic, dynamic and kinetic aspects of substrate binding within porous MOFs. Inelastic neutron scattering is an ideal technique for studying atomic and molecular motions, and in the field of gas storage, separation and purification it is developing our understanding of how these materials function at a detailed molecular level. This work will lead to the design and development of new functional materials with higher storage capacities and stronger binding energies.



A representation of the mobility and binding dynamics of acetylene, ethylene and ethane guests within the NDT-300 MOF host.

Engineering

Looking for strain in high-entropy alloys

Related publication: L.R. Owen et al. "An assessment of the lattice strain in the CrMnFeCoNi high-entropy alloy" *Acta Materialia*, 122 (2017): 11-18.

DOI: 10.1016/j.actamat.2016.09.032

Instrument: Polaris

Funding: EPSRC/Rolls-Royce Strategic Partnership EP/M005607/1 and EP/H022309.

 Nick Jones (University of Cambridge)

High-Entropy Alloys (HEAs) are made from nearly equal ratios of several different metals. These novel materials are of considerable interest, because they have potentially desirable properties. Alloying elements into a pure metal causes local distortions in the atomic array, and the strain fields associated with these distortions give rise to strengthening. Extending these concepts to HEAs give rise to the hypothesis that their structure would be highly strained and distorted. To test this hypothesis, a team of researchers used total scattering measurements on Polaris to examine CrMnFeCoNi, and compared it with several compositionally simpler materials. The data, published in *Acta Materialia*, showed that the strain in the HEA lattice is not anomalously large, and the results do not support the hypothesis that multi-component solid solutions must have extremely distorted lattices.

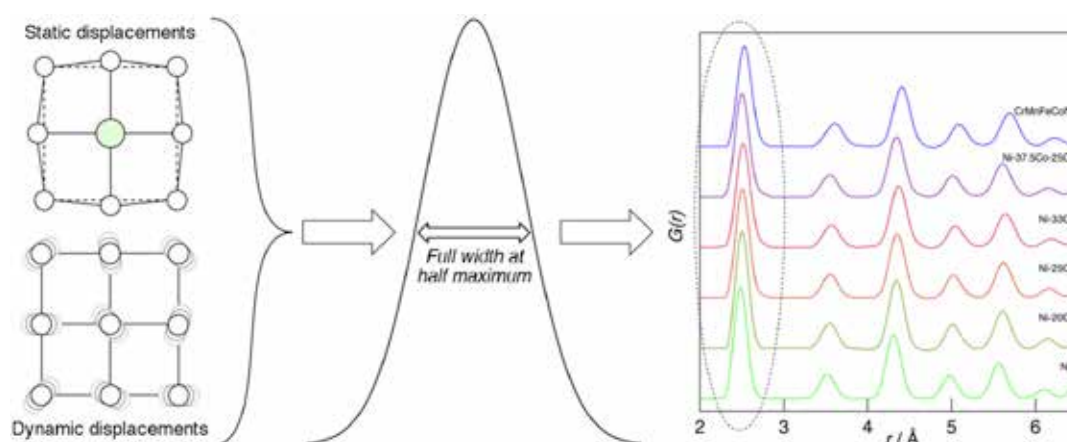


Image reproduced from L.R. Owen, E.J. Pickering, H.Y. Playford, H.J. Stone, M.G. Tucker, N.G. Jones, An assessment of the lattice strain in the CrMnFeCoNi high-entropy alloy, Acta Materialia, Volume 122, 2017, Pages 11-18, ISSN 1359-6454, <http://dx.doi.org/10.1016/j.actamat.2016.09.032>.

Neutrons illuminate stress/strain in high-temperature superalloys

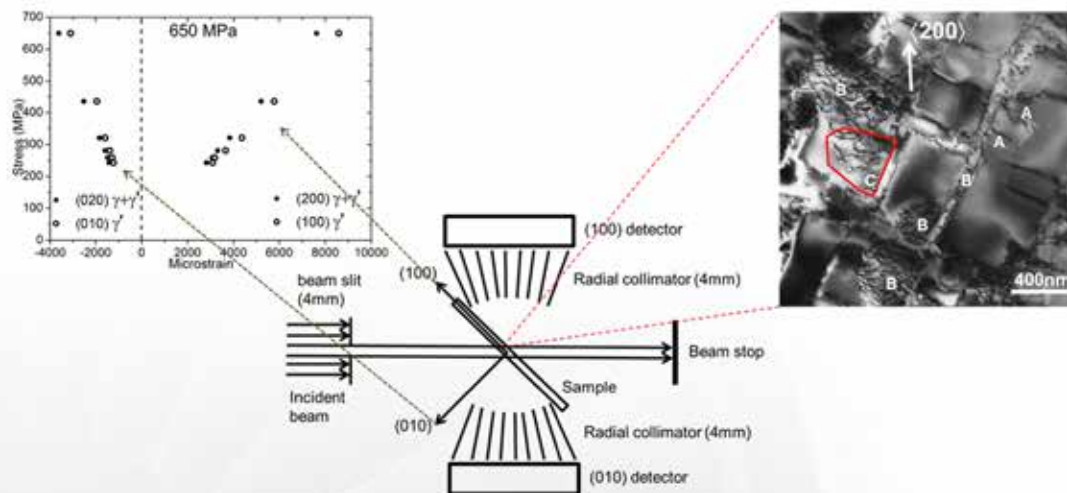
Related publication: Neil D'Souza et al. "The role of stress relaxation and creep during high temperature deformation in Ni-base single crystal superalloys – Implications to strain build-up during directional solidification" *Acta Materialia*, 106 (2016) 322-332.

DOI: 10.1016/j.actamat.2016.01.032.

Instrument: ENGIN-X

 Chinnapat Panwisawas (University of Birmingham)

The excellent high-temperature capability of Ni-base superalloys makes them one of the best materials for aerospace applications. A team of researchers from academia and industry has carried out a series of experiments to investigate how stresses and strains that develop during the manufacturing process can be alleviated. In the manufacture of turbine blades, directional solidification occurs as the mould is removed from the furnace and cools, with differential thermal expansion between the metal and ceramic resulting in thermal stresses and strains within the blade. Solution heat treatment is required to confer a homogenised microstructure. The team used *in-situ* neutron diffractometry on ENGIN-X to study stress relaxation occurring during high-temperature deformation. Their results, published in *Acta Materialia*, will be used to improve predictive stress/strain models.



Neil D'Souza et al. "The role of stress relaxation and creep during high temperature deformation in Ni-base single crystal superalloys – Implications to strain build-up during directional solidification" *Acta Materialia*, 106 (2016) 322-332. DOI: 10.1016/j.actamat.2016.01.032.

Heritage Science

Examining Iron Age coins sheds light on our past

Related publication: J. Corsi, et al. "Compositional and microstructural characterization of Celtic silver coins from northern Italy using neutron diffraction analysis", *Microchemical Journal*, 126 (2016): 501-508.

DOI:10.1016/j.microc.2016.01.006 .

Instrument: INES

Funding: Regione Piemonte (Italy); INFN-CHNET

 Antonella Scherillo (ISIS Neutron and Muon Source) and Jacopo Corsi (University of Torino)

The non-invasive nature of neutron studies makes them ideal for heritage science. A team of researchers has used time-of-flight neutron diffraction (TOF-ND) on INES to analyse the silver coinage of Celtic tribes who settled in northern Italy between the fourth and first centuries BCE. Unlike Greek and Roman coins, Celtic coins from this era have rarely been investigated. The study, published in *Microchemical Journal*, used neutron diffraction techniques to overcome surface alteration and provide bulky compositional and structural information for 33 specimens. The results show a clear debasement of the coins over time, attributed to inflation processes related to the increasing power of the Roman Republic in the region, and provide new insights into Iron Age minting techniques.



Silver coinage of Celtic tribes who settled in northern Italy between the fourth and first centuries BCE.

International Collaborations

ISIS Neutron and Muon Source has more than 20 international partnerships and agreements with 11 different countries.

These not only create new opportunities for researchers from partner countries to use ISIS neutron and muon instruments, but also provide additional resources, such as instrument upgrades, which benefit the whole ISIS user community.

Highlights of some of our partnerships and agreements are given below.



Sweden

5-year agreement with the Swedish Research Council from January 2015.



India

A 5-year agreement with India to provide contributions to the Zoom instrument.



Italy

Renewal of a 6-year agreement with Italy, contributing to several ISIS instruments.



USA



Japan



China



Spain



The Netherlands

Newton Funding

ISIS Neutron and Muon Source has active programmes to support Indian and Chinese researchers using the facility through the UK Newton Fund, which has been running since 2014.

The Newton Fund is part of the UK's Official Development Assistance (ODA) and aims to promote the economic development and social welfare of partner countries.

The programme aims to provide skills development and capacity-building to improve the ability of researchers from China and India to undertake and disseminate scientific research, whilst providing opportunities for ISIS to develop long-term relationships with partner countries.

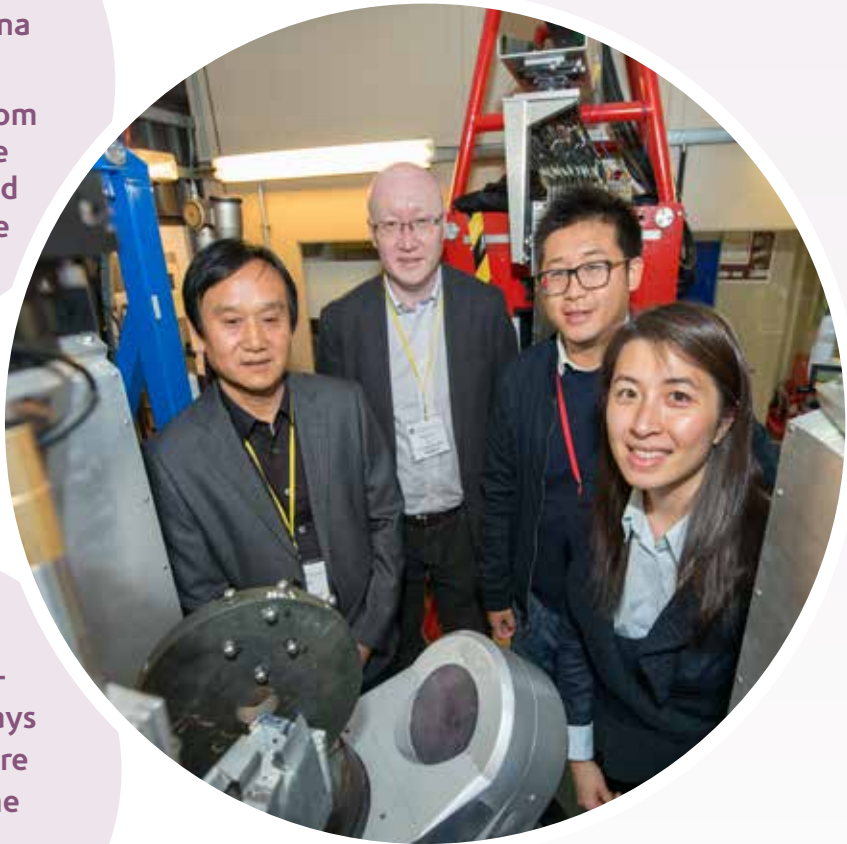
“Newton funds offer opportunity not only to perform state-of-art research but it opens a platform to train manpower”

Comments from a Newton Funded supported researcher

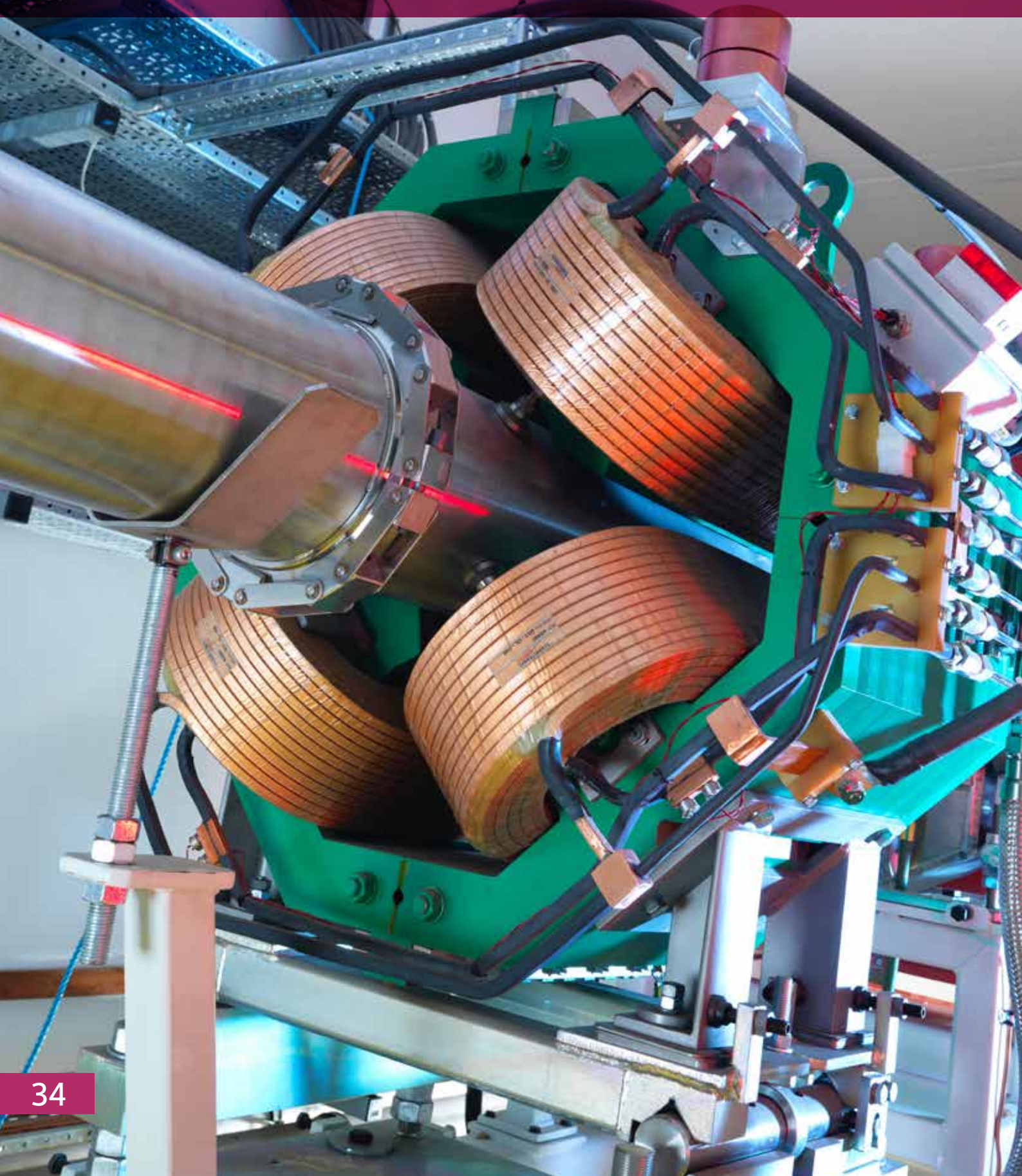
The Newton fund has led to 2 new agreements and partnerships with China and India.

Scientific proposals from China and India have more than quadrupled since the programme began.

Between 2014-2016 over 292 days of beamtime were supported by the Newton Fund.

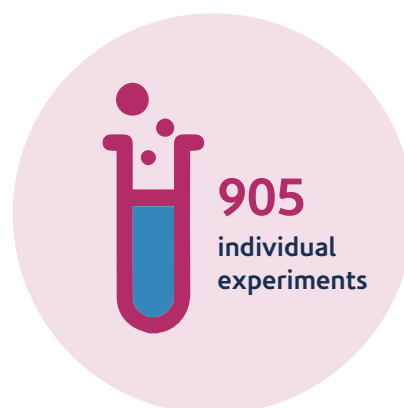
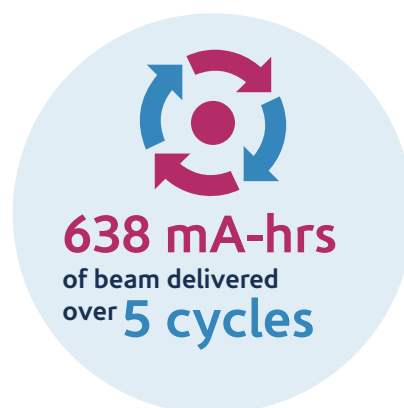
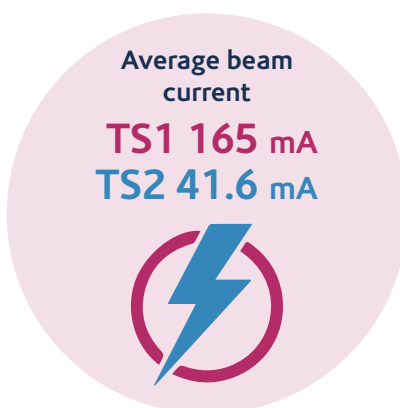


Technology



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 2016/2017 Cycle by Cycle

Cycle	16/1	16/2 (TS2 only)	16/3	16/4	16/5
	12 Apr -19 May 2016	28 Jun - 28 July 2016	13 Sept - 27 Oct 2016	15 Nov - 15 Dec 2016	14 Feb - 30 Mar 2017
Beam on target (hr)	802	627	709	590	864
Total beam current delivery for both targets (µA-hr)	165371	26031	143002	123006	180761
Combined beam current for beam on target (µA)	206	42	202	209	209
Target 1	166	0	163	167	164
Target 2	40	42	39	41	46
Averaged combined beam current per hour (µA)	214	40	202	212	211
Peak beam current over 24 hrs (µA)	186	36	170	190	167

Major Projects

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

Target Station 1

Target Station 1 (TS1) has run for over 30 years without significant maintenance or development work. The TS1 project seeks to develop and upgrade key elements of the target station, with the actual work likely to take place around 2020.

Preparation is already well underway with over 20,000 people hours already invested in the project. Highlights last year include: the creation of a characterisation rig that can take absolute flux and time of flight data, ortho/para ratio measurements for liquid hydrogen in both the target stations, and system and component design development and progression.

Finally as part of the project the team have created a virtual reality display of part of target station 1, allowing visitors and staff alike to fly through areas they would never normally access.

Target Station 2 Phase II Instruments

The ISIS Phase II project covered a range of activities on the second target station and consisted of a change of the Beryllium reflector and the delivery of four new instruments. The reflector change was successfully completed in 2016 and in the past year all four neutron instruments have continued to make significant progress into and towards their user programmes.

Details of developments of the four instruments in the Phase II project – LARMOR, IMAT, Zoom and ChipIR can be found in the Instrument Development section.

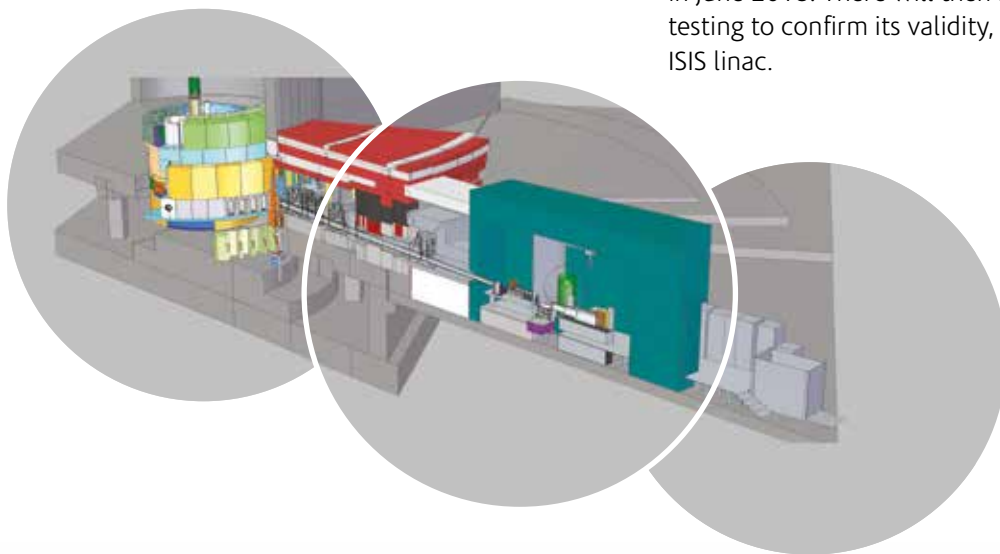


Dr Robert Bewley and Dr Daniel Pooley installing the TS1 Characterisation rig on the LARMOR instrument at ISIS's TS2 facility at STFC's Rutherford Appleton Laboratory

ISIS Supporting the European Spallation Source

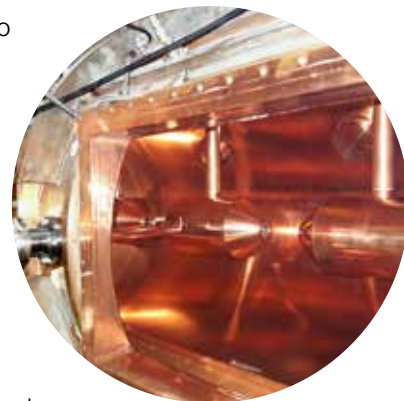
Staff at ISIS Neutron and Muon Source have been busy continuing their important contributions to several areas of the €1.8Bn European Spallation Source (ESS), currently being built near Lund in southern Sweden.

On neutron instruments, a major review of the SANS instrument Loki has been passed, and design studies are underway for a reflectometer called FREIA and, in conjunction with colleagues at CNR, a spectrometer called VESPA. In addition, work on data streaming is already proving to be useful to ISIS as well as ESS, with software developed for ESS being demonstrated on LARMOR at ISIS with similar synergies are planned for our work on data reduction. ISIS is also aiding the ESS in planning their support laboratories, drawing on our experience as an operating facility. Finally, the UK ESS programme office, which is based at ISIS, continues to oversee all of the UK's 10% involvement in ESS.



Linac tank 4

A project is underway to replace the ISIS linac's venerable Tank 4. A two-metre-long test section has proved the vacuum and radio-frequency (RF) characteristics successfully, with a Q-factor in excellent agreement with simulations. Assembly and testing of key components is well underway, such as compact magnet coils, yokes and cooling systems, as well as newly designed drift tubes (see image) which will improve RF power efficiency by 25%. Full-power RF testing is due to commence on the test section in October 2017, before the area is reconfigured to accept the real twelve-metre long tank. An order worth £750k was placed for the tank to be made in the Netherlands and it is expected in June 2018. There will then be a period of soak-testing to confirm its validity, before it is installed in the ISIS linac.



The Helium Recovery Project

Over the last 10 years the cost of helium has increased by over 300%. ISIS is a major user of helium, as liquid to cryogenically cool samples on the instruments and as gas in the target stations. Two thirds of ISIS experiments use liquid helium, and this looks set to increase.

In 2013 a project began to develop a helium recovery facility, with the aim of reducing the helium bill by capturing, compressing and storing helium, before making it available for re-use or by selling on.

The recovery facility has supplied Target Station 1 and the instruments and labs on Target Station 2 with recycled Helium for the last 2 operational cycles - a yearly saving for the target group alone is over £35K. Soon recycled helium for Target Station 2 and the instruments and labs on target station 1 will be available as well, which could save a further £100k / year. With the addition and commissioning of a Helium liquefier for the facility, the system is expected over the coming years to effect savings as high as £300k/year.

Instrument Updates



TOSCA

TOSCA is an indirect geometry spectrometer optimised for the study of molecular vibrations in the solid state. After a recent guide upgrade, completed in March 2017, the flux of TOSCA has increased by up to 100 times.

ENGIN-X is a dedicated engineering science facility at ISIS. In the past year a new low temperature stress-rig has been set up on ENGIN-X. The new stress-rig paves the way for research into the internal stresses in engineering materials at cryogenic temperatures – which is vital to our understanding of superconductors and their applications.



ENGIN-X



LARMOR

LARMOR is an advanced neutron polarisation instrument and one of the four instruments in the Phase II project. LARMOR is now a fully scheduled instrument with a broad ranging science program in hard and soft condensed matter, already publishing high impact work in the area of topological matter. LARMOR continues the strong collaboration with our partners at TU-Delft in the Netherlands, with the commissioning of the new TU-Delft Spin-Echo SANS (SESANS) equipment completed in September 2017.

Zoom is a small angle instrument which complements the existing SANS2D instrument by exploiting neutron polarisation techniques and is part of the Phase II Project. Zoom, which is co-funded by the Indian Department of Science and Technology's Nanomission project, has entered its commissioning phase and will enter the user programme in early 2018.



ZOOM



ChipIR

ChipIR is an innovative instrument to provide rapid testing of the effect of atmospheric neutrons on the microelectronics that society relies upon. ChipIR is one of the four instruments in the Phase II Project. ChipIR has now commenced its commercial testing programme for a range of microelectronics with applications in several industrial sectors.

LET is a cold neutron multi-chopper spectrometer for the study of dynamics in condensed matter. The instrument will shortly be equipped for uniaxial neutron polarisation analysis experiments. A broadband polarizer (for incident energies < 10 meV) has been installed and tested, and provides a neutron polarization of ~95% with a transmission of 40%. Initial experiments with uniaxial polarization analysis are planned for early 2018.

LET

MARI

MARI is a chopper spectrometer with continuous detector bank coverage. MARI is now 28 years old, but the June 2017 shutdown saw the instrument begin a significant upgrade to install $m=3$ supermirror neutron guides. This will bring the flux on MARI into line with the other the direct geometry spectrometers at ISIS. New choppers on MARI will allow the instrument to be run with simultaneous multiple incident energies (RRM mode).

MAPS was the first chopper spectrometer to employ a large array of position sensitive detectors, and the first to be designed solely for the purpose of measuring excitations in single crystals. As part of a comprehensive upgrade project (new moderator, new shutter and guides) significant improvements to the flux on MAPS are expected by the end of this year. New choppers on MAPS will allow the instrument to be run with simultaneous multiple incident energies (RRM mode).

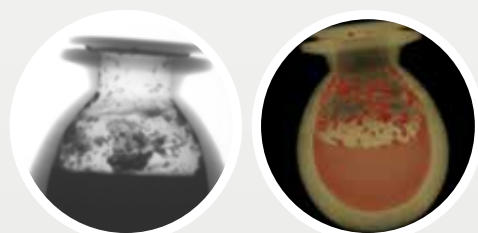
MAPS

IMAT

IMAT is a neutron imaging and diffraction instrument which will be used in a diverse range of disciplines such as engineering material sciences, battery research, earth science and cultural heritage. The instrument was formally opened in October 2016 and is now well into its commissioning. IMAT will undergo further commissioning work testing additional shielding and a new high-end neutron imaging camera.

One of the first user experiments on IMAT was on archaeological vases and pots from the Egyptian Museum in Turin. These first experiments were aimed at revealing the interiors of the closed objects and at finding clues about their manufacture and use.

Users setting up samples on IMAT



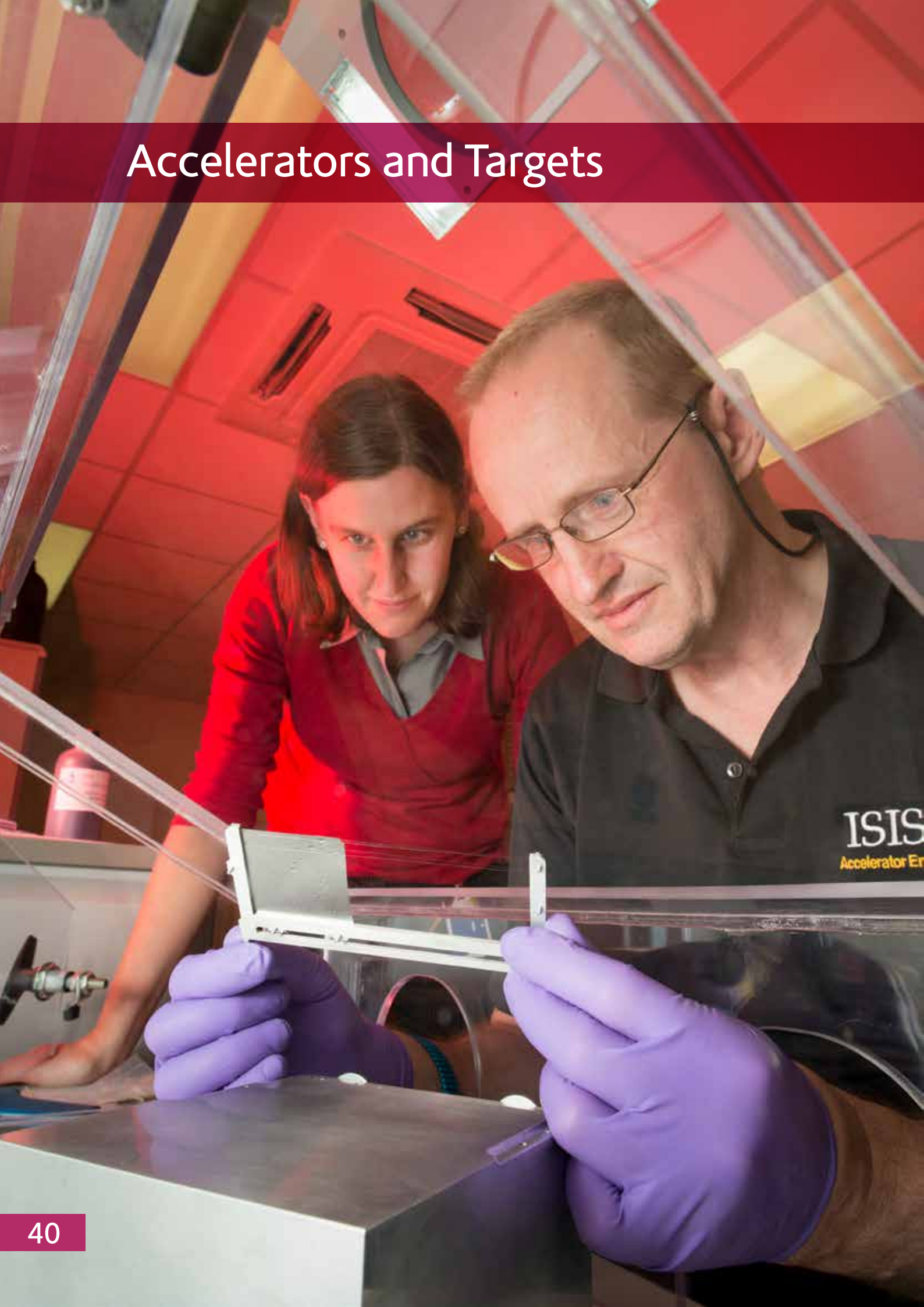
Neutron radiographies and tomographies of the vases and ceramic vessels were collected.



Dr Corrado Spinella, Director Department of Physical Sciences and Technology of Matter, CNR unveiling the IMAT inauguration plaque as Dr Andrew Taylor, STFC Executive Director, National Labs, looks on.



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.

New Ionisation Profile Monitor

A new ionisation profile monitor (IPM) that allows beam profile measurements to be taken without interfering with the beam has been constructed and tested by the ISIS diagnostics section, and was installed in the 2017 summer shutdown. The IPM uses Channeltron electron multipliers to detect ionised particles created by the beam as it passes through the monitor, then calculates the beam profile from this information, allowing for studies on sources of high intensity beam loss in ISIS.

Linac Tank 4

The ISIS linear accelerator (linac) consists of 4 radiofrequency (RF) accelerating tanks, accelerating hydrogen ions generated in the ion source to 37% of the speed of light before feeding them into the synchrotron for final acceleration. A project is underway to replace one of these – tank 4. See p 37 for more information.

Carbon Stripping Foil Tests with the ISIS Diagnostic Test Vessel

The Diagnostics Section have developed an off-line vacuum vessel with electron and ion guns to test components before installation in the synchrotron or extracted proton beamlines. This vessel has been used to perform tests of novel stripping foils without risk to the operations schedule. These experiments aim to increase foil lifetime, which will increase beam availability for users while while also improving safety.

Collaboration with Hiroshima University

Dr. Suzie Sheehy and Oxford DPhil student Lucy Martin visited the Hiroshima University Beam Physics group of Prof. Hiromi Okamoto in summer 2017 to collaborate on experiments using linear Paul traps to study accelerator beam dynamics phenomena. The ISIS Intense Beams group have been collaborating with Hiroshima University on this subject since 2013 and this has led to the development of the Intense Beam Experiment (IBEX). In January 2017 IBEX successfully trapped, extracted and measured ions for the first time. IBEX is based on a linear Paul ion trap and is designed to replicate the dynamics of intense particle beams in a flexible, compact system.

Dr. Suzie Sheehy and DPhil student Lucy Martin (2nd and 3rd from left front row) on their visit the Hiroshima University Beam Physics group of Prof. Hiromi Okamoto (far right).



Left: Mark Waite assembling a carbon stripping foil for ISIS as Hayley Cavanagh watches.

Computing

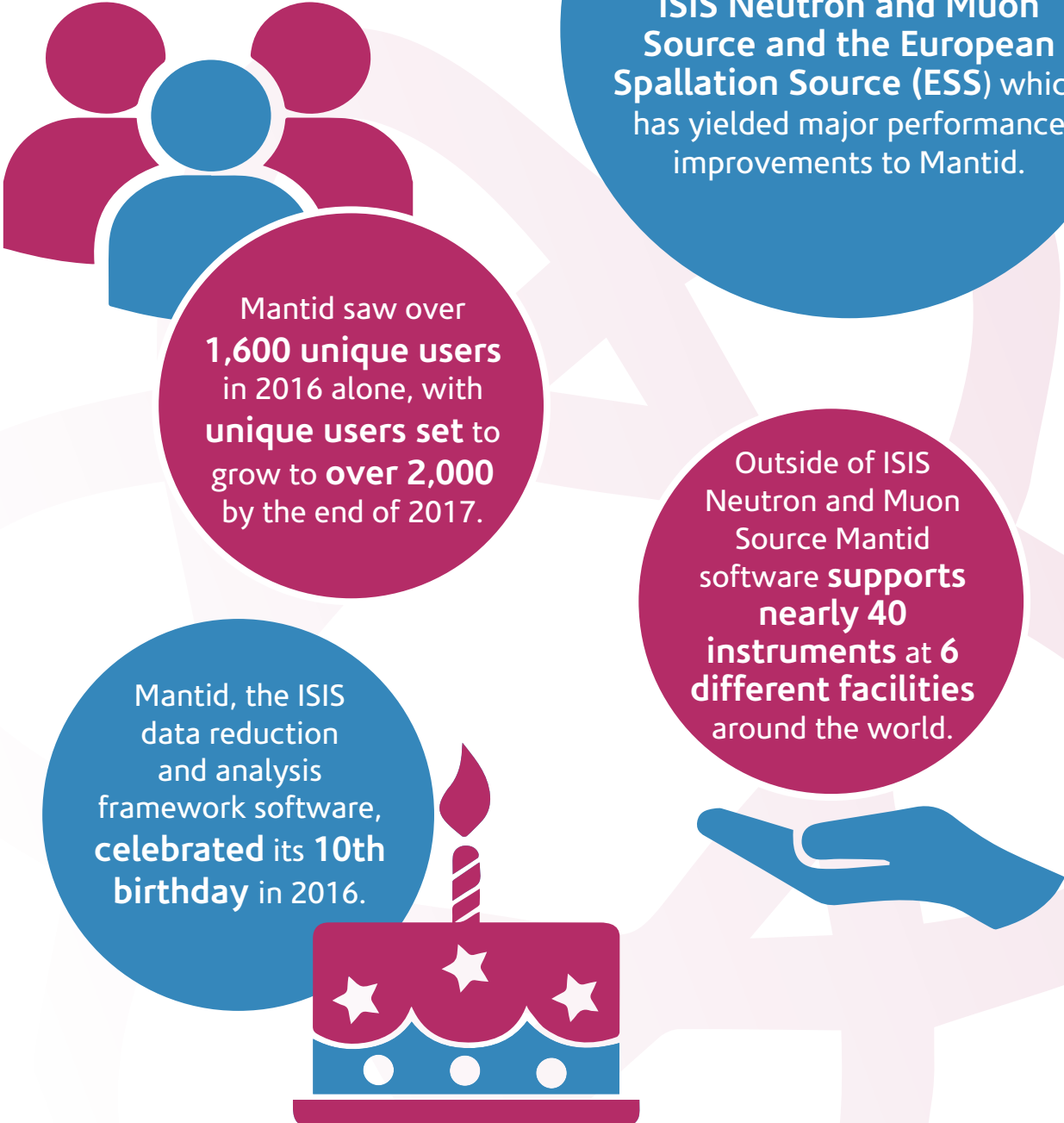


Computing

The ISIS Computing group is responsible for instrument control, data reduction software, data cataloguing and storage, maintaining and developing the computing network and back-end IT infrastructure including data storage, and providing IT support to business and science.

As well as supporting the current software used for instrument control at ISIS, the instrument control team's main project is developing the new 'IBEX' system based on EPICS. This will allow more complex device control and allow us to collaborate better with other international facilities.

The computing group works closely with STFC's Scientific Computing Department to provide access to the SCARF cluster for ISIS users, to maintain the 30+ year catalogue of ISIS data, and is working to provide a 'cloud' online data analysis facility to give ISIS users remote access to the resource they need to analyse their data.



A particular highlight from the last 12 months is the in-kind collaboration between **ISIS Neutron and Muon Source and the European Spallation Source (ESS)** which has yielded major performance improvements to Mantid.

Mantid saw over **1,600 unique users** in 2016 alone, with **unique users set to grow to over 2,000** by the end of 2017.

Mantid, the ISIS data reduction and analysis framework software, **celebrated its 10th birthday** in 2016.

Outside of ISIS Neutron and Muon Source Mantid software **supports nearly 40 instruments** at **6 different facilities** around the world.



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



18
Graduate
Students



49
co-sponsored
PhD students



25
vacation
students



20
work experience
placements



26
Apprentice
placements



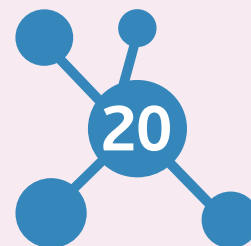
22
undergraduate
sandwich
students



1020 PhD students
used our instruments
gaining valuable skills
and knowledge of
neutron and muon
techniques



17
days of teacher
training



20
scientific
seminars



4063 total visitors,
including 1907
school students,
teachers and
members of
the public



22
events
organised by
the community



250
staff
talks
at meetings,
conferences and
workshops

Inspiring the next generation

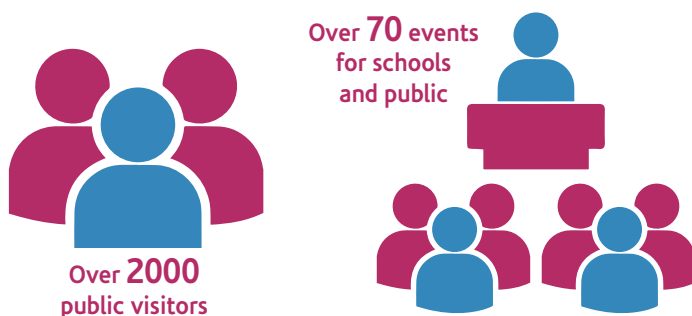


Inspiring the next generation

2017 has been a busy year in public engagement with over 2000 school pupils, teachers and members of the general public pouring into the facility for ISIS talks and tours of the experimental halls, hearing about the amazing science and engineering we undertake.

ISIS opens its doors to the public for several large events a year, including the Particle Physics Masterclass, Stargazing at RAL, Chemistry at Work Day and the RAL Apprentice Day. Education Access and Public Access Days at RAL continue to be popular, and feedback consistently shows tours of ISIS as a highlight of these events. 2017 also saw ISIS hosting a summer Open Day, with almost 450 visitors making their own slime, crystal gardens and electric motors, as well as experiencing virtual tours of the ISIS target area amongst many other activities.

In addition to our on-site activities, the past year has seen ISIS staff and students heading out to local schools, science festivals and careers fairs, engaging with the local community and inspiring the next generation of scientists and engineers. The 6-month display on neutron diffraction at the Wallace Collection National Museum in London came to an end in March 2017. The exhibit was centred around research on historical arms and armour undertaken at the facility, and allowed our research to reach a new and diverse audience, with visitor numbers in excess of 25,000.



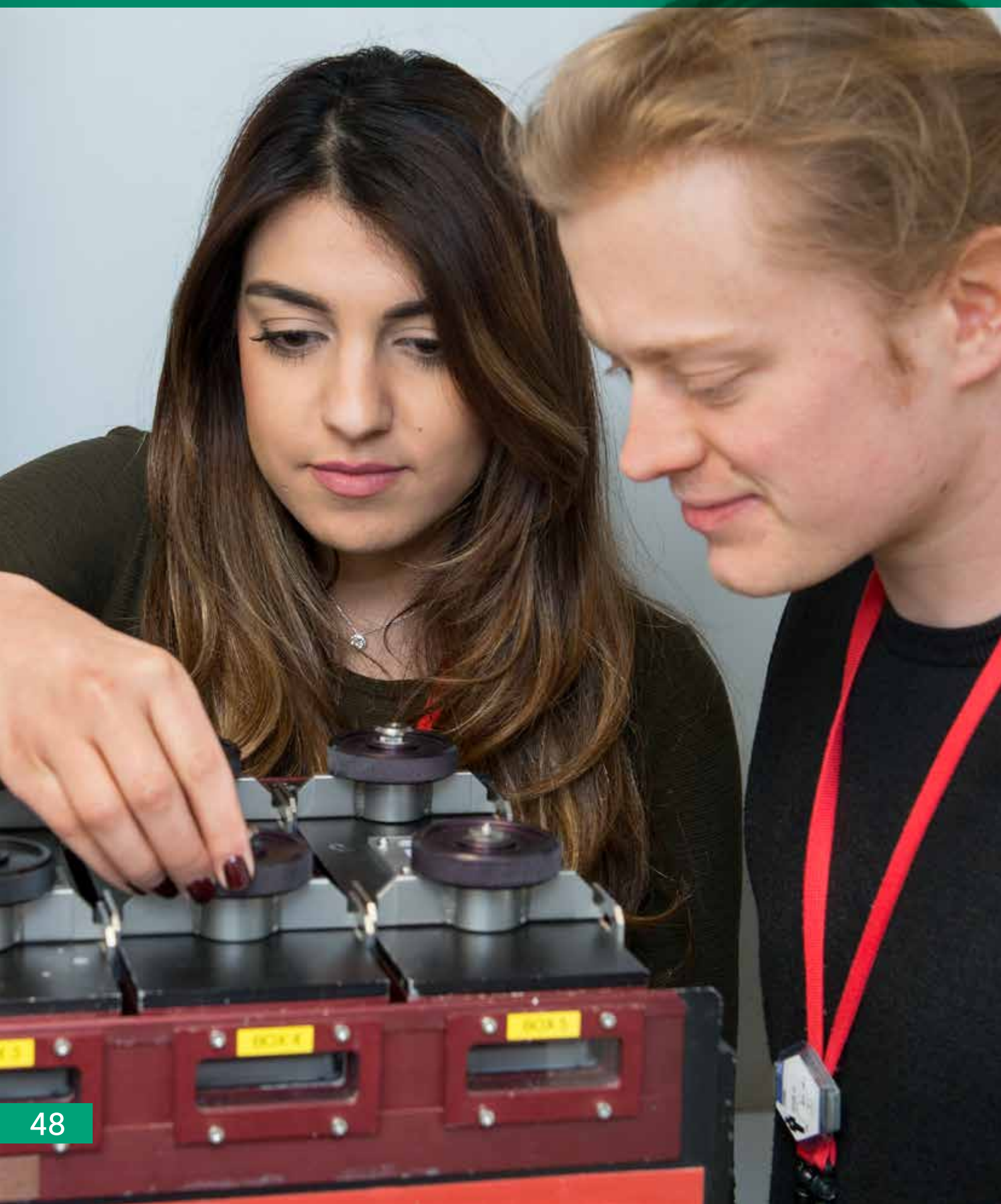
Chris Frost's liquid nitrogen show during Ashcroft Academy's visit to RAL on 3rd May

Case study: Chemistry at Work

This is the 3rd year we have been part of the RSC's flagship schools event, Chemistry at Work. This event welcomed 48 KS4 and KS5 school pupils for a day of talks and hands-on activities showcasing the range of opportunities for chemistry students. Students participated in several different workshops based around Chemistry at ISIS and were also treated to liquid nitrogen ice-cream and a Flash Bang Chemistry show.



Developing the student community



Developing the student community

The student community lies at the heart of ISIS Neutron and Muon Source, with nearly 100 co-sponsored PhD students, vacation and sandwich students working at the facility. In addition, there were over 1000 visits from PhD students to ISIS year for experiments. We look to encourage and grow the community in three key ways: training courses, supervision and on the job training.

Training Events

2016 saw a range of training events aimed at students including: the Oxford Neutron Summer School, ISIS/Diamond School for CDT students, ISIS student days, and the ISIS Neutron Training School plus a variety of more specialised and technical courses given through individual talks at external student events or contributing to university lecture courses.

In addition attendance at the student day held as a satellite to the UK Neutron and Muon Science and User Meeting more than doubled in 2017 compared to last year.

Supervision

ISIS staff are co-supervising over 80 students between them, in addition to managing sandwich students, apprentices or graduates within ISIS. PhD student co-supervision is always done in partnership with a university collaborator.

On the job training

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

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



Attendees for the UK Neutron and Muon Science and User Meeting student day.



Students learning how to use Single Crystal data analysis and Single Crystal structure refinement software at the 2017 ISIS Neutron training course.



A talk during the UK Neutron and Muon Science and User Meeting student day.

Events for the neutron community



Developing the wider neutron community

ISIS Neutron and Muon Source staff continue to organise, or have major input in organising, over 40 different events, workshops, conferences, user groups and seminars for the Neutron and Muon Community. In addition to this staff gave around 250 separate talks at a variety of meetings, including presentations at conferences and workshops, departmental seminars and more.

NIBS'16

The 5th International Symposium on Negative Ions, Beams and Sources (NIBS) was jointly hosted by STFC and the Culham Centre for Fusion Energy (CCFE), attracting over 100 international scientists and engineers to Oxford in September 2016. As well as discussing negative ion beams for accelerator and fusion applications, 88 peer review papers were produced.

Mantid Developer Workshop

The data reduction software Mantid had its 10th birthday this year, which happened to coincide with ISIS hosting the annual Mantid developer workshop 14th-16th June at Cosener's house. The workshop had software developers participating from Mantid's now four partner facilities: ILL, SNS, ESS and ISIS.

Faraday Conference 2017

The first meeting of its kind, the Faraday Conference aimed to bring the Physical Chemistry community together involving ISIS Neutron and Muon Source, ILL and ESS. The meeting showed the latest trends in research and encouraged collaboration, as well as strengthen links with industry.

ICANS XXII

ICANS XXII was the 22nd meeting of the International Collaboration on Advanced Neutron Sources (ICANS). ICANS is an informal network of laboratories whose scientists and engineers are involved in developing pulsed neutron sources and accelerator based spallation neutron sources. The collaboration was founded in 1977 and turned 40 this year. The 22nd meeting was hosted by ISIS in Oxford in March 2017.

UK Neutron and Muon Science and User Meeting

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

The Oxford School of Neutron Scattering

The 15th Oxford School of Neutron Scattering recently took place. The school aims to provide an in-depth grounding to theory, techniques, applications, facilities (pulsed and steady) and beamtime proposal. The Oxford School on Neutron Scattering is largely sponsored by ISIS but takes students from all over the world.



Attendees at the Oxford School of Neutron Scattering 2017



Attendees at Mantid's 10th developer workshop

Developing our people



Developing our people

ISIS has several initiatives to support our staff, from the thriving graduate and apprentice schemes to encouraging further study by part-time PhDs to professional memberships. In addition formal recognition of ISIS staff member expertise is given by other institutions through visiting or honorary appointments, professorships or lectureships. Staff have some 20 positions between them.

The prestigious BTM Willis prize for outstanding neutron scattering science was awarded to Dr Andrew Seel, formally a member of ISIS' Molecular Spectroscopy Group, at NMSUM.

Professor Carla Andreani, ISIS user and long-term collaborator of the facility, has been awarded the Giuseppe Occhialini Medal and Prize from the Italian Physical Society together with the Institute of Physics.

Matthew Ryder, a joint DPhil student at the University of Oxford and ISIS, won the 2017 British Zeolite Association's Founder's Award.

ISIS' Yanling Ma was awarded a prestigious Fellowship of the Institution of Mechanical Engineers (FIMechE).

Scott Lawrie & Ben Pine both completed their PhD's in the past year, in addition to working full time jobs at ISIS Neutron and Muon Source.

Uschi Steigenberger, former director of ISIS, has been honoured with an OBE for Services to Science.

Uschi Steigenberger, former director of ISIS, has been honoured with an OBE for Services to Science. Credit: Andrew Chappell



The prestigious BTM Willis prize for outstanding neutron scattering science was awarded to Dr Andrew Seel, formally a member of ISIS' Molecular Spectroscopy Group, at NMSUM.

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