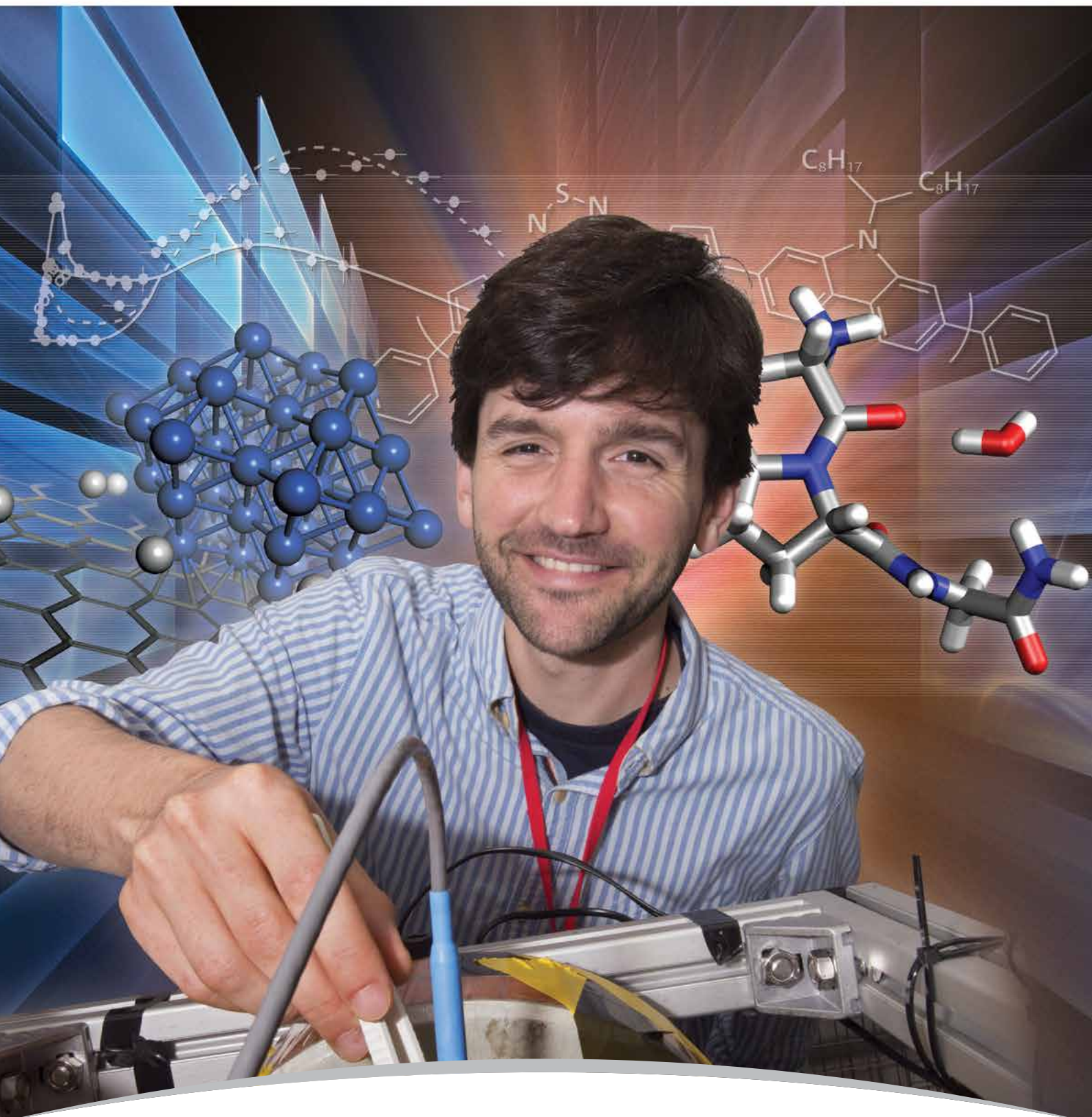


ISIS 2014

neutron and muon source annual review



Science & Technology
Facilities Council

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

ISIS 2014 production team: David Clements, Sara Fletcher, Oliver Glynn, Philip King, Kevin Knowles, Anders Markvardsen, Julian Norris, Stewart Parker, Andrew Seel and Rob Washington.

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November 2014

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ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2014 details the work of the facility over the past year, including science highlights, descriptions of major instrument and accelerator developments and the facility's publications for the past year.

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Foreword



In November 2013 ISIS was reviewed by an international panel chaired by Professor Joel Mesot, Director of the Paul Scherrer Institute. The review concluded that “ISIS has, since its creation, been able to create a culture of innovation that has had a profound impact on and will continue to change the way neutron scattering is performed worldwide”. This seems a fitting and very welcome conclusion as ISIS approaches its 30th birthday - the anniversary of first neutrons on December 16 1984 - but the story is far from over! These pages showcase numerous examples of continuing innovation and impact from ISIS users and staff.

2014 brings both welcome and less welcome news concerning neutron scattering. After more than 20 years of effort by numerous people, the European Spallation Source has finally started construction. When the first ESS workshop was held at Coseners House in 1991 the presentations were on overhead transparencies and nobody’s attention was diverted by email or mobile phones. Maybe we need to be a bit quicker at turning our visions into reality if we are to remain scientifically relevant? The BER-II reactor at the Helmholtz Zentrum Berlin will close in 2020 and will almost certainly not be the only European neutron source closing on that timescale. Although ESS will bring fantastic new capabilities, these will not be effectively exploited without a surrounding ecosystem of complementary neutron sources. So we need to start planning now for what will be next after ESS.

After several years of restricted operations for budget reasons, the situation for ISIS looks more promising from 2015. With increased UK funding, including from the Newton fund to support users from China, India and South Africa, and from Sweden to support the development of their user community, we plan to significantly increase our capacity. We will return all instruments to full user operation, bring the TS2 Phase II instruments on line and increase operating days. This will benefit both the UK and our partners. The design study for the TS1 target/moderator upgrade will be complete in mid-2015 and we are already looking for the necessary funding. There are continuing opportunities for improved performance through instrument and moderator development. And towards the end of 2015 we will launch the process of gathering ideas for ISIS-II, a new accelerator which should start construction in about 2025-30 as ESS moves into steady state operation. Whatever form ISIS-II takes there will certainly have to be an emphasis on energy and cost effective ‘science production’. So, I am already looking forward to a sense of déjà-vu when I read the conclusions of the 2043 international review...

The House of Commons Business, Innovation and Skills Select Committee including Adrian Bailey MP, Paul Blomfield MP, Mike Crockart MP and Robin Walker MP visited the ISIS TS2 facility on 17 June 2014.

ISIS International Review Panel members Thomas Schulthess (ETH Zurich), Mike Rowe (NIST Centre for Neutron Research) and Joel Mesot (Paul Scherrer Institut) being shown the Oxford Instruments – ISIS ‘ISISstat’ by Oleg Kirichek (ISIS).

Professor Robert McGreevy, ISIS Director and Professor Cristina Messa, Vice President, CNR, Italy, signing an agreement to renew ISIS’ long-standing partnership with Italy. With Professor Carla Andreani, CNR, Professor Roberto Di Lauro, Italian Scientific Attaché, and Professor Guiseppa Gorini, CNR.

L-R Greg Clarke MP, now Minister for Universities, Science and Cities and Deputy PM Nick Clegg with ISIS Director Robert McGreevy on a visit to the facility in January 2014.

Target Station 2 *five years of success!*

The second target station at ISIS was officially completed in August 2009. Five years on we look at some of the achievements, scientific and technical, and the opportunities to come as the second phase of instruments starts commissioning.

The aim in building TS2 was twofold: to provide increased capacity at ISIS through more instruments, and to enhance the capabilities of the facility through optimising the target, moderators and instruments. TS2 was designed to provide colder neutrons, a broad spectral range and high resolution, enabling science in emerging areas including soft condensed matter, biomolecular science and advanced materials.

The first user experiment was run in May 2009. Over 150 papers have been published, encompassing a wide range of disciplines. This year the first two phase 2 instruments, Larmor and ChipIR, have started commissioning, ready for first users in 2015, and IMAT and Zoom are well underway (see pages 24-25).

Highlights so far have included:

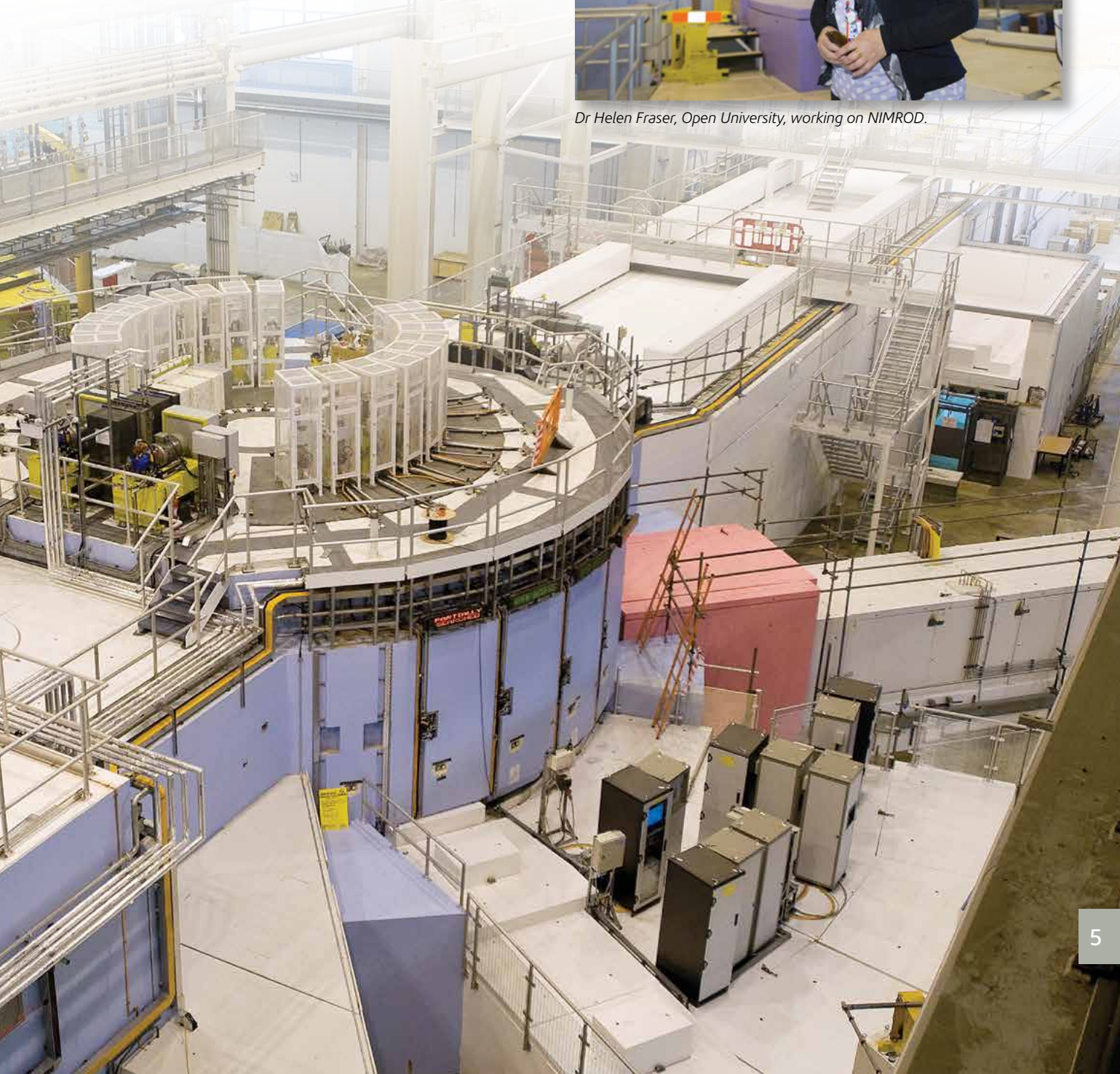
- Nimrod has been used to study iron nanoparticles relevant to iron therapies used to combat anaemia, to elucidate structure-function relationships. Its wide Q-range has been invaluable: "Nimrod allows us to collect data ranging from particle size and shape to details of bond lengths within the core and interactions at the surface. We can look at our particles in solution, dried or with isotopic substitutions, which gives us the maximum opportunity to decipher the structure.", says Dr Helen Chappell of the MRC's Biomineral Research Group.
- The magnetic structure of $\text{CaMn}_7\text{O}_{12}$, which exhibits electric polarisation alongside long-range magnetic order, was determined on Wish. The high resolution available on Wish was important for resolving the complex incommensurate helical magnetic structure (Phys Rev Lett, Johnson *et al* 2012).
- A detailed study of the model magnetic system $(\text{C}_7\text{H}_{10}\text{N})_2\text{CuBr}_4$ was completed on LET thanks to the instrument's ability to allow multiple incident neutron energies to be used simultaneously, together with the ability to use high magnetic fields coupled with mK temperatures (Schmidiger *et al*, Phys Rev Lett 2013).



- Small angle scattering on Sans2D has been used to elucidate the solution structure of immunoglobulin IgG used in drug preparations, enabled by the low background and wide Q range of the instrument (Rayner et al., J. Mol Biology 2013).
- Neutron reflectometry on Inter has been used to study the penetration of colicins into lipid membranes, relevant to anti-bacterial action. This real-time study was enabled by Inter's unique kinetics capabilities (Clifton et al., Biol Chem 2012).
- Polref has been used to look at lubricant additives, to understand the interactions between the various components, with the aim of improving performance from the bottom up (Wood et al., Langmuir 2013).
- The Offspec interferometer has been used to examine the gravitationally induced phase shift when a beam of neutrons is split and recombined (de Haan et al., Phys Rev A 2014).

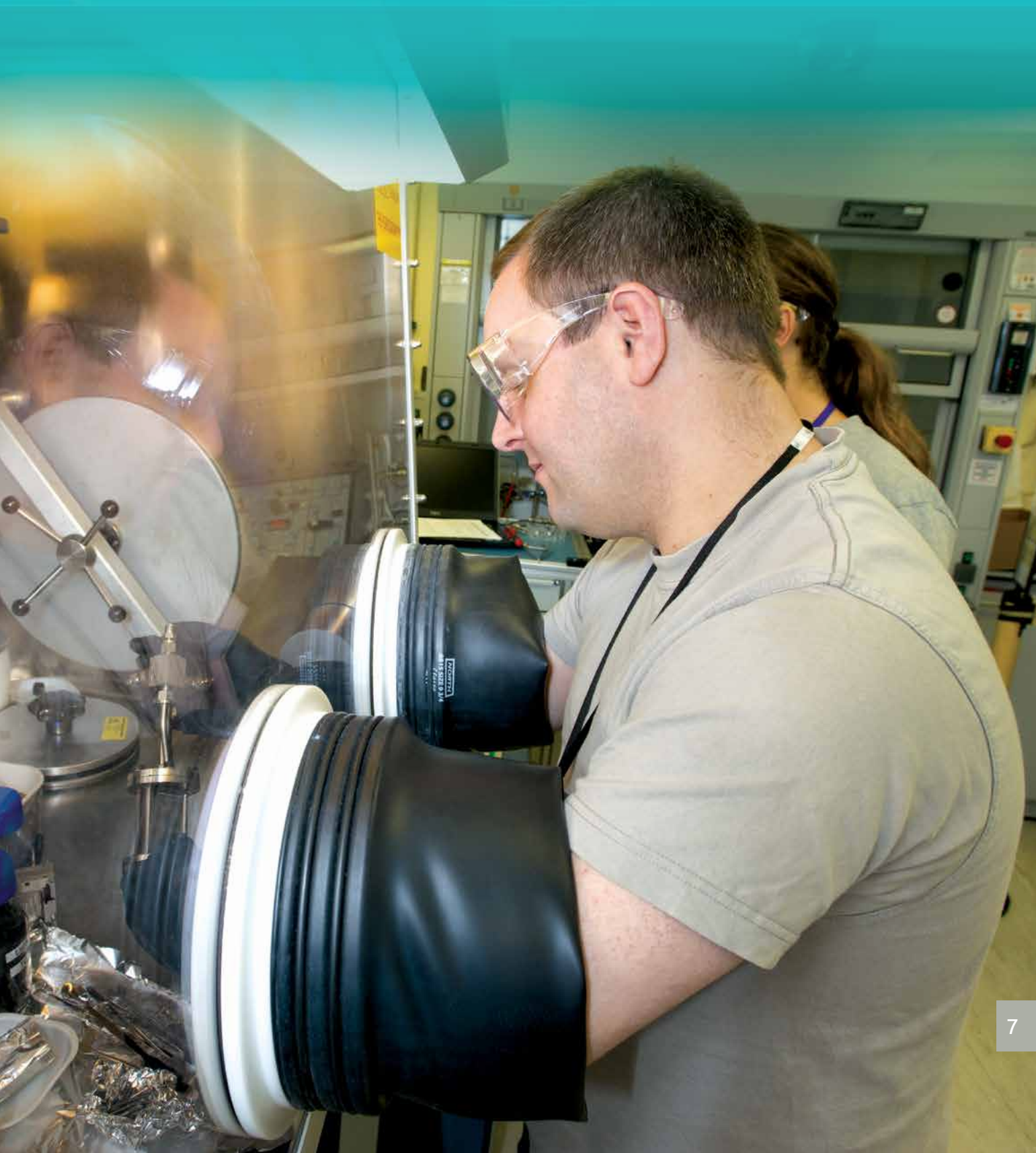


Dr Helen Fraser, Open University, working on NIMROD.



Science

Every year over 400 papers are published based on research at ISIS. These span a wide range of scientific disciplines, from pharmacology, cultural heritage and engineering to fundamental chemistry and magnetism. This section gives a snapshot of ISIS research from some of these areas.



Applied materials

New ruthenium oxides from hydrothermal chemistry

CI Hiley, MR Lees, RI Walton (University of Warwick), JM Fisher, D Thompsett (Johnson Matthey plc), S Agrestini, (Max-Planck Institut CPFS, Dresden), RI Smith (ISIS).

Instrument: GEM **Support:** EPSRC Industrial CASE award with Johnson Matthey plc

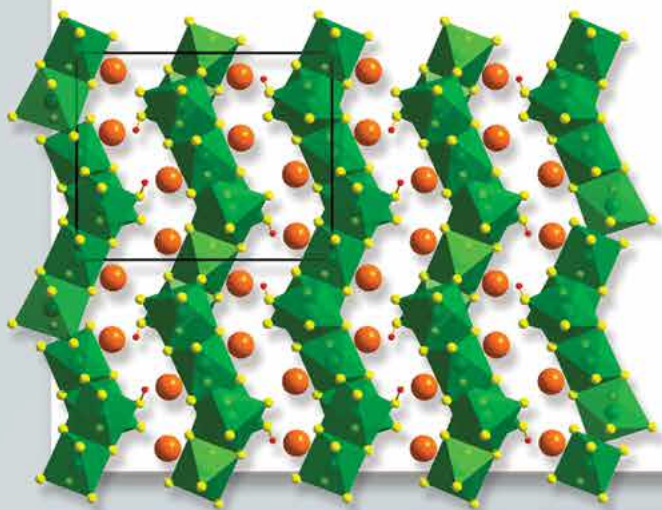
Oxides of the precious metal ruthenium are the focus of fundamental research due to the wider interest in the physics of 4d and 5d metal oxides. Ruthenium oxides are also of use in catalysis, such as electrolytic and oxidation reactions. Synthesis of mixed oxides usually requires high temperatures and, if high oxidation states are required, oxygen pressure

is also needed. In this study, mild, solution-based synthesis (240°C) for crystallising novel oxides has been explored. Three novel materials, all containing ruthenium(V) and each with interesting structural and magnetic properties, have been isolated. $\text{Ca}_{1.5}\text{Ru}_2\text{O}_7$ is a defective pyrochlore; SrRu_2O_6 is a layered material with a PbSb_2O_6 structure, whilst $\text{Ba}_2\text{Ru}_3\text{O}_9(\text{OH})$ has a previously unreported structure type. SrRu_2O_6 is antiferromagnetic with an ordering temperature above room temperature, whilst $\text{Ca}_{1.5}\text{Ru}_2\text{O}_7$ shows evidence for magnetic frustration at low temperatures. For each of the polycrystalline materials neutron diffraction, measured using GEM Xpress, was used to refine their structures, complementing X-ray data, and for SrRu_2O_6 allowing determination of the magnetic structure.

Contact: r.i.walton@warwick.ac.uk

Further Reading: CI Hiley *et al.* *Angew. Chem., Int. Ed.* **53** (2014) 4423-4427.

The puckered, layered structure of the new oxyhydroxide $\text{Ba}_2\text{Ru}_3\text{O}_9(\text{OH})$, with sheets of edge- and corner-shared Ru-centred octahedra (green) and interlayer Ba atoms (orange).



Muons show the pathway and speed of Li diffusion in battery materials

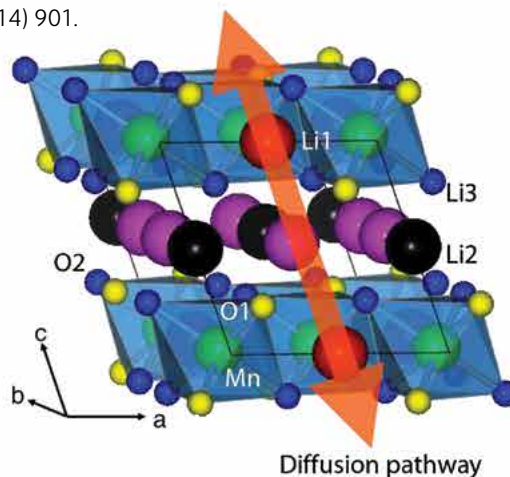
J Sugiyama, H Nozaki, K Mukai, M Harada (Toyota Central Research & Development Labs., Inc), M Månsson (PSI & EPFL), A Hillier (ISIS).

Instrument: Muons **Support:** Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan

For battery materials it is very important to know how ions move in the material, as ions carry charge. In order to obtain such information on a new cathode material, Li_2MnO_3 , muon-spin relaxation ($\mu^+\text{SR}$) measurements with zero applied magnetic field (ZF) and longitudinal-field (LF) were performed at ISIS. The results revealed the presence of a dynamic fluctuation of a nuclear magnetic field due to Li^+ -diffusion. From the muon results, the Li^+ ions were found to diffuse mainly along the c-axis through the Li^+ ion in the $[\text{Li}_{1/3}\text{Mn}_{2/3}]\text{O}_2$ layer. Also, based on the field fluctuation rate, a self-diffusion coefficient of Li^+ ions (D_{Li}) at 300 K was estimated as $4.7(4) \times 10^{-11} \text{ cm}^2\text{s}^{-1}$ with the thermal activation energy $E_a = 0.156(3) \text{ eV}$.

Contact: e0589@mosk.tytlabs.co.jp

Further Reading: J Sugiyama *et al.*, *Solid State Ionics* **262** (2014) 901.

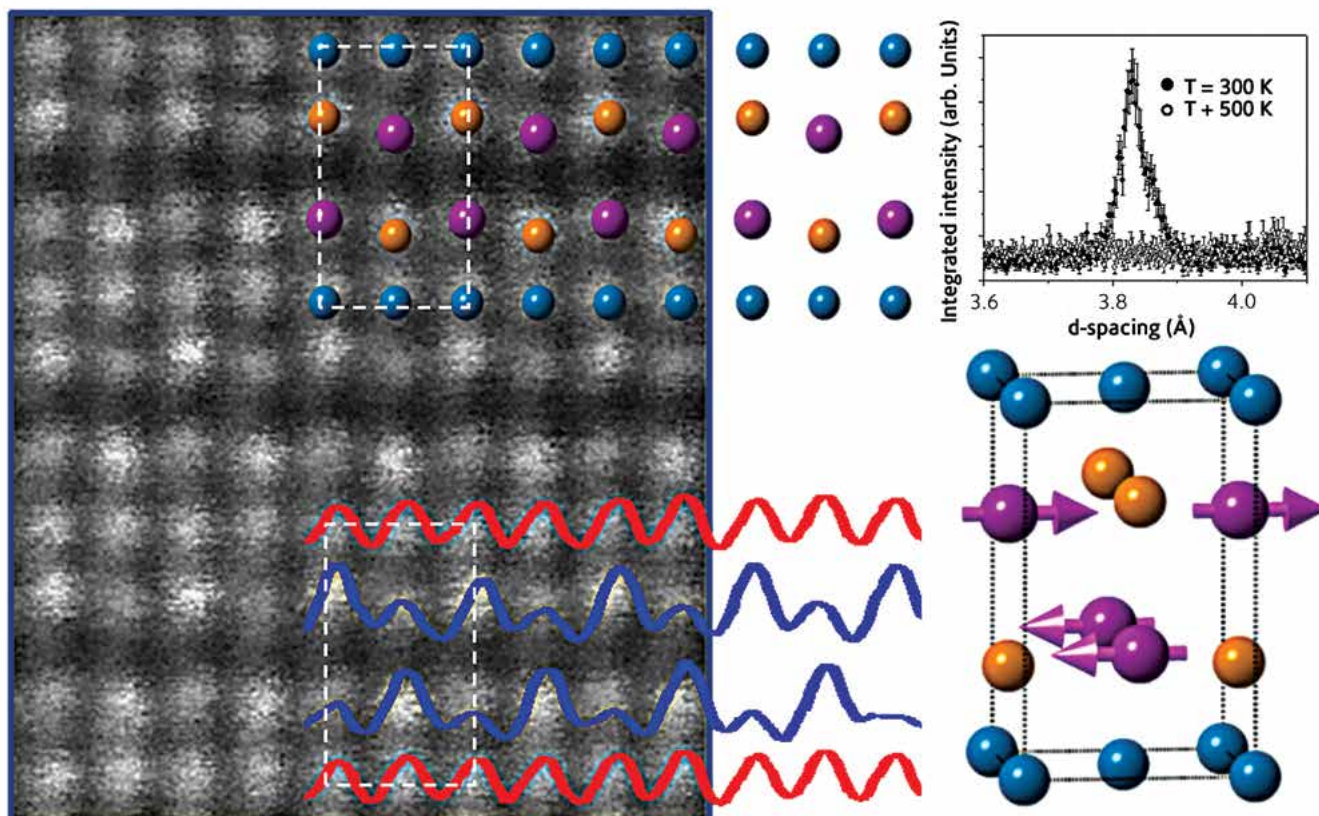


In the crystal lattice of Li_2MnO_3 , the diffusion pathway of Li^+ is deduced along the c-direction (orange arrow) from the $\mu^+\text{SR}$ measurements.

CuMnAs thin films for antiferromagnetic spintronics

P Wadley, K Edmonds (University of Nottingham), D Khalyavin, S Langridge (ISIS).

Instrument: WISH Support: ERC Advanced Grant No. 268066. EPSRC Grant EP/K027808/1



STEM image of the bc plane. (bottom centre) Intensity profiles showing the distinct elemental intensities. (top centre) model of CuMnAs showing perfect agreement (Cu - blue, Mn - purple and As - orange). (lower right) Unit cell of CuMnAs with spin structure. (upper right) Neutron diffraction intensity for the magnetic CuMnAs (100) peak.

The use of ferromagnetic materials for storage and other functionality is widespread in the microelectronics industry, and has been pushed towards its fundamental limits. Possible alternatives to using ferromagnets are compounds with another type of magnetic ordering, called antiferromagnetism, wherein the neighbouring spins point in opposite directions. CuMnAs had never been grown in thin film form but was predicted by theory to be a high temperature antiferromagnet (AF). Thin film AFs are very hard to characterise because they have no net magnetisation and cannot be measured in traditional ways. Here neutron diffraction was used in a prototype experiment

to determine the magnetic ordering and operating temperature (T_N) of CuMnAs thin films. The results show that CuMnAs is indeed an AF with T_N well above room temperature making it a promising candidate for AF microelectronics applications and research.

Contact: Peter.wadley@nottingham.ac.uk

Further Reading: Wadley *et al* Nature Communications, **4** (2013) 2322.

Applied materials

Importance of spin-orbit interaction for the electron spin relaxation in organic semiconductors

L Nuccio (Queen Mary University of London and University of Fribourg), M Willis, RM Wilson, I Hernandez, T Kreouzis, WP Gillin, AJ Drew (Queen Mary University of London), L Schulz, C Bernhard (University of Fribourg), S Fratini (CNRS), F Messina, M D'Amico, M Cannas (University of Palermo), FL Pratt, JS Lord I McKenzie (ISIS), M Loth, B Purushothaman, J Anthony (University of Kentucky), M Heeney (Imperial College London), K Sedlak (PSI).

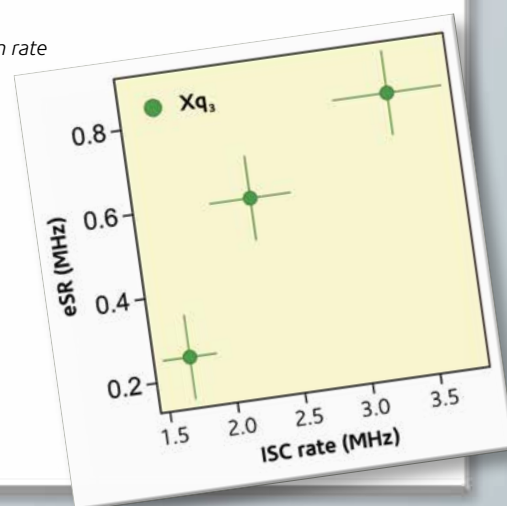
Instrument: Muons **Support:** Leverhulme Trust, EPSRC, SNF, P.O.R Regione Sicilia

Organic semiconductors (OSCs) are promising materials for spintronics due to their very long spin relaxation time. Spin relaxation in the OSC causes a loss of spin polarization, and it has a detrimental effect on spintronic device performance. OSCs are mainly composed of light elements, so the spin-orbit interaction (SOI) was neglected as a possible cause of spin relaxation, while the hyperfine interaction (HFI) was considered a good candidate. In order to differentiate between the SOI and HFI contributions to the spin relaxation, in this study a light atom in the OSC is replaced with heavier ones. This modifies the SOI, which depends on the atomic number whereas the HFI does not. The electron spin relaxation rate in these molecules is measured through μ SR, showing that it depends on the strength of SOI, probed through time-resolved photoluminescence by measuring the exciton singlet to triplet conversion rate. This provides direct evidence of the existence of a sizable SOI-based mechanism for the electron spin relaxation in OSCs.

Contact: laura.nuccio@gmail.com

Further Reading: L Nuccio *et al.*, Phys. Rev. Lett. **110** (2013) 216602.

Electron spin relaxation rate as a function of the intersystem crossing rate, used as a measurement of the strength of SOI, in the $Alq_3/Gaq_3/Inq_3$ series.



Bifurcated polarization rotation in bismuth-based piezoelectrics

DS Keeble (University of Warwick), ER Barney (University of Nottingham), DA Keen (ISIS), MG Tucker (ISIS & Diamond), J Kreisel (CRP Gabriel Lippmann, Luxembourg), PA Thomas (University of Warwick).

Instrument: GEM **Support:** EPSRC & SCRA

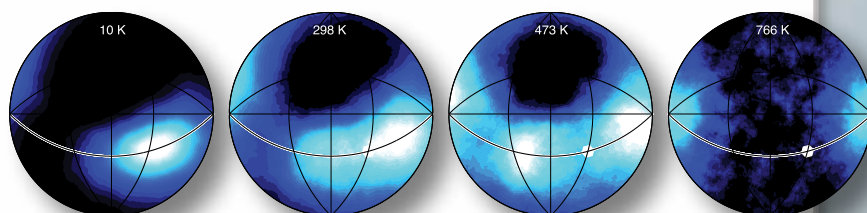
Piezoelectrics are a class of material where the electric and strain fields are coupled; this means a piezoelectric changes shape if you put a voltage across it, and develops a voltage if you squeeze it. In the search for good piezoelectrics (i.e. ones with a strong coupling) that don't rely on toxic lead, sodium bismuth titanate (NBT) is very popular. However, the atomic structure of NBT is understandably rather complex – the sodium and bismuth ions randomly occupy atomic environments which are nominally identical, despite the two ions being physically and electronically different. The authors of this study used neutrons to probe how the overall crystal structure manages to accommodate this disordered lattice of differing ions; how the behaviours of the ions themselves differ; and what influence temperature has on this interaction. It is shown that the bismuth ions dominate what is observed on average, and that as the material is warmed from -260°C to nearly 500°C the bismuth

population splits into two types of off-centering that counter-rotate through a plane.

Contact: dean.keeble@diamond.ac.uk

Further Reading: DS Keeble *et al.*, Adv. Funct. Mater. **23** (2013) 185-190.

Stereographic projections showing the bifurcated polarization rotation in sodium bismuth titanate. Light areas represent common directions of displacement from the local environment.



Suppression of thermal conductivity by rattling modes in thermoelectric sodium cobaltate

DJ Voneshen, E Cemal, S Uthayakumar, DG Porter, JP Goff (Royal Holloway University of London) K Refson (STFC), E Borissenko, M Krisch, A Bosak (ESRF), A Piovano, E Cemal, M Enderle (ILL) Mj Gutmann (ISIS) M Hoesch (Diamond) M Roger (CNRS) L Gannon, AT Boothroyd (University of Oxford).

Instrument: SXD **Support:** EPSRC Grants EP/J011150/1 and EP/J012912/1.

Thermoelectric materials are of great interest due to the global need to reduce energy consumption, such as converting waste heat in car exhausts into electrical power, or cooling hotspots on computer chips using solid-state refrigerators.

This study probes the origin of the thermoelectric effect in sodium cobaltate. Inelastic X-ray and neutron studies are used in conjunction with cutting edge computational modelling to identify low-energy Einstein-like rattling-modes in the phonon structure of sodium cobaltate. These modes involve large anharmonic displacements of sodium ions within multi-vacancy clusters, and suppress the thermal conductivity of the material by a factor of six compared to vacancy-free systems. These results have great impact for the design of thermoelectric materials and the future of power recovery and refrigeration.

Contact: Jon.Goff@rhul.ac.uk

Further Reading: D.J. Voneshen *et al.*, *Nature Materials*, **12**, (2013) 1028-1032.

Cutting energy consumption by utilising waste heat in car exhausts requires an understanding of thermoelectric materials.

Thermally robust anion order in oxynitride materials

L Clark, JP Attfield (University of Edinburgh), J Oró-Solé, A Fuytes (ICMAB-CSIC, Spain), KS Knight (ISIS).

Instrument: HRPD **Support:** EPSRC, STFC and the Royal Society, UK; and MINECO, Spain.

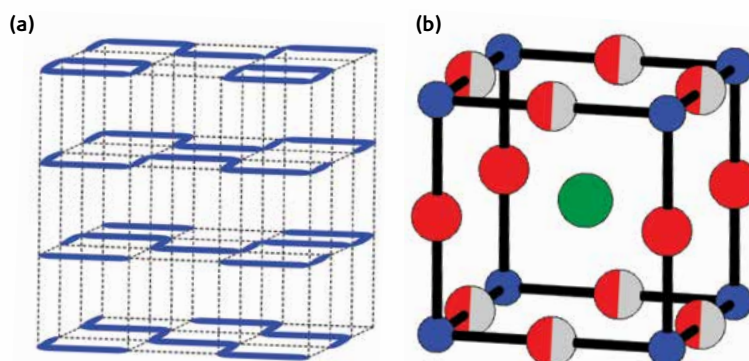
Transition metal oxynitrides such as SrTaO₂N and LaTaON₂ with perovskite-type crystal structures have important optical and electronic applications, including photocatalysis for water splitting, high-permittivity dielectrics, and non-toxic pigments. The issue of whether and how the oxide and nitride anions are ordered has been controversial, but recent studies have revealed a partial order as layers of disordered anion-chains. This study using neutron and electron diffraction has enabled the first full structure refinements of the anion-ordered superstructures of SrTaO₂N and LaTaON₂, giving detailed structural insights into the links between covalency, anion order and octahedral tilting. From high temperature measurements, the anion order is estimated to be stable up to at least 2000°C, far above reported preparation conditions for these materials, revealing a

remarkably robust segregation of the anions into layers of chains when the materials are synthesized.

Contact: j.p.attfield@ed.ac.uk

Further Reading: L Clark *et al.*, *Chem. Mater.*, **25** (2013) 5004.

(a) Anion chains (heavy lines) in layers within oxynitride perovskites. (b) The unit cell seen by neutron diffraction where the half-shaded O_{0.5}N_{0.5} atoms average over the local configurations in (a).



Fundamental *magnetism*

Observation of spontaneous magnon decay in a triangular lattice antiferromagnet

J Oh, MD Le, J Jeong, J-G Park (Seoul National University), J-H Lee, W-Y Song (SungKyunKwan University), H Woo, TG Perring (ISIS), WJL Buyers (Chalk River Laboratories), SW Cheong (Rutgers University)

Instrument: MAPS **Support:** Institute for Basic Science (Korea), National Research Foundation of Korea, US Department of Energy.

Just as the vibrations of atoms in a solid become quantised as phonons, the analogous spin excitations are magnons, and both are considered to be particles with definite energy and momentum. Nonetheless, the expected magnon-magnon interactions should lead to quasiparticle decay, so it was a puzzle since early research in the 1970s that magnons appear to be extraordinarily stable, in that no decay of one magnon into (for example) two was observed. It was subsequently determined that this is because the collinear nature of most magnetic order forbids, by symmetry, the third order interaction required for magnon decay. LuMnO_3 , in contrast, has a non-collinear spin arrangement, so that this term is allowed,

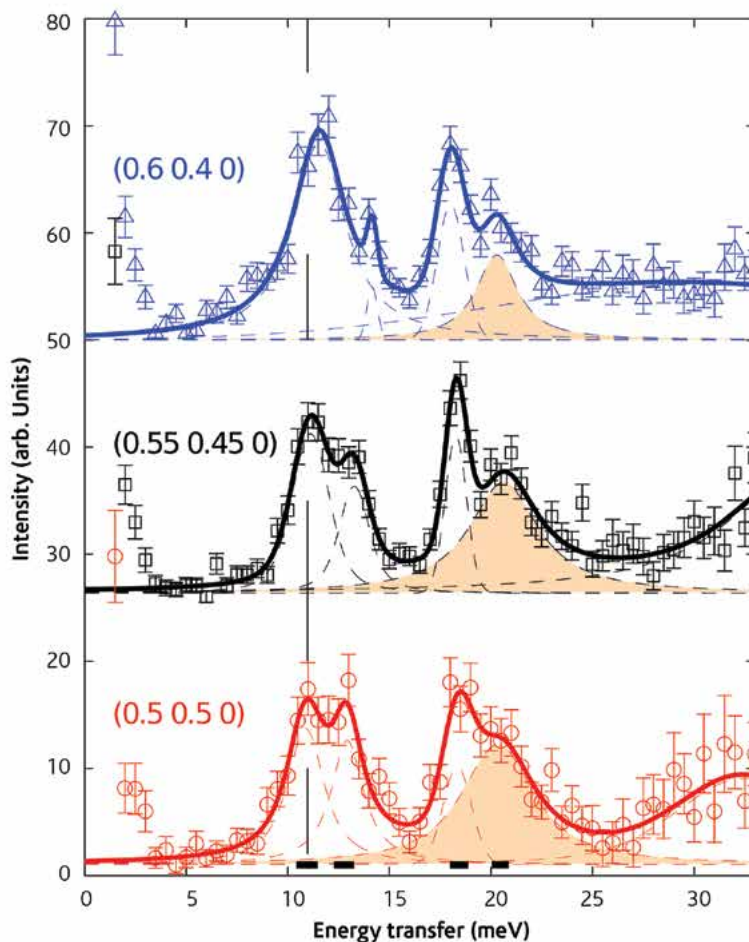
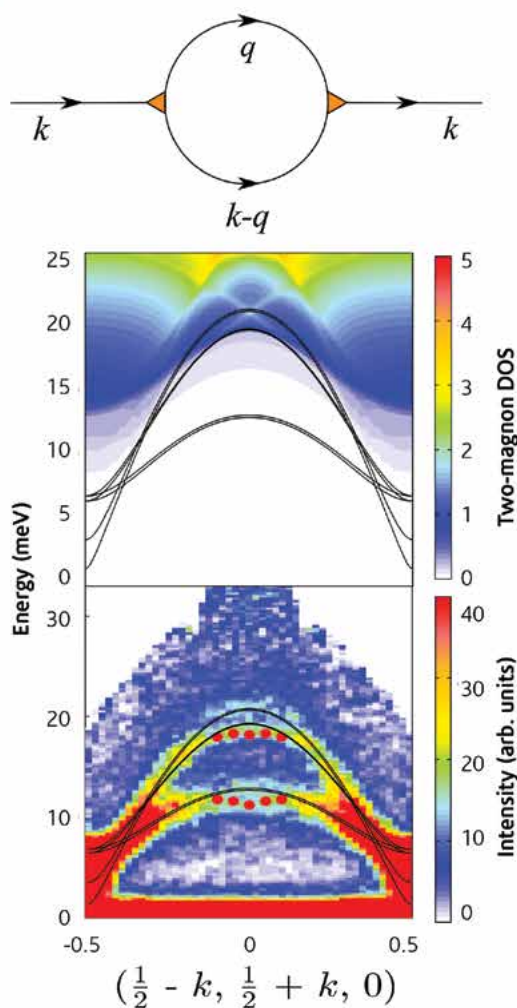
permitting for the first time measurement of the full spectrum of magnon decay in a 2D magnet. The key signatures are the q-dependent renormalization and the broadening of the inelastic neutron scattering line width at high energies only in parts of the Brillouin zone.

Contact: jgpark10@snu.ac.kr

Further Reading: J Oh *et al.*, Phys. Rev. Lett.

111 (2013) 257202.

Schematic diagram of magnon decay and inelastic neutron scattering data showing line width broadening near where the 1-magnon dispersion crosses the 2-magnon continuum attributed to magnon decay.



When is a ferroelectric not a ferroelectric?

Y Shi (National Institute for Materials Science, Japan), Y Guo (University of Oxford), X Wang (National Institute for Materials Science, Japan), AJ Princep (University of Oxford), D Khalyavin, P Manuel (ISIS), Y Michiue, A Sato (National Institute for Materials Science, Japan), K Tsuda (Tohoku University, Japan), S Yu, M Arai (National Institute for Materials Science, Japan), Y Shirako, M Akaogi (Gakushuin University, Japan), N Wang (Institute of Physics, Beijing), K Yamaura (National Institute for Materials Science, Japan), AT Boothroyd (University of Oxford).

Instrument: WISH **Support:** EPSRC grants EP/J017124/1 and EP/J012912/1

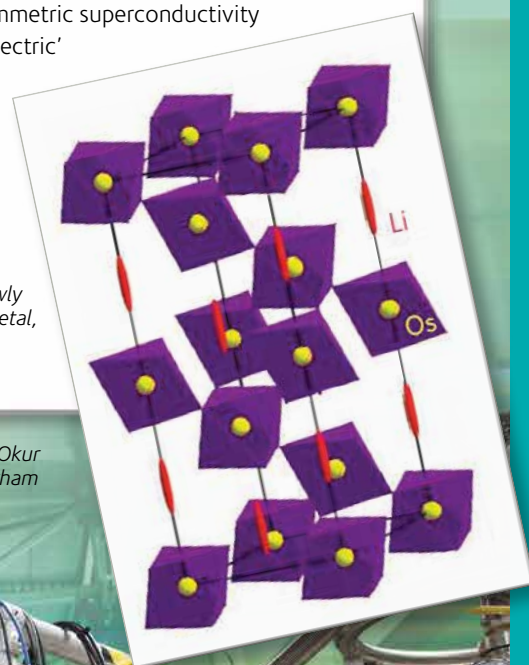
Ferroelectrics are insulating materials having an electrical polarisation that can be switched by an applied voltage. Ferroelectricity cannot occur in metals because it would be screened by the conduction electrons. In this work a new material, lithium osmate (LiOsO_3), is detailed that remains a metal down to the lowest temperatures and yet undergoes a structural phase transition identical to that in the well-known ferroelectrics LiNbO_3 and LiTaO_3 . Neutron diffraction on WISH showed that the phase transition in LiOsO_3 is characterised by a large shift in the position of the Li ions, a structural effect known to cause ferroelectricity in LiNbO_3 and LiTaO_3 . The discovery represents the first example of a so-called 'ferroelectric metal', a concept first postulated over 50 years ago by Nobel prize-winner Philip Anderson

and co-worker Eugene Blount, and establishes a new class of materials which could have interesting properties, possibility including non-centrosymmetric superconductivity stabilised by the 'ferroelectric' structural instability.

Contact: a.boothroyd@physics.ox.ac.uk

Further Reading: Y. Shi *et al.*, *Nature Materials* **12** (2013) 1024.

Crystal Structure of the newly discovered 'ferroelectric' metal, LiOsO_3 .



l to r; Ross Colman, Esma Okur and Hiroyuki Okazaki, Durham University, on HIFI.



Fundamental *magnetism*

Exotic magnetism on the quasi-FCC lattices of the double perovskites La_2NaTO_6 ($T = \text{Ru, Os}$)

AA Aczel (ORNL, USA), PJ Baker, T Guidi, DT Adroja (ISIS), DE Bugaris, J Yeon, H-C zur Loye (University of South Carolina, USA).

Instruments: Merlin and LET **Support:** US Department of Energy, Office of Basic Energy Sciences

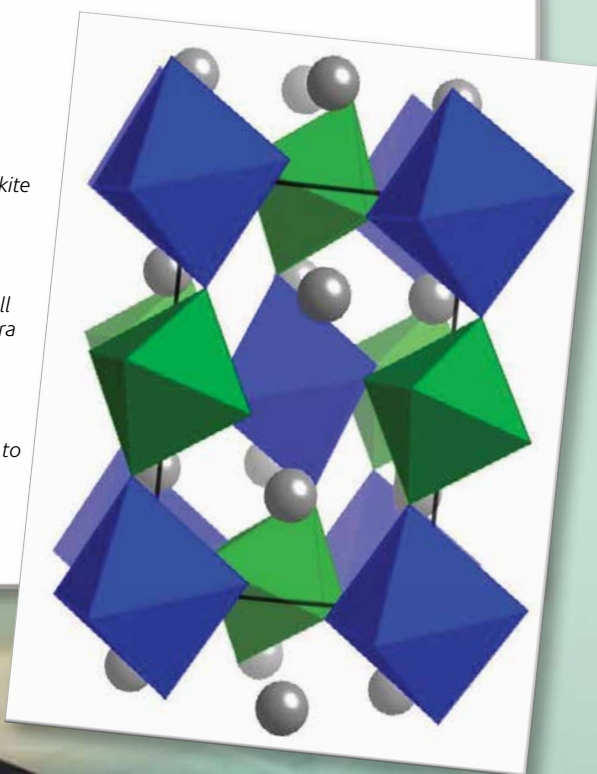
Many interesting properties have been revealed in studies of 3d transition metal oxides, including superconductivity and colossal magnetoresistance, but comparatively little work has been done on 4d and 5d transition metal oxides. In this study, neutron scattering and muon spin relaxation are used to investigate the magnetism of the 4d/5d double perovskites La_2NaTO_6 ($T = \text{Ru, Os}$). Incommensurate magnetic order is revealed on the face-centered-cubic (FCC) Ru/Os magnetic sublattices. This has not been predicted theoretically, but may arise via a delicate balance of exchange interactions. In the Ru system, inelastic neutron scattering also reveals a sizable spin gap in the magnetic excitation spectrum. Magnetic anisotropy is generally minimized in the more familiar octahedrally-coordinated 3d³ systems, so the large gap observed for $\text{La}_2\text{NaRuO}_6$ may result from the significantly enhanced value of spin-orbit coupling in this 4d³ material. These findings suggest that the magnetism in 4d and 5d transition metal oxides may be quite different from their 3d counterparts.

Contact: aczelaa@ornl.gov

Further Reading: AA Aczel et al, Phys. Rev. Lett.

112 (2014) 117603

Double perovskite structure, with the large blue octahedra representing NaO_6 , the small green octahedra depicting $(\text{Ru,Os})\text{O}_6$, and the isolated grey spheres corresponding to La atoms.



Tim Stevenson, left, and Omar Matar, University of Leeds, on POLARIS.

Doping dependence of spin excitations in iron pnictides superconductors

M Wang, X. Lu, H. Luo, X Zhang (Institute of Physics, Beijing, China), C Zhang, G Tan, Y Song, M Wang (Rice University, USA), EA Goremychkin, TG Perring (ISIS), TA Maier (Oak Ridge National Laboratory), Z Yin, K Haule, G Kotliar (Rutgers University), P Dai (Rice University, USA).

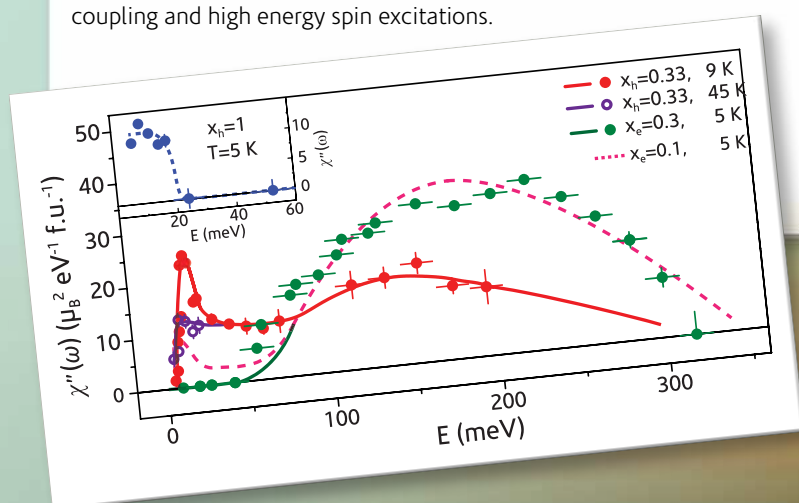
Instruments: MAPS and Merlin **Support:** Ministry of Science and Technology of China 973 programs, US Dept of Energy

In conventional Bardeen-Cooper-Schrieffer (BCS) superconductors, superconductivity occurs when electrons form coherent Cooper pairs below the superconducting transition temperature T_c . Although the kinetic energy of paired electrons increases in the superconducting state relative to the normal state, the reduction in the ion lattice energy is sufficient to give the superconducting condensation energy. For iron pnictide superconductors derived from electron or hole doping of their antiferromagnetic (AF) parent compounds, the microscopic origin for superconductivity is unclear. Here neutron scattering is used to show that high- T_c superconductivity only occurs for iron pnictides with low-energy itinerant electron-spin excitation coupling and high energy spin excitations.

Since these absolute spin susceptibility measurements for optimally hole-doped iron pnictide reveal that the change in magnetic exchange energy below and above T_c can account for the superconducting condensation energy, it is concluded that the presence of both high-energy spin excitations giving rise to a large magnetic exchange coupling J and low-energy spin excitations coupled to the itinerant electrons is essential for high- T_c superconductivity in iron pnictides.

Contact: pdai@rice.edu

Further Reading: Meng Wang *et al.*, Nat. Comm. **4** (2013) 2874.



Energy dependence of dynamic susceptibility for $Ba_{1-xh}K_{xh}Fe_2As_2$ and $BaFe_{2-xe}Ni_{xe}As_2$ integrated in a Brillouin zone.

Felicity Dear, University College London, on OSIRIS.

Carbon

Hydrogen storage study of nickel-decorated graphene by means of muon spin relaxation

M Gaboardi, M Aramini, G Vlahopoulou, D Pontiroli, G Magnani and M Riccò (University of Parma, Italy), A Bliersbach, P Mauron, A Züttel (Empa, Dübendorf, Switzerland), G Bertoni, G Salviati (IMEM-CNR, Parma, Italy).

Instrument: EMU **Support:** SNSF "HyCarBo" project (Grant no. CRSII2-130509)

Graphene is potentially an ideal hydrogen storage system, thanks to its huge specific surface area (2630 m²/g) and potential ability to chemisorb up to 7.7 mass% H₂. Unfortunately, the high energy needed to dissociate the

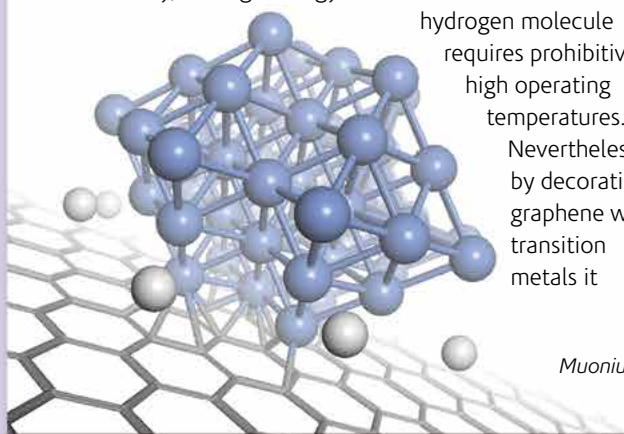
hydrogen molecule requires prohibitively high operating temperatures.

Nevertheless, by decorating graphene with transition metals it

is possible to catalyse H₂ dissociation at more moderate temperatures. Muons can probe atomic hydrogen interaction with graphene through the analysis of the spin evolution of muonium atom (μ^+e^-), a light hydrogen isotope. When graphene is decorated with nickel, a large fraction of muonium is captured to form C-Mu groups. The local modification of graphene around the nickel nanoparticle induces a larger affinity to hydrogen (muonium) with respect to the unperturbed plane, and the overall hydrogen chemisorption is enhanced.

Contact: mattiagianandrea.gaboardi@fis.unipr.it

Further Reading: M. Gaboardi *et al.*, *J. Mater. Chem. A* **2** (2014) 1039.



Muonium (white balls) is captured on graphene planes near nickel nanoparticles (blue).

Environmentally friendly cement is stronger than ordinary cement

J Jacobsen (The Niels Bohr Institute and ESS), MS Rodrigues (UNICAMP), MTF Telling (ISIS), AL Beraldo (UNICAMP), SF Santos (USP), LP Aldridge (ANSTO and Monash University) and HN Bordallo (The Niels Bohr Institute and ESS).

Instrument: IRIS **Support:** The Niels Bohr Institute, the European Spallation Source AB, CNPq-Brazil, Grant #2009/17293-5 and Grant#2010/16524-0, São Paulo Research Foundation (FAPESP).

The manufacture of Portland cement accounts for roughly 5% of all human-generated greenhouse-gas emissions. To reduce this effect, binder materials containing amorphous fine-grained silicates, an effective method of improving concrete durability, are replacing cement during concrete production. The resulting material is referred to as 'green

cement'. Sugar cane straw ash, originating from agricultural waste, is one of these new binders. Quasi-elastic neutron scattering demonstrates that the improved durability of green cement is directly linked to the nano-scale details of the pore structure. Concrete performance is critically related to the structure of the cement paste blocking water ingress, and results clearly indicate that it is the increased confinement of water due to the formation of a specific hydrogen bond network, rather than pore blocking, that drives the improved durability of concretes manufactured using binder materials. These results prompt further developments and applications of this work to both reduce greenhouse-gas emissions as well as to produce more durable concrete.

Contact: bordallo@nbi.ku.dk

Further Reading: J Jacobsen *et al.*, *Sci. Rep.* **3** (2010) 2667.

Sugar cane substitution in cement reduces greenhouse-gas.

The use of SANS in the study of radiation damage in nuclear graphites

Z Mileeva, DK Ross (University of Salford), SM King (ISIS).

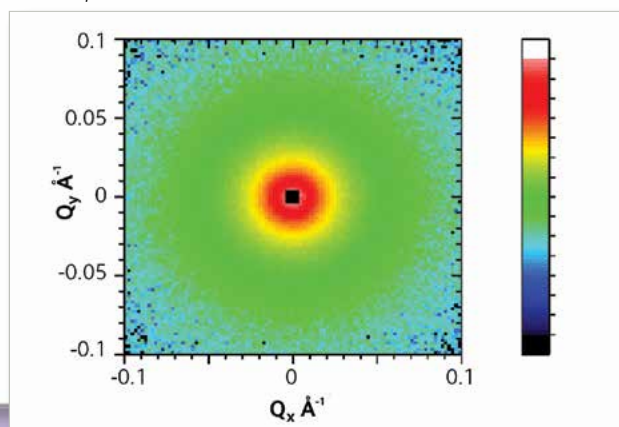
Instrument: SANS **Support:** EPSRC through consortium grant (EP/1003223/1).

The UK electricity supply depends on AGR reactors operating well beyond their original design life. This demands a high integrity graphite moderator which depends on the porosity of the graphite and this is a function of neutron dose. Small Angle Neutron Scattering (SANS) examines porosity on a length scale from ~ 0.5 to ~ 50 nm. Three important results have been obtained in this work: a) the pores have a fractal nature a) the pores have a fractal nature (a non-integer power law distribution over several orders of magnitude); b) saturating the graphite with a contrast-matching liquid shows that 65% of the porosity is accessible from the surface of the sample; c) The SANS decreases linearly with temperature (at all Q) when measured up to 2000°C – suggesting complete disappearance by around 3000°C . This confirms that the pores are Mrozowski cracks, created by the shrinkage of the graphite in the direction normal to the graphene sheets when cooled during production.

Contact: d.k.ross@salford.ac.uk

Further Reading: Z.Mileeva, D.K.Ross and S.M. King, Carbon **64** (2013) 20-26.

Contour plot of SANS from Gilsocarbon slab heated to 2000°C .



Probing the evolution and morphology of hard carbon spheres

VG Pol, CK Lin, J Wen, KC Lau, LA Curtiss, DJ Miller, SA Deshmukh, Sankaranarayanan, MM Thackeray (Argonne), S Callear, DT Bowron, WIF David (ISIS).

Instrument: Nimrod

The properties of carbon materials depend on their structure on the nanometre scale, which in turn depends on how the material was formed. In the case of heating plastic bags to very high temperatures, the challenge is to understand how the chain-like molecules of polyethylene evolve into hard carbon spheres with a hardness approaching that of diamond. Understanding this process helps to tailor the properties of the carbon end product for a particular technological application, such as carbon electrodes in lithium-ion batteries.

The researchers in this study used X-ray diffraction to monitor the evolution of polyethylene, and neutron diffraction at ISIS to determine the nm scale internal structure of the carbon spheres. They found that the polyethylene starts to decompose at around 105°C . The hydrocarbon product remains molten until about 500°C , when it rapidly decomposes, accompanied by a sharp increase in pressure. On cooling, the spheres form abruptly at about 350°C . Neutron diffraction showed that on the nm scale the carbon adopts a predominantly

layered structure. Heating the carbon spheres to 2800°C increases the carbon (graphitic) layering which improves their electrochemical properties.

Contact: thackeray@anl.gov

Further Reading: V.G. Pol *et al.*, Carbon **68** (2014) 104-111.

Waste carrier bags could help improve batteries.



Pharmaceuticals

Polymorphism in cisplatin anticancer drug

MPM Marques, R Valero (University of Coimbra, Portugal), SF Parker, J Tomkinson (ISIS) and LAE Batista de Carvalho (University of Coimbra, Portugal).

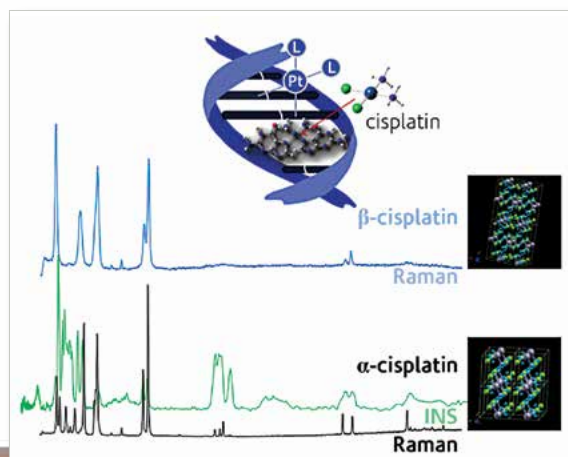
Instrument: Tosca **Support:** Portuguese Foundation for Science and Technology– PEst-OE/QUI/UI0070/2011, European Commission under the 7th Framework Programme through the Key Action: Strengthening the European Research Area, Research Infrastructures – Contract n°: CP-CSA_INFRA-2008-1.1.1 Number 226507-NMI3.

Cisplatin ($\text{cis}-(\text{NH}_3)_2\text{PtCl}_2$) is one of the most widely used anticancer agents, particularly towards testicular, head and neck tumours. Polymorphism, the ability to exist in more than one crystal form, is a key issue in pharmaceutical science since equilibrium between distinct polymorphs may affect the drug's properties and therapeutic effect. Cisplatin's polymorphic equilibrium between the two known alpha and beta species was elucidated by simultaneous Raman and INS spectroscopies, coupled to theoretical approaches. Alpha is predominant at very low temperatures (below ca. -170°C), while beta occurs at room temperature and higher. Both species coexist at intermediate temperatures, their relative population depending on the sample's history and follows a marked hysteresis. Simultaneous INS and Raman experiments, under exactly the same conditions, allowed a clear picture of cisplatin's polymorphic behaviour to be attained. Elucidation of the polymorphic equilibrium of this extensively used chemotherapy drug is paramount for optimising its pharmaceutical preparation, as well as transport and storage conditions.

Contact: pmc@ci.uc.pt

Further Reading: MPM Marques *et al.*, *J.Phys.Chem. B* **117** (2013) 6421.

Alpha and beta cisplatin polymorphs (INS and Raman spectra) and cisplatin-DNA interaction.



Tumours and time of flight: a promising bio-nanocomposite for the treatment of breast cancer

ML Martins (University of Copenhagen), MJ Saeki (UNESP), MTF Telling (ISIS), JPRL Parra (UNESP), RI Smith (ISIS), HN Bordallo (University of Copenhagen).

Instrument: Polaris **Support:** CAPES, FAPESP, DanScatt and the Science Without Borders

Breast cancer is the most common cancer in women in the UK. It tends to spread to different parts of the body, in particular the bones. By developing a bio-nanocomposite – formed by first encapsulating magnetic nanoparticles in a polymeric shell and then impregnating the surface with apatite nanocrystals (a main component of bone tissue) – this affinity can be used to fight the disease. Antitumour drugs can be further incorporated onto the carrier. The benefit of this magnetic

delivery technique is that the drug carrier can be guided directly to the breast cancer site by external magnetic fields. It will then bind to tumour cells alone, due to apatite inclusions, leading to increased uptake of the drug at the target site, with reduced side effects. The properties of this magnetic nanoparticle-based targeting system, such as particle size and amount of apatite modification, can all be probed using neutron techniques, the results of which will lead to further device optimisation and, ultimately, more efficient drug delivery.

Contact: bordallo@nbi.ku.dk

Further Reading: Martins, M.L. *et al.*, *Journal of Alloys and Compounds* **584** (2014) 514–519.

Penicillin's auto-catalytic self-activation

Z Mucsi (University of Toronto), GA Chass (Queen Mary University of London), P Ábrányi-Balogh (University of Szeged), B Jójárt (University of Szeged), DC Fang (Beijing Normal University), AJ Ramirez-Cuesta (ISIS), B Viskolcz (University of Szeged) and IG Cszimadia (University of Toronto).

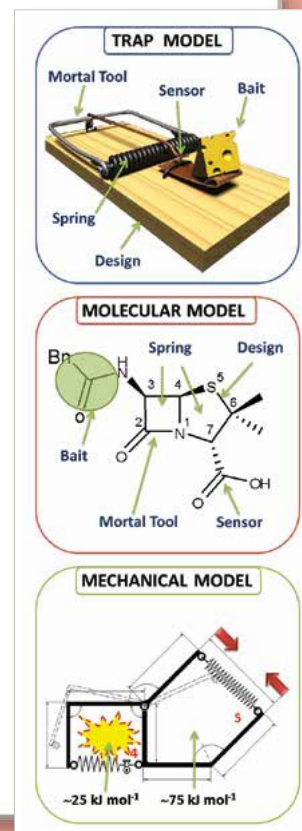
Instrument: Tosca **Support:** EPSRC, UK (EP/H030077/1 & EP/H030077/2), Royal Society, UK (IE120096), National Natural Science Foundation of China (21073016), TÁMOP-4.2.2.A-11/1/ KONV-2012-0047, Hungary

Although penicillin is recognised as one of the great discoveries of the 2nd millennium, the appearance of resistant bacteria has significantly reduced its utility and viability. Continued characterisation of its structure and mechanism aids in the understanding and design of novel antibiotics with desired effects and great precision. Since its discovery by Fleming in 1928 and subsequent mass production, it has remained a mystery as to how penicillin escapes the body's hydrolytic effects, while maintaining its ability to hone-in on and disable the bacterial transpeptidase enzyme, efficiently blocking cell wall synthesis. To resolve this ability to switch from a non-active to a highly-reactive form, the dynamic structure-activity relationship of penicillin has been investigated by inelastic neutron spectroscopy, reaction kinetics, NMR and multi-scale theoretical modeling (QM/MM, DFT and post-HF ab initio). Results show that by a self-activating physiological pH-dependent two-step proton-mediated process, penicillin changes geometry to activate its irreversibly reactive acylation,

facilitated by systemic intramolecular energy management and cooperative vibrations. This dynamic mechanism is confirmed by the 1st characterisation of a natural antibiotic by neutrons.

Contact: g.chass@qmul.ac.uk
Further Reading: Z Mucsi, *et al.*, *Phys. Chem. Chem. Phys.*, **15** (2013) 20447-20455.

Trap composed of bait (to entice prey), sensor (detect prey), spring (energy reservoir) and mortal tool (kill prey). Components and systemic aspects are analogously reflected in penicillin's molecular structure.



Construction and physiochemical characterisation of a multi-composite, potential oral vaccine delivery system (VDS)

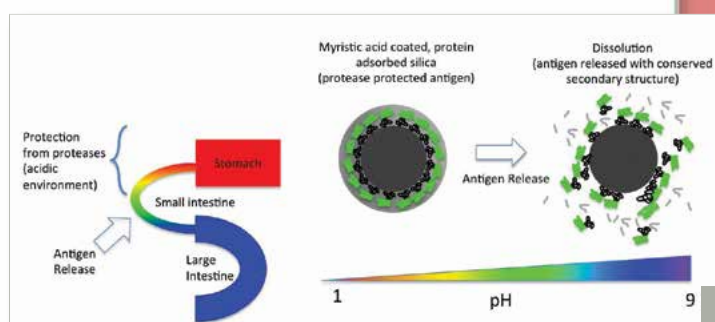
MW Pettit, PDR Dyer, PC Griffiths, F Pullen, B Alexander, B Cattoz (University of Greenwich), RK Heenan, SM King, (ISIS), UKR Schweins (Institut Laue - Langevin), SR Wicks, JC Mitchell, SCW Richardson (University of Greenwich).

Instruments: Sandals and LOQ **Support:** University of Greenwich and STFC

This prize-winning, interdisciplinary research highlights small angle neutron scattering studies undertaken at ISIS, characterising a potential oral vaccine delivery system. This system was initially proposed for use in livestock, impacting upon food security. Through careful design, there exists the potential for this technology to also translate into an oral vaccination system for people. This technology has the capacity to make an impact through the application of synthetic biology, that is, designing antigens that can be delivered to different compartments within the body, with world-class analytics (such as neutron scattering). This high degree of analytical precision helps tell us, at the nano-scale, if what we have made is what we think it is, a process critical for success! Surprisingly, the protein stabilisation involved in the vaccine delivery system may also have the capacity to reduce the cost of vaccination, as it may help negate the need for vaccines to be stored and shipped at ultra-low temperatures.

Contact: S.C.W.Richardson@Greenwich.ac.uk
Further Reading: Pettit *et al.*, *International Journal of Pharmaceutics* **468** (2014) 264–271.

Myristic acid coated, antigen-adsorbed silica was stable at low pH (i.e. in the stomach). At a higher pH the antigen was released (distal to the stomach).



Water

Water acts as an aid in nucleating protein folding in solution.

S Busch (University of Oxford), CD Bruce (Erskine College, USA), CD Lorenz (King's College London), and SE McLain (Oxford).

Instrument: Sandals **Support:** EPSRC Fellowship grant

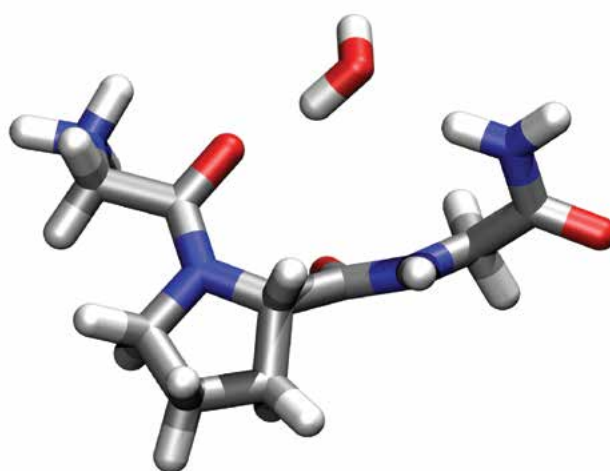
In nature, protein folding is not a random process, yet how a given peptide sequence is transformed into its functional macromolecular structure remains unknown, particularly with respect to the role that water plays in this process. Using a combination of neutron diffraction with isotopic substitution in conjunction with EPSR modelling, NMR and MD, the structural interactions between the glycine-proline-glycine (GPG) peptide in water have been assessed.

Contrary to the 'hydrophobic' model of protein folding in water, for GPG in solution, hydrogen-bonding interactions appear to be the primary driving force in inducing this common β -turn sequence to fold. Specifically the results from this combined study suggest that water is mediating the interaction between the ends of the peptide, nucleating the turn in solution. The results suggest that in solution it is highly likely that hydrophilic forces are just as important in driving protein folding as the hydrophobic effect, especially for the initiation of this process in vivo.

Contact: sylvia.mclain@bioch.ox.ac.uk

Further Reading: S. Busch et al. *Angew. Chem.*, **52** (2013) 13091-13095. S. Busch et al., *PCCP*, **15** (2013) 21023-21033.

Structure of the GPG peptide in solution, showing a water-mediated peptide folding interaction (taken from the MD trajectory)



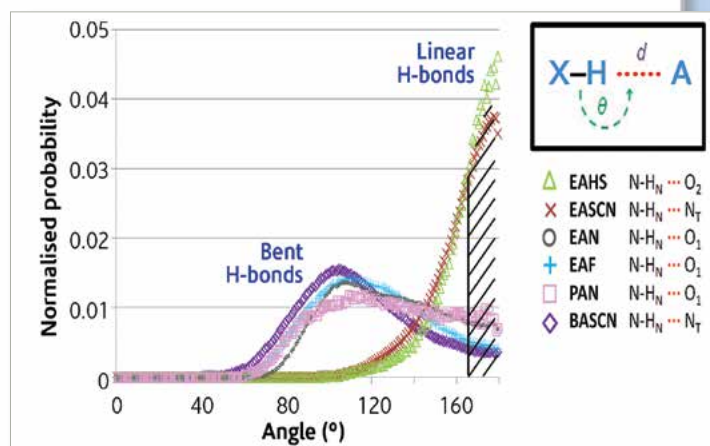
The nature of hydrogen bonding in protic ionic liquids.

R Hayes (University of Newcastle, Australia), S Imberti (ISIS), GG Warr (University of Sydney, Australia), R Atkin (University of Newcastle, Australia).

Instrument: Sandals **Support:** Australian Research Council Discovery Projects and Australian Research Council Future Fellowship for RA.

The nature of hydrogen (H-) bonding in a range of protic ionic liquids (PILs) has been determined through model fitting to neutron diffraction data. Despite their pure ionic composition, H-bonds are a hallmark of all PILs as ions are formed due to proton transfer from a Brønsted acid to a Brønsted base. Strikingly, this study shows that a significant proportion of H-bonds in all the PILs are bent (angles $< 165^\circ$) but that the directionality of the H-bonds formed can be tuned via variation in ion structure. Moreover, a clear relationship between H-bond strength and macroscopic physical properties is evident in the data. It is demonstrated that weak H-bonds (longer $> 2.0 \text{ \AA}$, bent $X-H \cdots Y$ angle) fluidize PILs whilst strong H-bonds (shorter $< 2.0 \text{ \AA}$, linear $X-H \cdots Y$ angle) impart more solid-like properties. These findings enable us to suggest design rules for PIL solvent selection by tailoring the degree of H-bonding in the bulk.

Protic ionic liquid nanostructure controls the H-bond strength and structure by dictating the relative orientations of the cations and anions to each other.



Contact: rob.atkin@newcastle.edu.au

Further Reading: Hayes, R.; Imberti, S.; Warr, G. G.; Atkin, R. *Angewandte Chemie*, **52** (2013) 4623.

The structures of salicylate surfactants with long alkyl chains in non-aqueous media

CL Lee, SS Lam, AF Routh (University of Cambridge), PJ Dowding, AR Doyle, KM Bakker (Infineum UK Ltd), SE Rogers (ISIS).

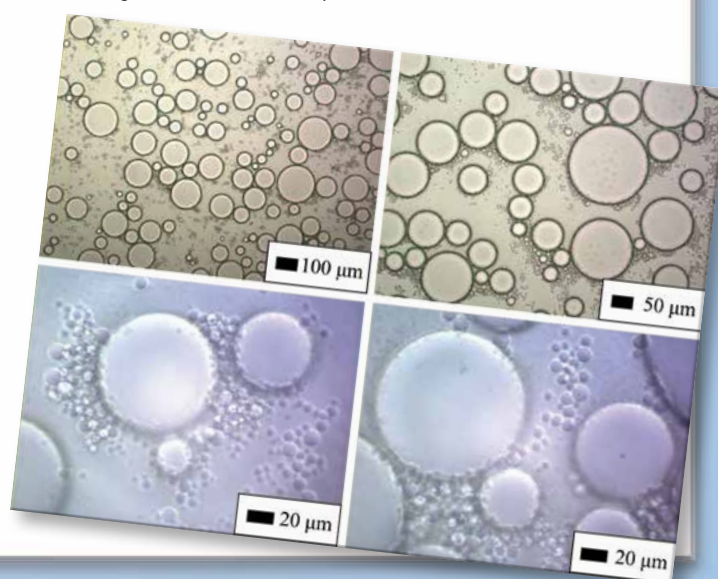
Instrument: SANS **Support:** Dorothy Hodgkins Trust and Infineum UK Ltd

Alkyl salicylate surfactants are commonly used to stabilise metal carbonate nano-particles in engine oil formulations. Colloidal stability of these surfactants, in the harsh environment of an engine, is crucial and this study investigates the effect of moisture. These surfactants form a variety of self-assembled structures in organic media. The structure is dependent on the presence or lack of water, as well as the oil type and surfactant head-group counterions. On length scales of tens of nanometers, SANS measurements show that the counterions with the smallest solvated ion size (sodium, potassium) form spherical micelles and the larger counterions (calcium, magnesium) form cylindrical shaped micelles. On length scales of a few microns, optical microscopy shows a range of multiple emulsions forming with bi-disperse emulsion droplets forming in the calcium salicylate system.

Contact: afr10@cam.ac.uk

Further Reading: CL Lee *et al*, *Langmuir*, **29** (2013) 14763–14771.

5 wt % calcium salicylate surfactant in dodecane with 50 μL of water added to 3g of solution after 1 day.



Competing quantum effects on the melting of water

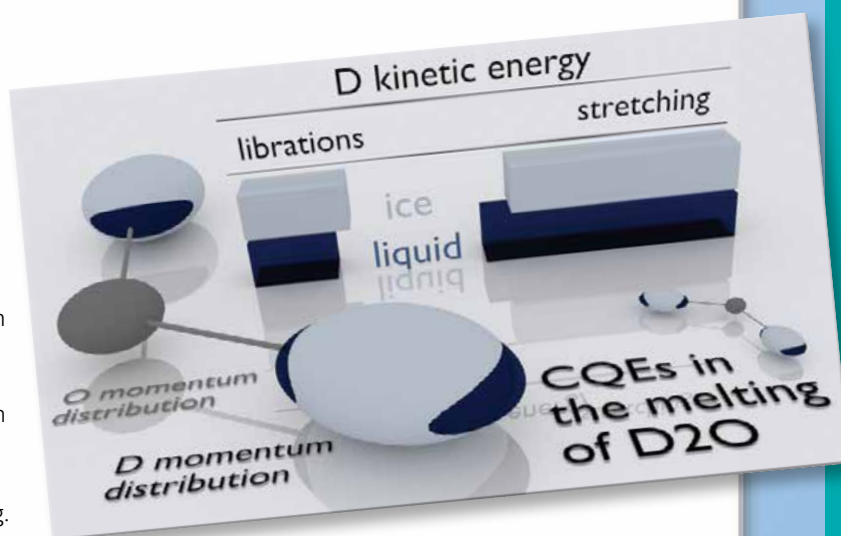
G Romanelli (Università di Roma Tor Vergata), M Ceriotti (Ecole Polytechnique Fédérale de Lausanne), DE Manolopoulos (University of Oxford), C Pantalei (CEA, Saclay), R Senesi (Università di Roma Tor Vergata), C Andreani (Università di Roma Tor Vergata).

Instrument: Vesuvio **Support:** CNR-STFC Agreement No. 06/20018 concerning collaboration in scientific research at the spallation neutron source ISIS

It is well known that liquid and solid water have different structure and density. Moreover, in the two phases, atoms in the water molecule have different dynamics, resulting in a measurable change in particle kinetic energy. In this work the kinetic energies and momentum distributions of all atoms in D_2O liquid and ice have been measured and resolved along different molecular axes using the VESUVIO spectrometer. This study was supported by ab-initio path integral simulations and shows that changes associated with stretching and vibrational motion are of opposite sign. This finding provides evidence of ‘competing’ quantum effects, giving a partial cancellation in the changes in the total mean kinetic energy. Thus the rearrangement of atoms in the solid liquid transition is accompanied by a peculiar interplay between quantum zero-point motion and hydrogen-bonding.

Contact: giovanni.romanelli@uniroma2.it

Further Reading: Giovanni Romanelli, *et al*. *The Journal of Physical Chemistry Letters*, **4** (2013) 3251–3256.



Competing quantum effects: directional components of kinetic energy change with opposite signs during the melting of heavy water.



Technology

Cutting-edge science at ISIS is underpinned by cutting-edge technology. ISIS has an ongoing programme of development on the machine and instruments, extending capabilities and improving performance.



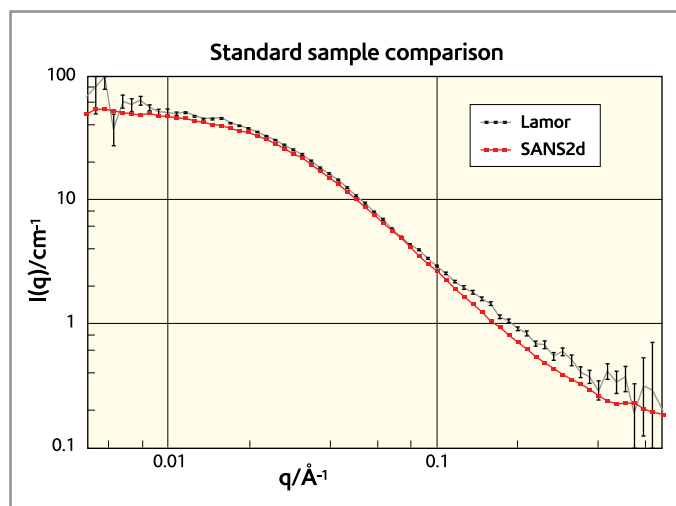
Advances in instrumentation & techniques

TS2 Phase 2 instrument updates

LARMOR

Larmor opened its shutter for the first time on 20th March 2014 for the start of scientific and engineering commissioning. Once it is fully operational in 2015/16 the instrument will provide access to a number of advanced Larmor precession techniques such as Spin-Echo Small Angle Neutron Scattering (SESANS) and Larmor diffraction as well as traditional SANS. The spin-echo equipment is being provided through a collaboration with TU-Delft and the NWO in the Netherlands. The commissioning program has proceeded well and has demonstrated that SANS results are obtained that are consistent with existing ISIS instrumentation. Commissioning will continue in early 2015 when the work has been completed to enable the instrument to view the coupled moderator of the ISIS second target station. This will improve performance considerably and enable the user science program to begin in the first half of 2015.

Progress is regularly updated on the Larmor twitter page <https://twitter.com/LarmorISIS>



CHIPIR

ChipIR will be the first instrument dedicated to studying how silicon microchips respond to cosmic neutron radiation. Our increasing demand for electronic devices has led components to become smaller than ever before, but smaller devices are more vulnerable to the effects of cosmic neutrons. Placing electronic systems in the neutron beam enables us to predict the frequency of neutron strikes and observe the consequences.



ChipIR is on schedule to receive first users in March 2015. The shutter was opened for the first time in June 2014, which revealed a higher than predicted neutron flux. This has meant a short-term delay to the schedule, but we are working to resolve this and expect to be back on schedule later in the year.

ChipIR is funded by the Department for Business, Innovation and Skills. Once it becomes operational in 2015 we expect significant industrial usage, particularly from the aerospace, electronics and computing industries.

IMAT

Construction of the IMAT instrument has continued this year with key achievements including the delivery of 2 neutron imaging cameras for tomography studies and the successful installation of a 44m long supermirror guide. Work will continue in 2014 with the installation of the instrument blockhouse and experimental equipment including a 7-axis sample positioner capable of manipulating 1.5 tonne samples.



From summer 2015 IMAT will enable neutron radiography, tomography and novel energy selective imaging analyses at ISIS. Eventually diffraction capabilities will be added which will make this a unique facility for materials science applications with a main emphasis on engineering studies.

ZOOM

Zoom will be a flexible, high count rate, small angle neutron scattering instrument. The instrument will have the option to polarise neutrons. A flexible sample area set up, whereby the detector vacuum tank and sample area can change position, will accommodate large sample equipment, as well as allowing a future upgrade to use focussing devices to reach very small Q (VSANS).

This year the 12 m long stainless steel 0.1 mbar vacuum tank has been installed. The detector motion system, capable of moving the detector between 6 to 10 m away from the sample, has been installed inside the tank. The sample positioning system has been delivered and is waiting to be installed, as is the double disk chopper. The polariser, guide and collimation unit and the shutter collimation are in design to be delivered next year. The super mirror bender for neutron transport is in design with the supplier and will be delivered by the end of the year.

Don Abram and Ian Maxwell from Daresbury's Technology ETC working on Zoom.



Rep Rate Multiplication (RRM) makes Merlin even more competitive

A new chopper system has been installed on Merlin making repetition rate multiplication (RRM) possible for the first time on this instrument. RRM involves sending several pulses of different neutron energies onto the sample in a single ISIS timeframe. In single energy mode, users request their desired energy, e.g. 50 meV, and get a single data set in return, whereas in RRM mode, up to 5 separate incident energies can be measured simultaneously, allowing a survey of data sets to be gathered in a fraction of the time.

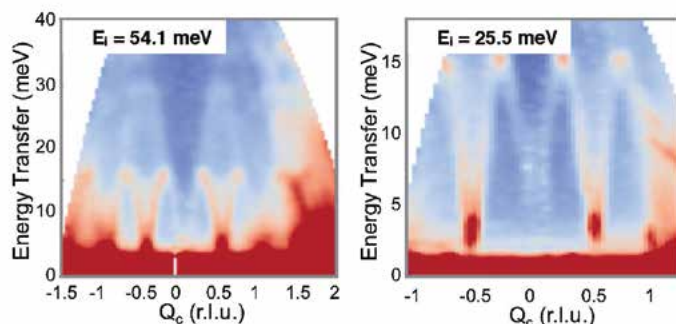
The technique has already been used to great effect on LET up to a maximum energy of 20 meV. Now RRM on Merlin allows collection of data between ~10 meV and 200 meV. Significantly the quality of the data produced is state of the art making Merlin highly competitive on the international stage.

SANS2d

Two new arrays of 8mm diameter, 1m long, ^3He gas tube detectors have enhanced the performance of SANS2d due to efficiency improvements of 30-40% compared to the original multi-wire devices. The arrays of 120 tubes will also take much higher count rates and are more robust in the case of failure as individual tubes can be replaced. Design and installation was required for a completely new cable handling system for a greatly increased set of cables to the movable detectors, a new screened room, and a method to deliver detector high voltage via air-filled tubes inside the vacuum of the SANS2d tank.

Below: Ed Spill with the new SANS2d detectors just after installation in the sample vacuum tank

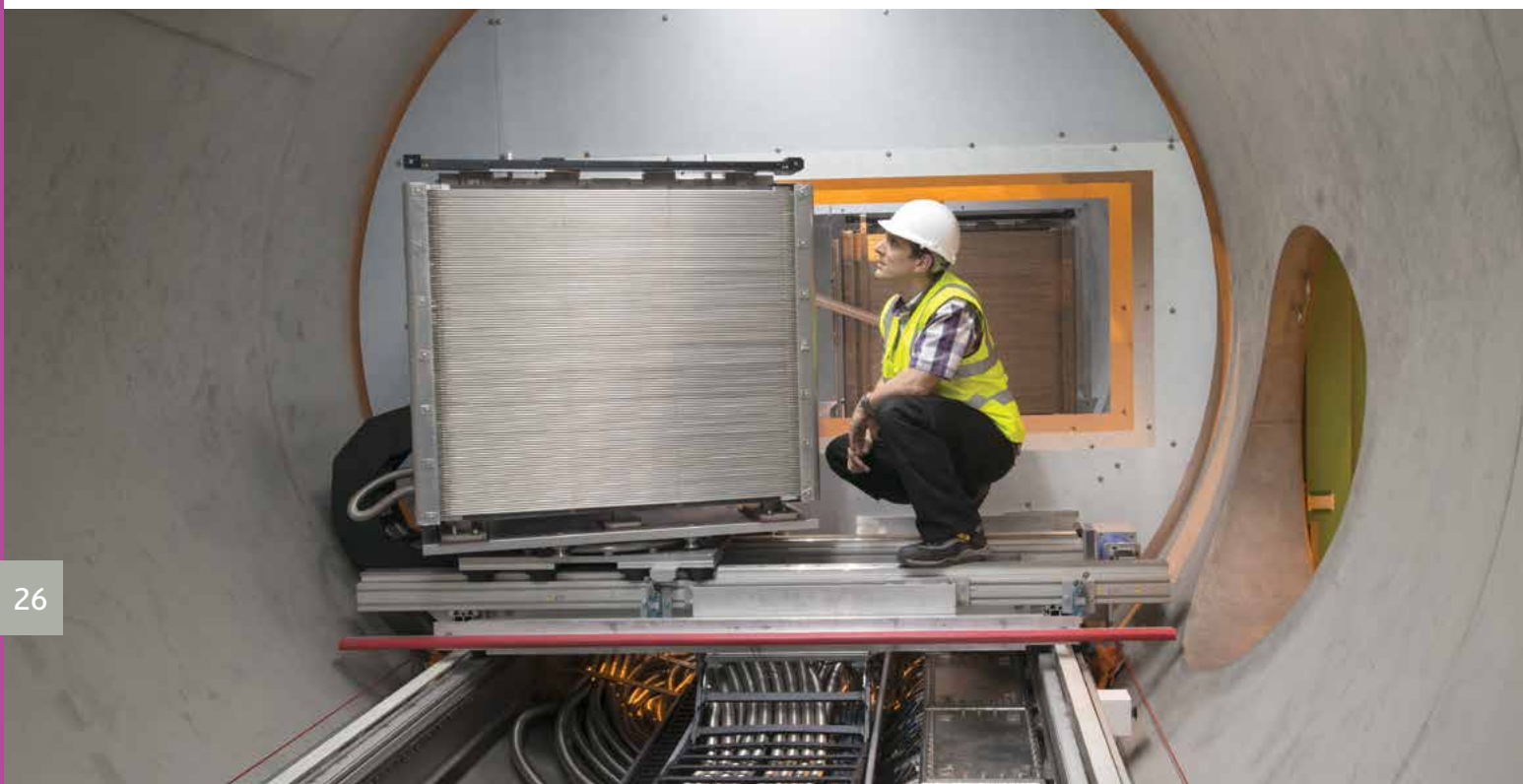
Ross Stewart, leader of the ISIS Excitations group, says, "This development adds new capability to the ISIS neutron spectroscopy suite and shows that despite lower source flux, Merlin can compete with the best in the world."



Simultaneously measured neutron spectra from a 3g crystal of copper germinate (CuGeO_3) measured on Merlin in RRM mode.

In-silico neutron spectroscopy goes Mantid

Mantid is the ISIS data reduction and analysis framework which is now also in use at other neutron sources around the world. Development is an ongoing process, and a variety of instruments have seen Mantid taken forward this year. For example, Mantid has been upgraded considerably for the analysis and interpretation of neutron spectroscopic data on Tosca and the low-energy spectrometers Iris and Osiris. New interfaces and algorithms have been included to allow integration into Mantid of computational modelling tools such as nMoldyn to allow comparison of experimental data with model predictions.



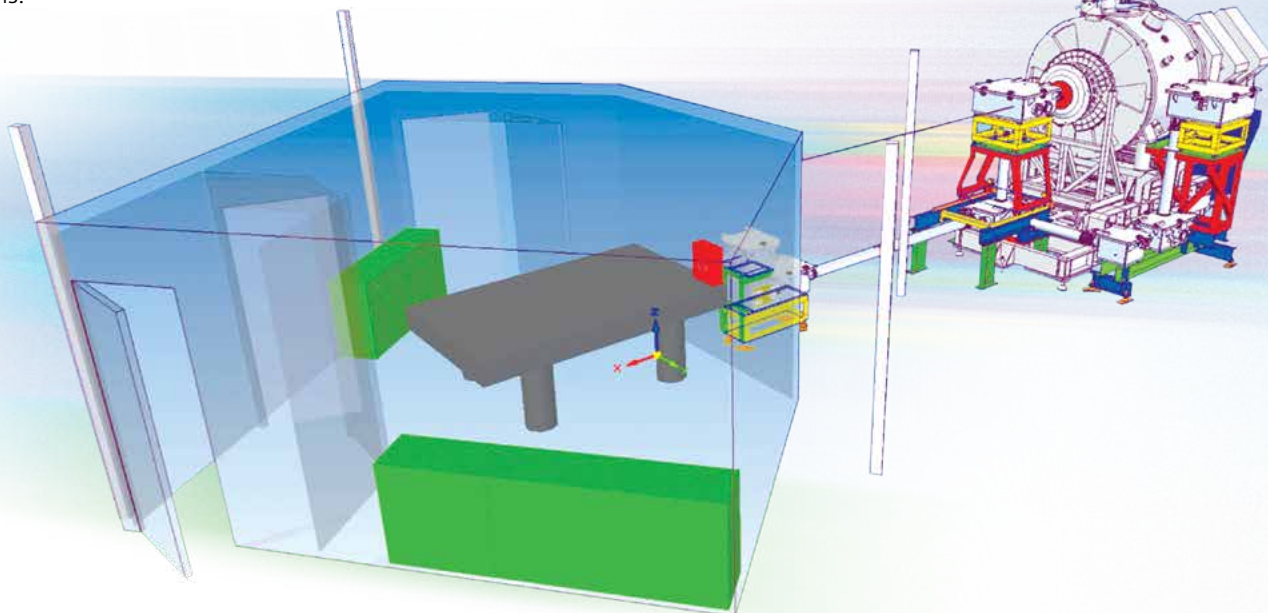
Upgrade to the muon beamlines

The European muon beamline was originally constructed in the mid 1980's. An upgrade to the beamline has been designed which should give a significant increase in the flux available to the muon instruments. The first two magnets in the beamline are located very close to the muon production target, and therefore receive high doses of radiation. New radiation-tolerant quadrupole magnets have been designed and built by a joint team from ISIS and the STFC Technology Department which use a coil insulation system based on concrete. The first of these magnets has been manufactured on site at RAL and is currently being tested ahead of a installation during the long shutdown.



Lasers on HiFi

In December 2013 a new laser system was installed on the HiFi muon spectrometer, expanding the scope of science possible at the ISIS muon facility. The upgrade is part of a collaboration between ISIS and Queen Mary University London and funded by the European Research Council. The new laser system will enable users to perform optically excited muon spectroscopy on materials. The pulsed laser can be used to excite molecules or electrons within a sample, with muons then implanted to measure the excited state. The aim is to understand how light excites a molecule, and to follow the subsequent evolution of the molecule's charge distribution and magnetic moment – enabling detailed investigation of dynamics in soft matter systems.



New *in-situ* neutron diffraction cell for electrode materials

A novel neutron diffraction cell has been constructed to allow studies of the structural changes in materials used in battery applications *in-situ* during charge/discharge cycling. An important aspect of the design is its modular nature, allowing flexibility in both the materials studied and the battery configuration. The cell is based on a number of circular disk-shaped components. It is constructed by stacking these, so that different cell configurations can be assembled depending on the type of battery under investigation, or to maximize the quantity of electrode material exposed to the neutron beam. The cell is flexible in the sense that different configurations may be assembled for experiments *in-situ*.



Moving on to EPICS

The range and complexity of experiments performed at ISIS is always increasing, and thus the instrument control software needs to evolve to meet these new challenges. After an evaluation exercise, a project has begun to replace the existing control software with a new system based on the EPICS open source tools. EPICS-based systems are widely used around the world, including at Diamond Light Source and the US Spallation Neutron Source, to provide real-time control systems.

The recently built LARMOR instrument has been running the first iteration of the new control system, which it used successfully during its recent commissioning. The software will undergo further development during the ISIS long shutdown and be deployed to other ISIS instruments over coming years.

EMMA refurbishment

EMMA (Equipment Materials and Mechanics Analyser) is a refurbishment of the HET beamline. It will be used to test detectors, shielding material, software and other beamline components. A new block house has been constructed to form a dedicated detector and electronics testing facility. The new blockhouse paves the way for a portable detector lifting trolley to be installed, providing the ability to lift detectors into the beam and remotely move them in 2 axes in steps as small as 0.1mm for testing purposes.

Below: ISIS scientist Rob Dalglish on Offspec

Demonstrating the spin-echo technique on Offspec

Many products in everyday use are suspensions of very small particles: milk and paint, for example. If the microscopic particles in these suspensions aggregate into large clusters, the properties of the suspension are often changed, sometimes in desirable ways – such as when cream forms on the top of the milk – and sometimes in less useful ways. Understanding the formation of these aggregates can help us design materials that resist clumping. Roger Pynn from Indiana University and colleagues used a new neutron scattering technique, only available at ISIS, to study aggregation in a model system composed perspex particles, so small that a million of them could fit on the head of a pin. They changed the force of attraction between the particles by adding small amounts of polystyrene. Above a critical amount of polystyrene, large aggregates are formed. Nevertheless, the distance of a perspex particle to its nearest neighbours and the number of nearest neighbours remains essentially the same independent of the amount of polystyrene.



Accelerators and targets

TS1 target upgrade



The ISIS first target station – TS1 – has been operating since ISIS started up in 1984. With the experience gained from the recent construction of TS2, and the ability to use computer modelling to simulate target station performance, there is now a significant opportunity to enhance TS1.

ISIS neutronic, instrument and engineering teams have been busy this year working on the TS1 Upgrade Feasibility Project. The work on the project has seen a base lining of the neutronics and engineering of the existing target station and the development of new target, reflector and moderator proposals which will, at a minimum, double the useful neutronic output for the existing instrument suite. This flux increase will deliver real improvements to the scientific capabilities of the existing instruments and, of course, future instrument developments.

Whilst investigating the current target design, a target team was able to obtain rare footage around the target and the void vessel. By modifying existing equipment, the team were able to move a camera system up to the void vessel and inspect the proton beam pipe, instrument windows and door sealing face.

Upgrading the extracted proton beam

Upgrade of the muon target section of the proton beamline for TS1 will take place during the 2014 long shutdown. Six quadrupole magnets, which were original built for the Nimrod accelerator (the precursor to ISIS) in the 1960s, will be replaced with new magnets built to the same design as those in TS2. These new quadrupoles will have a wider aperture than the existing magnets which is helpful in squeezing the beam at the muon target. The quadrupole arrangement has been designed such that operations can continue with any one magnet within the section failed.

Phase 2 reflector

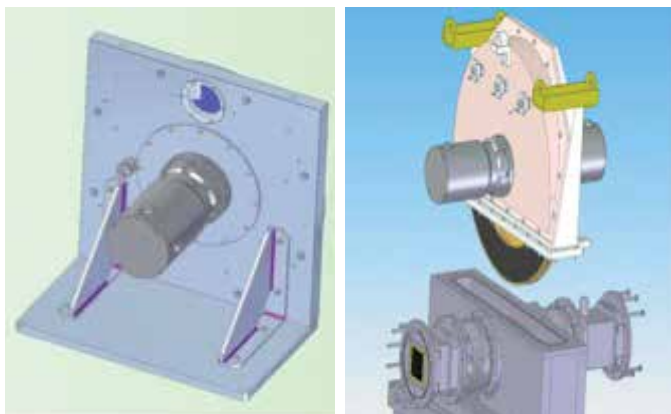


Andy Robinson and Graham Wallace assembling the MK II Beryllium Reflector onto the ISIS Second Target Station (TS2) test stand.

The new reflector plays a key role in the TS2 Phase II upgrade by opening up a view of the target for two new instruments – ChipIR and LARMOR - with the option to add more instruments in the future as funding becomes available. In addition development of the moderators, located within the reflector, is continuing and these are very likely to change shape as new moderator materials are tested. In view of this the new reflector design incorporates sections that can be easily removed and replaced to accommodate any changes in moderator size, shape or volume.

The TS2 test stand has made it possible for the reflector assembly to be pre-aligned ready for installation during the long shutdown as well as to fully test the water flow through the cooling circuit and develop tooling and methods for working on the reflector, in the remote handling cell, when it's in service.

Neutron chopper vacuum drive system



Allowing neutron disc choppers to run with an internal vacuum could improve the neutron flux and the capabilities of instruments. The development of IMAT, which would benefit from this approach, gave the Design Section the ideal opportunity to design and develop a vacuum neutron disc chopper. In the last year a new drive system has successfully passed site acceptance tests at ISIS and is now on long-term trials. Once these are successfully completed the neutron chopper team will be able to offer the conversion over to vacuum to all the instruments on ISIS.

Head-tail instability studies and GSI-Darmstadt collaboration

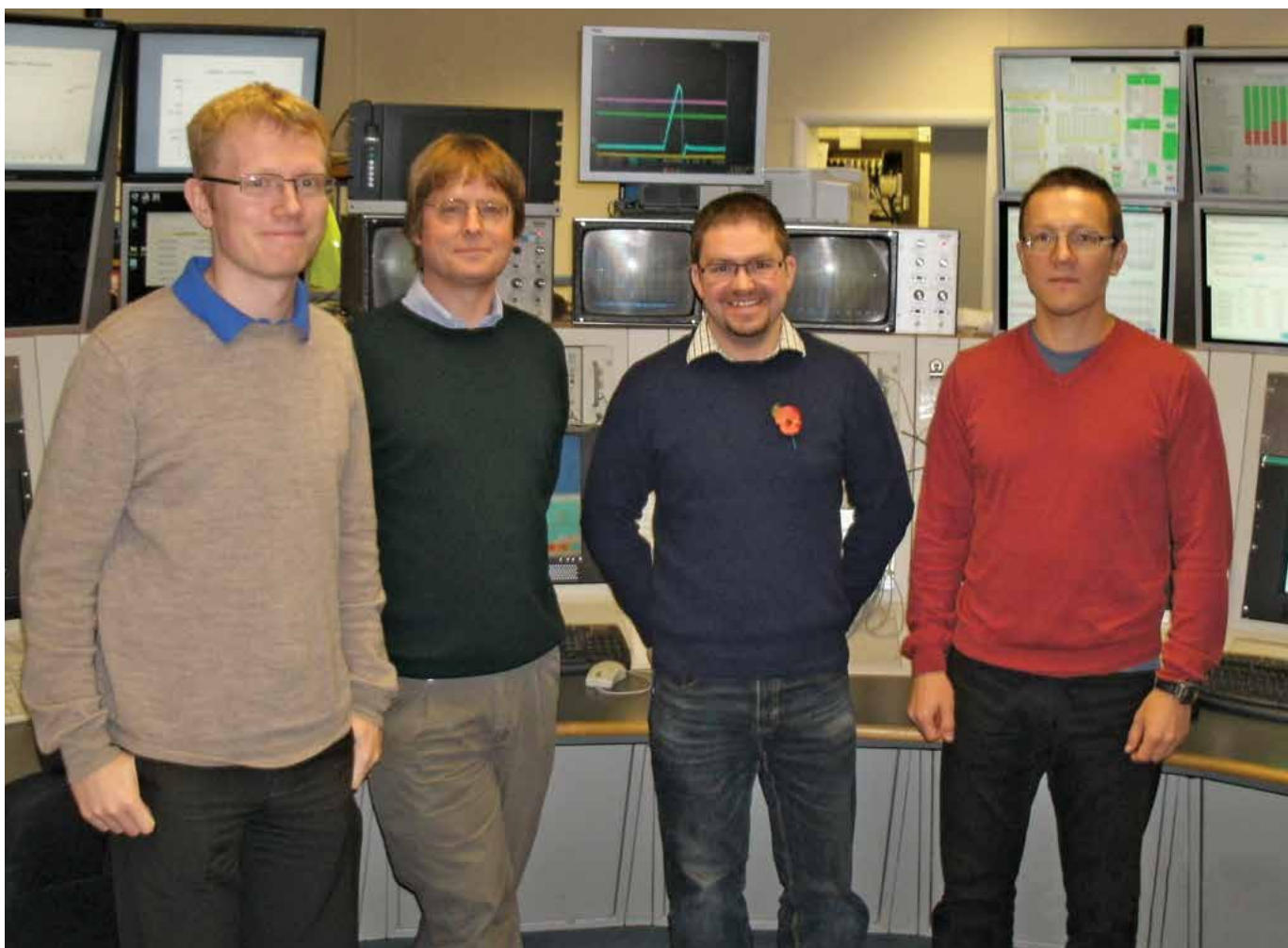
The ISIS Accelerator Physics group started a collaboration with Dr Vladimir Kornilov of GSI-Darmstadt who visited ISIS for a week in November to help with experimental studies of the transverse head-tail instability on the synchrotron.

Extensive sets of measurements were taken with RF in single and dual harmonic modes, at a wide range of intensities. Some interesting new features were noted including a lower and upper intensity threshold to the

instability, and the ability to shift the instability (usually seen around 2 ms in the ISIS cycle) to 0.5 ms.

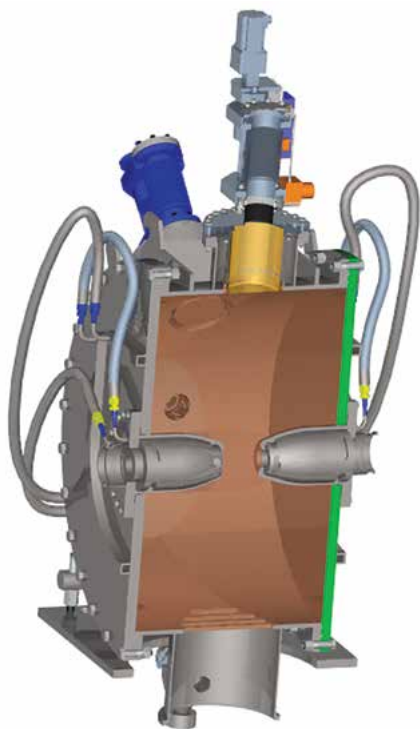
A greater understanding of the instabilities seen on ISIS and determination of their causes will help the group increase operating beam intensity and design future upgrades.

Rob Williamson, Chris Warsop, Bryan Jones with Vladimir Kornilov of GSI in the ISIS Control Room during new head-tail beam instability studies.



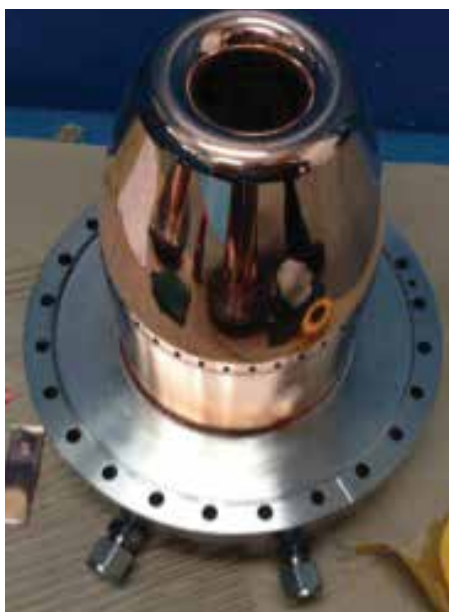
New debunching cavity for the ISIS injection systems

When ISIS was first built many of the components for the accelerator were taken from older machines that had already been decommissioned. One such component is the debunching cavity, installed in the High Energy Drift Space between the linear accelerator and the synchrotron. The cavity acts to reduce the



A CAD cross section of the newly designed cavity.

energy spread of the beam while maintaining the beam's average energy, and was originally designed in the 1960s for operation in the 50 MeV Proton Linear Accelerator (PLA), sited at RAL until 1969. Due to its age, complexity and a lack of detailed information regarding its design and some past failures, the cavity posed a risk to the continued operation of ISIS. A new debunching cavity has, therefore, been designed and is currently in its final stages of manufacture. The new design should give improvements in efficiency, maintainability and reliability. Testing will be taking place in the coming months in the new Linac Test Area, with an installation planned for the long shutdown.



One of the two RF drift tubes ready to be installed.

Main magnet power supply upgrade programme

In April the group took delivery of the new main magnet power supply DC Bias from Danfysik. This is a 1.44MW power supply and when commissioned it will be the highest power unit in use on ISIS with over twice the power capability of the 680kW extraction septum power supplies. The power supply is currently being connected and will undergo final acceptance testing in July. When operational in February 2015 this power supply will improve the existing stability of the biased sine wave current used to drive some of the synchrotron magnets. It will also allow the synchrotron main magnets to operate in a mode suitable for higher injection energies as foreseen as part of the ISIS upgrade program.

Replacement chokes



Steve West inspecting the new ISIS MMPS main chokes during installation in R6A back in May 2009.

Throughout the year work has continued on commissioning the replacement chokes for the synchrotron main magnet circuit. These have now been commissioned to $\frac{3}{4}$ of their nominal operating level of 660Amps DC and 400 Amps AC. Performance so far has been excellent and the aim is to commence operation with the new chokes in February 2015.

Other developments



New EPB1 power supplies

Installation and commissioning of the new power supplies for EPB1 magnets has continued throughout the year. These power supplies are of a modular construction and operate with sufficient power modules to provide n+1 redundancy. In the event of a power module failure, the power supply detects the failure and isolates the failed power module from the output with the remaining power modules providing the required output whilst maintaining the specified output stability. This process occurs within 1mS without causing a beam trip.



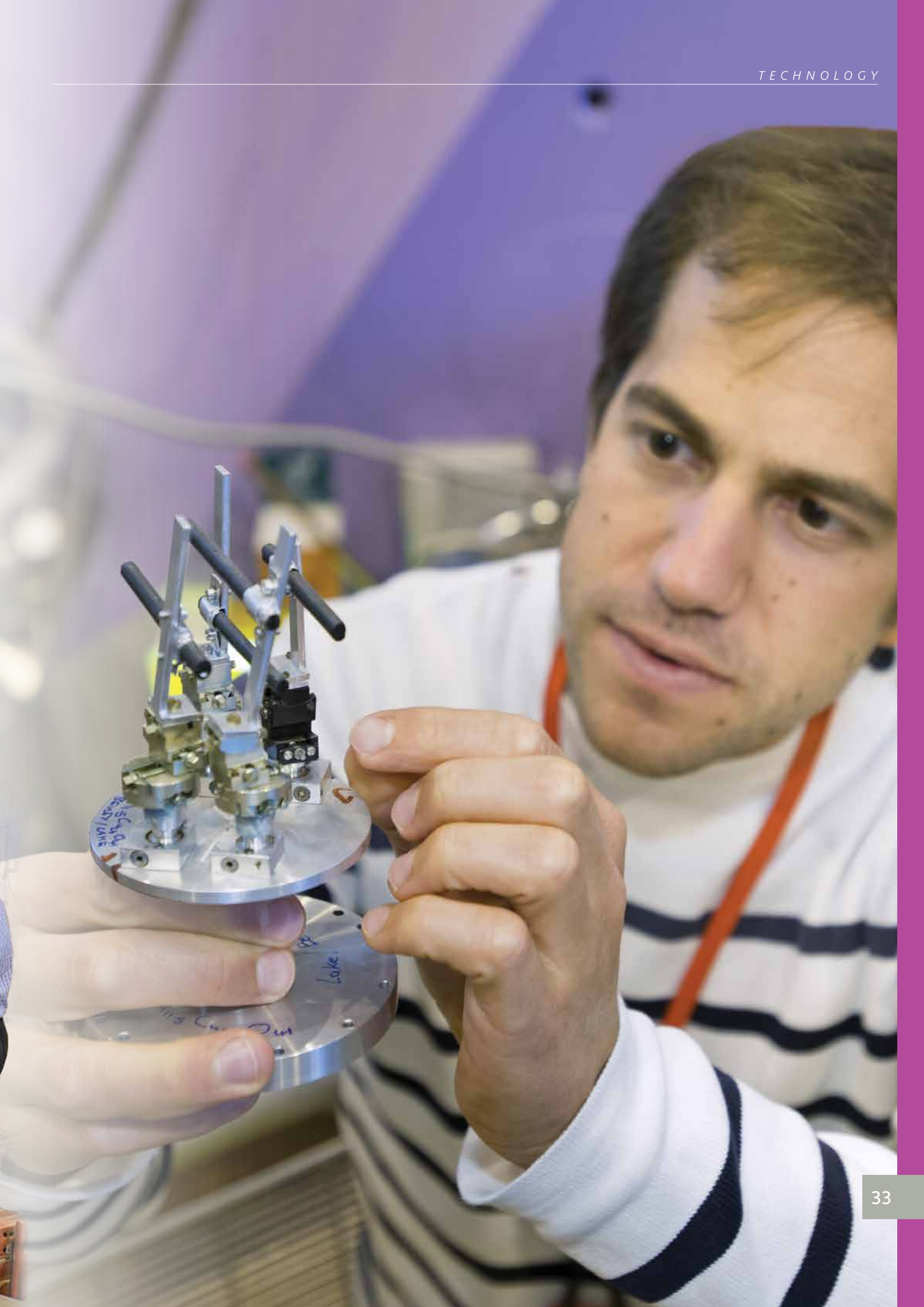
Top left: Following a review of plant efficiency the magnet cooling circuit on Extracted Proton Beam 2 has been rebalanced, lowering running costs and reducing overall system stress. Paul Masterson with the kit.

Centre left: ISIS vacuum staff have been trained to strip down and repair a variety of vacuum pumps. As a result they can now successfully carry out repairs and maintenance on these pumps inhouse, saving both time and money. Shown here Roy Symes and Andrew Eales.

Bottom left: Tony Millington, head of the new Survey group, with a new laser scanner set up within the EC muon upgrade mock-up.

Below: An upgrade to the demineralised makeup plant has reduced the dissolved oxygen and carbon dioxide levels, increased the PH, and improved the conductivity level and overall stability. Shown here, Stuart Morse and Andrew Woods.

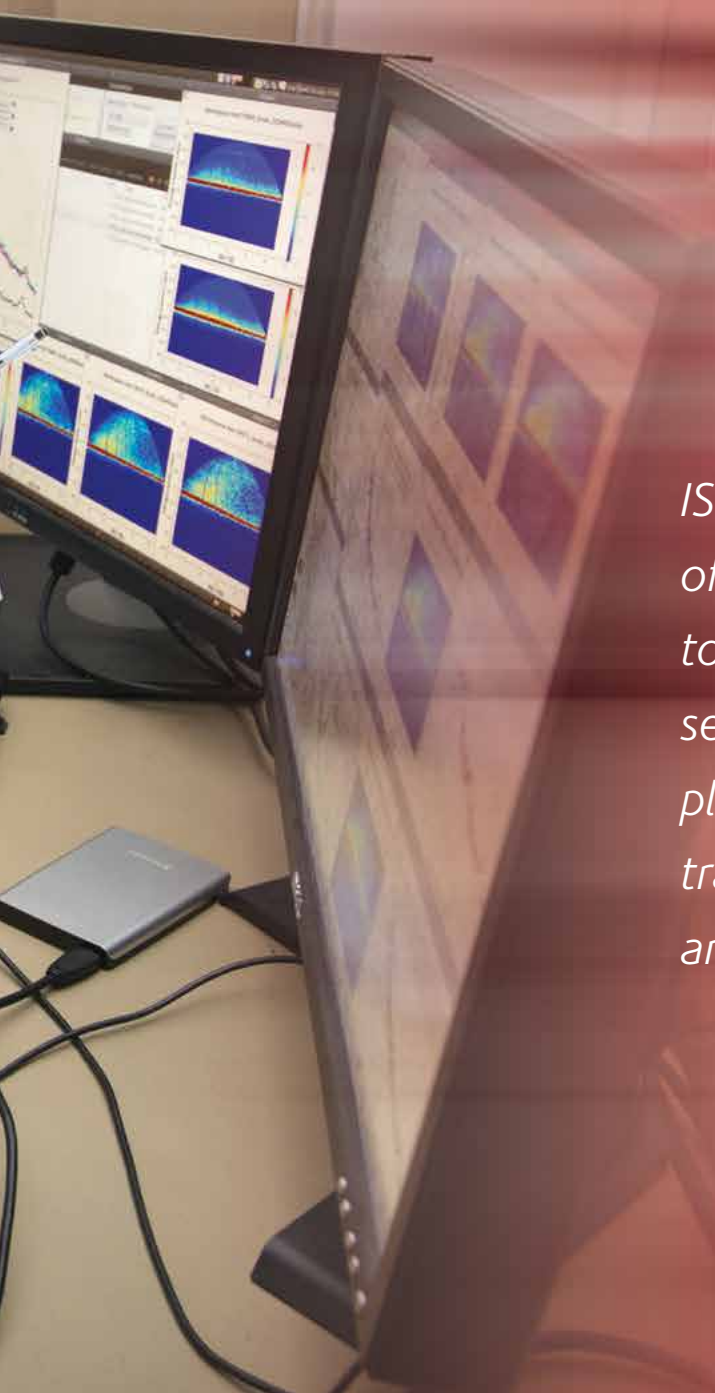




Working



with industry



ISIS collaborates with a wide range of companies, from small start-ups to multinational corporations, with sectors including chemicals and plastics, healthcare, aerospace, transport, manufacturing, automotive and the energy industry.

Industry and innovation

There are a range of mechanisms for collaborating – through partnerships with academia, by paying to go the commercial route, or through the ISIS Collaborative R&D programme (IRCD). The IRCD scheme was set up in 2011 to widen the use of ISIS by industry and increase the economic benefit to the UK. The scheme has been very successful, with 22 companies now involved, and several more in negotiation. In 2013/14 a total of 59 companies accessed ISIS through the various schemes.

Case Study

Breaking the barriers to a solar future

Researchers at the University of Sheffield, University of Durham and ISIS in collaboration with start-up company Ossila are using neutron reflectometry to look the formation of plastic solar cell films with the goal of developing devices which efficiently harness the power of the sun whilst being cheaper and easier to manufacture than the current silicon solar cells.

“Current photovoltaic devices are expensive and difficult to install, and over the last decade there has been little increase in efficiency, which in turn has limited their uptake. Plastic polymer solar cells could change the game – they can be manufactured much more cheaply and quickly, and are easier to install – but first we need to make them more efficient and stable. With the University of Sheffield we are using ISIS to understand how the length of polymer chain affects efficiency and therefore how we can optimise these devices to make them really competitive.”

James Kingsley, Ossila



Case Study

Testing new welding techniques for the nuclear industry with AREVA

Introduction of new designs, novel fabrication methods or modifications to existing plant in the nuclear power generation industry are subject to intense scrutiny to ensure that safety is not compromised. Multi-national corporation AREVA has designed the new European Pressurised Reactor (EPR) to meet stringent demands for increased safety and reduced cost of electricity generation. A twin EPR power station at Hinkley Point in Somerset is planned and will be constructed using modern welding technology.

Together with the Open University, AREVA has been using Engin-X to map residual stress in mock-ups of welded nuclear components for the purpose of validating models simulating their new processes for over five years.

Professor John Bouchard from the Open University led the research. He says, "This was a challenging experiment as we were working close to the operational limit of Engin-X. However the results were in good agreement with earlier measurements and validated the advanced weld prediction model developed by AREVA. We are confident that the knowledge we've gained will support implementation of this new welding process".

Case Study

Building safer ships with Lloyd's Register

Ultrasonic peening (UP) is a technique for improving the fatigue performance of welded joints. Little research has been done on how UP-treated welds behave when they are subjected to real world conditions such as compressive overload or variable amplitude loading. Lloyd's Register provides quality assurance to the marine industry, and they have been using ENGIN-X to investigate UP welded joints in these conditions. Understanding the process and its benefits will allow improved control of fatigue cracking, lower maintenance costs, and extending the life of welded connections in marine and other industries.

David Howarth of Lloyd's Register says, "For many years the advantages of adding a compressive stress in the area of the weld toe have been known but could not be practically applied to large ship structures. The advent of ultrasonic peening provides the ship builder with the freedom to do this without affecting the speed of construction seen in modern shipyards. The ability to understand how residual stresses perform under realistic conditions has been a great help to the industry in pushing the process forward."



Education



& outreach

ISIS recognises the need to develop our people, help train the next generation of scientists and engineers and to provide inspiration for thousands of students to study STEM subjects in higher education.

Inspiring the next generation

How often do you get to visit a particle accelerator, to stand on the roof as millions of protons travel beneath your feet at almost the speed of light? For our staff it's a regular occurrence so it's easy to forget how exciting it can be!

At ISIS we recognise we have a responsibility to inspire the next generation of scientists, and with our science spanning disciplines from physics, chemistry and biology to cultural heritage, environmental science and materials science, we are well placed to showcase what a scientific career can offer!

ISIS is a highlight of the trip for many visitors taking part in STFC's public and education access days. This year we welcomed over 600 under-18 year-olds to the facility, with 400 attending in one week as part of the Particle Physics Masterclass! In addition many of our staff are STEM ambassadors and frequently visit local schools and science fairs with hands on activities explaining their science. Finally we provide training for science teachers, equipping them with first-hand knowledge of our cutting edge research to take back to the classroom.

Visitors on a public access day get a look inside Engin-X



ISIS scientist Chris Frost shows visitors how to detect cosmic rays as part of Stargazing Live.



Equipping the scientists and engineers of the future

ISIS plays a key role in training scientists in the skills they need to use the facility in the future. Our scientists are currently co-supervising around 50 PhD students, and 674 students took part in experiments at ISIS over the year. In October 2013 we organised the Oxford Neutron School, where 60 PhD and post-doctoral researchers received an introduction to the theory, techniques and applications of neutron scattering. In May 2014 we ran a week-long school on the use and applications of muon spectroscopy, giving students the chance to get hands-on experience on the muon instruments, and the neutron training course, run for over 40 students in March, provided a similar combination of lectures and practical experience.

"The school showed us everything that can be done with neutrons. Now I know about alternative techniques that could be applied to my project."

Neutron school delegate

Neutron school delegates outside TS1.



Apprentices

The STFC apprenticeship scheme takes on young people for a four year programme where they undertake three to six month placements in various STFC departments. ISIS has been involved in the scheme for 22 years, and we take on about 10 apprentices every year. The scheme presents a great alternative to further education, providing budding engineers with competitive skills and experience.

“Some of the best times I’ve had at work have been on the beamlines, coming up with wonderful ways of fixing things, but it’s really the communication with the scientists and engineers I enjoy, because you feel more a part of the experiment and the science, as it’s happening.”

Apprentice Jamie Pinnel



Apprentice Jamie Pinnel.

Taking our staff to the next level

Nick Webb, Mike Dudman and Dan Coates from the ISIS Design Division are all ex apprentices who have been sponsored by STFC to complete a BEng in Mechanical Engineering Design. Taking the degree alongside their full-time jobs was a challenge, but all three were delighted to be awarded first class with honours.

Two other ISIS staff, Dan Crossman and Mike van de Mortel also received their degrees this year in Electrical and Electronic Engineering from the University of the West of England. Congratulations to all five new graduates!

Nick Webb, Mike Dudman and Dan Coates with their certificates.



Conferences & workshops

Crystallography Users Meeting

11-12 November 2013

The annual joint meeting between the ISIS crystallography user group and the Physical Crystallography Group (PCG) & Structural Condensed Matter Physics (SCMP) was an exciting blend of information, ideas and inspiration. The unprecedentedly large turnout over the two days was evidence of the value of such a meeting to the various scientific communities present, as well as the breadth of expertise and quality of science on display. Overall, with so many opportunities to foster ideas, friendships and collaborations, the meeting was a resounding success for new students and old-timers alike.

Frontiers and Horizons in Electron Volt Neutron Spectroscopy

January 2014



January 2014 saw over 40 scientists from across the globe coming together at Cosener's House in Abingdon, UK, for a two-day meeting on the latest science and developments in instrumentation in the field of electron Volt (eV) neutron spectroscopy. The meeting was jointly organised by the ISIS Molecular Spectroscopy group, CNR, Università degli Studi di Roma Tor Vergata and Università degli Studi di Milano in Italy.

Muon Site Calculation Meeting

19 March 2014

The latest in a series of meetings discussing methods for calculating the muon site in materials was held at RAL in March 2014. With a focus on the application of DFT techniques to μ SR, the meeting brought together over 40 scientists from Europe and Asia for an afternoon of presentations and discussion. Talks included investigations of the muon site for a number of topical systems, including cuprate and heavy fermion compounds, calculation of hyperfine coupling constants for the interpretation of level crossing spectra and an introduction to the utility of the CASTEP software for this type of work.



(L to R) Isao Watanabe (RIKEN-RAL), Shukri Sulaiman (USM), Steve Cox (ISIS) and Roberto De Renzi (Parma) during the muon site calculation meeting

3rd UK-China Steel Research Forum & 15th Chinese Materials Association-UK

10-11 July 2014



The 3rd UK-China Steel Research Forum was held in conjunction with the 15th Biennial Conference of Chinese Materials Association in the UK on Materials Science and Engineering. Jointly organised by steel researchers from

the UK and China, with support from industry leaders, steel research institutions and research funding bodies from the UK and China, the event attracted over 80 delegates. Invited speakers included Futao Chen, Minister Counsellor of Science and Technology, Chinese Embassy, Chris Grovenor, Head of the Department of Materials, University of Oxford, Rachel Thomson, Acting Dean of the School of Aeronautical, Loughborough University (UK), Harry Bahdasha, FRS, University of Cambridge, (UK) and Chenguang Bai, Vice- President, Chongqing University (China), Universities represented included the University of Cambridge, Tsinghua University, University of Science and Technology Beijing. Companies who attended included

Rolls Royce, Tata Steel, TWI, and China Iron & Steel Research Institute Group. The conference was chaired by Dr. Shu Yan Zhang, senior scientist from ISIS. Scientists, engineers, technologists and industry leaders were able to discuss and exchange the recent advances in the research of materials science and engineering, in particular on steel research and development in the two countries. It provided a unique and valuable opportunity for academic institutions and industrial companies to develop joint research projects to foster research collaborations between the UK and China.

UK Neutron and Muon Users Meeting (NMUM)

10-11 April 2014

The 2014 NMUM meeting saw 150 ISIS and ILL users come to Warwick for a series of facility updates, science talks and breakout session for users to feedback their view on key areas that affect them. In addition it provided students with the opportunity to showcase their work in a poster prize session, with the winners delivering a science talk on the final day.



Seminars

ISIS seminars continue to attract a wide variety of national and international speakers.

April 13

Kostya Trachenko (Queen Mary, University of London)

New understanding of liquid heat capacity and dynamic crossovers in the supercritical state

Aldo Isidori (University of Frankfurt)

Rotationally-invariant slave-bosons for strongly correlated superconductors

June 13

Nandini Trivendi (ISIS/CMPCity Joint Seminar)

Emergence of a Novel Pseudogap Metallic State in a Disordered 2D Mott Insulator

Gunnar Möller (ISIS/CMPCity Joint Seminar)

Vortex Lattices and supersolidity of bosons in flat bands

Aninda J Battacharyya (Bangalore)

Examples of Confinement Effects in the Context of Electrochemical Processes

Professor Juan Manuel Pérez-Mato
(University of Pais Vasco – Bilbao, Spain)

Symmetry of incommensurate magnetic structures and its consequences

André-Marie Tremblay (ISIS/CMPCity Joint Seminar)

Insulators, metals, pseudogaps and cuprate superconductivity

George Sawatzky (ISIS/CMPCity Joint Seminar)

Orbital Physics

July 13

Luis Carlos Pardo (Universitat Politècnica de Catalunya)

FABADA: a Bayesian fitting tool

Massimo Giovannozzi

CERN

Manipulation of transverse beam distribution in circular accelerators: Beam splitting by particle trapping into resonance islands

Dr Phi Bentley

European Spallation Source, Lund

Reducing High Energy Backgrounds on Spallation Source Instruments

Kjartan Thor Wikfeldt

University of Iceland

Large geometrical isotope effects and quantum tunneling in hydrogen-bonded ferroelectrics from ab initio simulations

Aug 13

Amitava Bhattacharyya

ISIS / University of Johannesburg

Magnetic And Transport Properties of Rare Earth Based Intermetallic Compounds

Sept 13

Ian Wood

Department of Earth Sciences, UCL

Crystallography and the Deep Earth

Henry Glyde

University of Delaware

Bose-Einstein Condensation, Superfluidity and Elementary Excitations in Quantum Liquids

Professor Feri Mezei

European Spallation Source, Lund

ESS Target Station – Status and recent progress

Jim Stovall

The Conceptual Design of an Injector Linac for The Chinese Institute of Atomic Energy

Dec 13

Iain McKenzie

TRIUMF

Soft Condensed Matter Studied With Radioactive Local Probes: ^2D NMR and μSR of Polymers and Liquid Crystals

Tom Fennell

PSI

Magnetoelastic excitations in the pyrochlore spin liquid $\text{Tb}_2\text{Ti}_2\text{O}_7$

Jan 14

Andrew Goodwin (University of Oxford Chemistry)

Exploiting neutron total scattering: disordered networks, cooperative paramagnets, membrane proteins, and Bayesian modelling

Sergey Kulikov (Joint Institute for Nuclear Research, Dubna)

The first pelletized cold neutron moderator start up for the IBR-2 reactor

Feb 14

Dr Luke Clifton (ISIS)

Making and Destroying Models of the Gram Negative Bacterial Outer Membrane

Prof. Kanetada Nagamine (KEK / RIKEN Atomic Physics Laboratory)

Prospects of the Ultra Slow Muon project

Konstantin Kamenev (School of Engineering, University of Edinburgh)

An engineering approach to developing high-pressure instruments for neutrons and X-rays

Mar 14

Martin Own Jones (ISIS)

The evolution of hydrogen storage

Dr Alan Drew (Physics Department, Queen Mary, University of London)

Spin and charge dynamics in organic semiconductors measured using local probes

Frank Kruger (ISIS/UCL)

Spirals close to ferromagnetic quantum criticality

Other events

Organised by ISIS or with major input from ISIS in the 13/14 financial year.

April 13

UK-Korea meeting on spintronics

NMUM 2013

EPICS Spring Conference

May 13

Quantum Design Workshop

June 13

ISIS Facility Access Panel meeting

ISIS/SNS Bilateral Target Workshop

ISIS User committee meeting

Theoretical and Experimental Magnetism Meeting

BRSg: Magnetic Resonance Group Summer Meeting and AGM

Dynamics of Molecules and Materials-II

International Conference on Neutron Scattering (ICNS) 2013

Sept 13

Maps/Mari/Tosca Review

Oxford School of Neutron Scattering 2013

Rigaku SmartLab Users Workshop

Radiation Effects on Components and Systems 2013 (RADECS 2013)

Oct 13

2nd STEP Meeting for Materials and Engineering Diffraction

Denim (Design and Engineering of Neutron Instruments)

Workshop on fast neutron applications at spallation sources

Nov 13

Joint ISIS Crystallography User Group Meeting and Winter Meeting of the PCG-SCMP

ISIS International Review

Dec 13

ISIS Facility Access Panel meeting

ISIS User Committee meeting

Jan 14

VI Workshop on Electron Volt Neutron Spectroscopy: Frontiers and Horizons

Feb 14

Neutron Training Course

Muon site calculation meeting



A year

This year has seen ISIS extend our presence on the international stage, with both staff and users winning international recognition and with the signing of significant collaboration agreements with international partners.

around ISIS



Prize-winning science

Prestigious fellowship for ISIS scientist

ISIS senior scientist and STFC Fellow Dr Alan Soper has been elected as a Fellow of the Royal Society. Alan Soper is distinguished as the world leading experimentalist on the structure of water and aqueous solutions, and an internationally outstanding expert on the structure of liquids in general. Besides making major and seminal contributions to the study of water and other aqueous systems, including complex systems of high chemical and biological importance, he has been influential in studies of many other liquids and glasses, and has developed novel diffraction instruments and techniques that have revolutionised the field. He has also pioneered the wider use of computer simulation as a tool for building three-dimensional models of the disordered states of matter based on measured data.

Bath researcher scoops top neutron scattering prize



Dr Anita Zeidler (University of Bath) receives the B.T.M. Willis prize from Dr Ali Zerbakhsh, Chair of the IOP/RSC Neutron Scattering Group.

Dr Anita Zeidler (University of Bath) has been awarded the prestigious '2014 B.T.M. Willis Prize' for neutron scattering in recognition of her studies of a wide range of materials including water, and their interactions at the atomic and molecular level. Anita has played a major role in better understanding the structure and dynamics of liquid and amorphous materials under extreme

conditions, for example high-temperatures and high-pressures. "Neutron techniques are an essential tool in my goal to better understand the structure and dynamics of amorphous materials. I am very honoured to win this prize and, building on this success, my focus will be on further advancing neutron scattering research to unravel the complexity of liquid and amorphous materials," said Dr Zeidler on her achievement.

ISIS user receives the 2014 Yamazaki Prize

Professor Roberto De Renzi from the University of Parma has been awarded the 2014 Yamazaki Prize for muon science. He is recognised for his sustained and exceptional contributions to the development of the muon spin relaxation (μ SR) technique to investigate solid-state physics. The prize is awarded by the International Society for Muon Spectroscopy (ISMS). Professor Stephen Blundell, ISMS President, said, "Roberto De Renzi's work has made effective bridges between NMR and muon techniques and he is particularly well known for his work in magnetism and superconductivity."

ISIS collaborations

UK and China to bring together neutron expertise

An agreement has been signed to promote collaboration between ISIS and the China Spallation Neutron Source (CSNS), part of the Chinese Academy of Sciences. The CSNS is currently under construction in Dongguan city, Guangdong Province and is set to become China's national facility in 2018. The memorandum of understanding commits the two facilities to establishing a series of cooperative research programs in various technologies relating to pulsed spallation neutron sources, with the aim of sharing development tasks to make the most efficient use of resources.



ISIS scientist Shu Yan Zhang gives Governor Zhu of Guangdong Province a tour of Engin-X during a visit in September 2013 to highlight collaborations with the region.

NPL and ISIS collaboration

A new research collaboration was announced in February 2014 between the UK's National Physical Laboratory (NPL) and ISIS in order to achieve a greater understanding of materials and how changing conditions may alter their performance. NPL have signed a Memorandum of Understanding with the ISIS facility to both increase collaboration between the two organisations and jointly develop innovative capabilities to enhance our understanding of materials, particularly multiferroics, and how they perform under different conditions. Long term the research findings from the collaboration should be of real benefit to UK industry in the fields of micro-electronics with the aim of making computers (including mobile devices) smaller and faster while using less power.

ISIS signs up to continued collaboration with Italy



ISIS Director Robert McGreevy signs the agreement, with Cristina Messa, Vice President of CNR.

The Science and Technology Facilities Council (STFC) and the Consiglio Nazionale delle Ricerche (CNR, the Italian National Research Council) signed an agreement in March 2014 worth €15M to further develop collaboration between the two countries in the field of neutron scattering using the STFC ISIS facility. In the last five years Italian involvement with ISIS has included over 300 Italian scientists having produced 200 publications based on research undertaken at the facility. Italian science at ISIS spans a wide range of areas from fundamental studies through to biomaterials, materials for energy and cultural heritage studies. Future collaboration is aimed at ensuring the mutually beneficial development of instrumentation and techniques.

ISIS-ESS Collaboration

ISIS signed a Memorandum of Understanding with the European Spallation Source (ESS) in January 2014 concerning an extensive programme of technological collaboration, ranging from accelerator diagnostics to data analysis. The ESS is being developed in Lund, Sweden and construction is due to start this year. By sharing existing technologies and expertise ISIS can help ESS to reduce its construction risks and costs, and by adopting common technologies we will reduce future development costs for both partners. The UK has also pledged construction support for the ESS build, and ISIS will be essential for delivering parts of this contribution.

Facts



& figures

In 2013-2014 801 experiments were run, 3154 days were delivered to the user programme and 446 journal papers were published based on ISIS research.

Facility Access Panels *membership*

ISIS Facility Access Panels (FAPs) meet twice a year to review all proposals submitted to the facility based on scientific merit.

FAP 1	FAP 2	FAP 3	FAP 4	FAP 5	FAP 6	FAP 7
Diffraction	Disordered	Large scale structures	Excitations	Spectroscopy	Muons	Engineering
D Gregory	C Hardacre	D Barlow	A Boothroyd	N Skipper	D Paul	J Bouchard
D Allan	M Arai	W Bouwman	M Braden	C Andreani	M Aronson	C Davies
D Arnold	P Bingham	K Edler	P Dai	F Bresme	H Dilger	T Holden
J Claridge	E Bychkov	T Hase	B Lake	S Golunski	N Morley	A Lodini
E Cussen	C Cabrillo	S Lee	S Raymond	M Karlsson	A Suter	J Quinta da Fonseca
M Hofmann	L Dougan	T Nylander	H Ronnow	M Krzystyniak	I Terry	R Reed
C Knee	J Holbrey	S Prescott	N Shannon	M P Marques	T Veal	H Stone
A McLaughlin	G Monaco	D Scott	C Stock	A Nogales Ruiz	I Watanabe	M Yescas
S Skinner		E Sivaniah		A Sartbaeva		
A Thompson		I Tucker		R Senesi		
P Vaqueiro-Rodriguez						
I Wood						
S Hull	A Hannon	J Webster	J Taylor	F Fernandez-Alonso	A Hillier	S Y Zhang
M Tucker	D Bowron	M Skoda	R Ewings	F Demmel	S Cottrell	J Kelleher

ISIS User Committee Membership December 2013

The ISIS User Committee represents the user community on all aspects of facility operation.

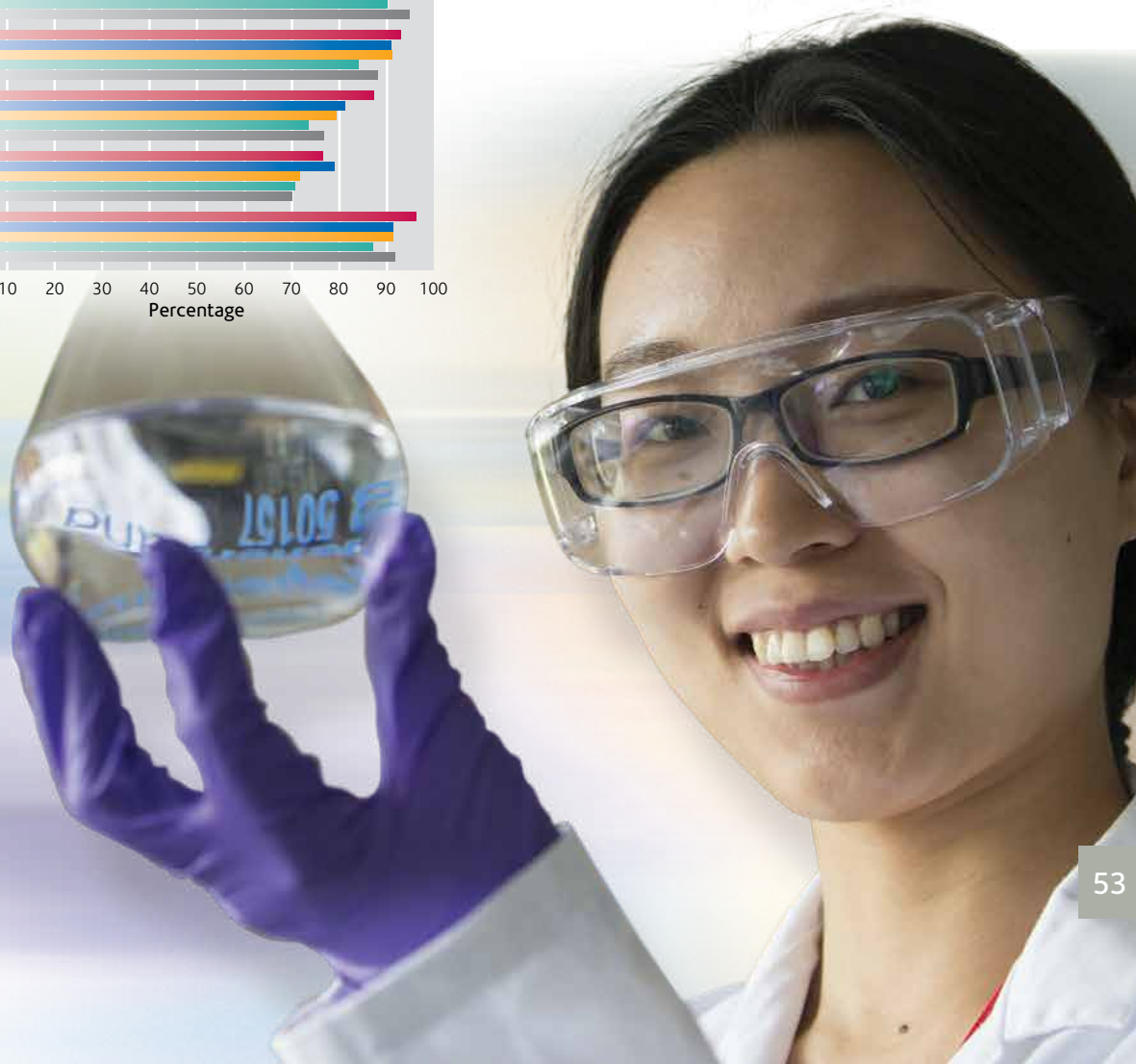
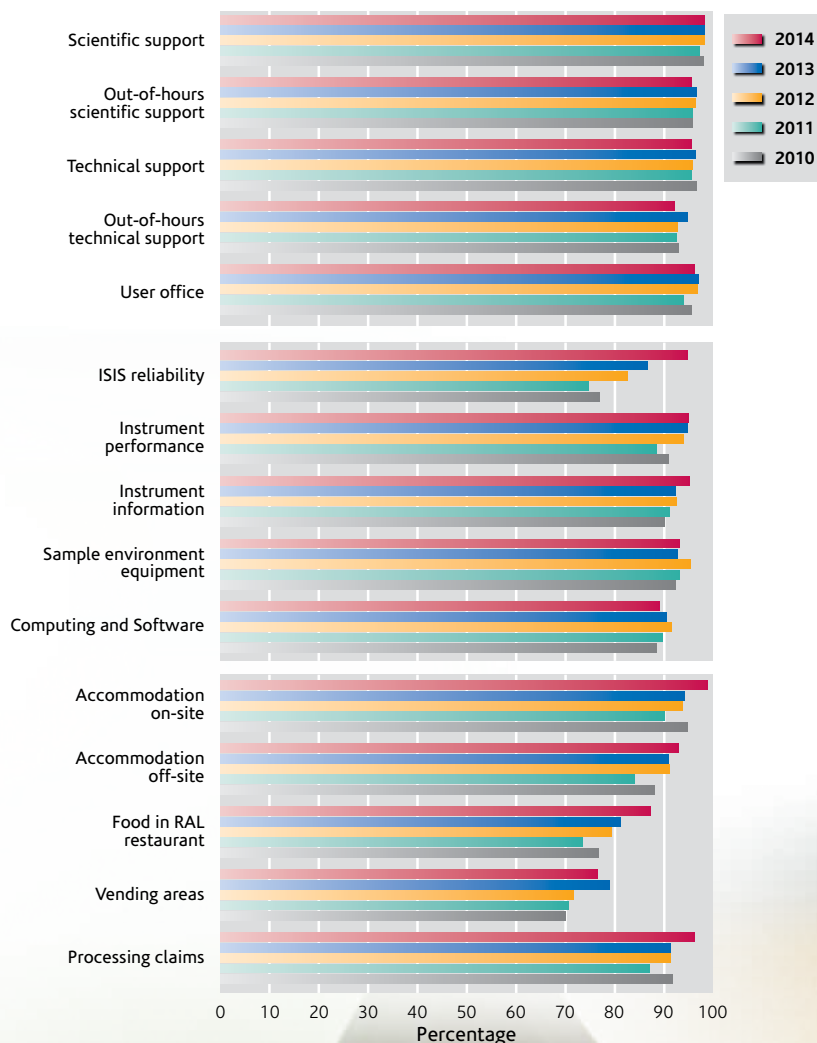
IUG1 Crystallography	Peter Slater Anthony Powell	University of Birmingham Herriot Watt University
IUG2 Disordered Systems	John Holbrey Beau Webber	Queen's University, Belfast University of Kent
IUG3 Large Scale Structures	Ali ZARBAKSH Jeremy Lakey	Queen Mary College, London University of Newcastle upon Tyne
IUG4 Excitations	Jon Goff (Chair) Phil Salmon	Royal Holloway, University of London University of Bath
IUG5 Molecular Spectroscopy	Christoph Salzmann Sylvia McLain	University College, London University of Oxford
IUG6 Muons	Don Paul Alan Drew	University of Warwick Queen Mary College, London
IUG7 Engineering	David Dye Michael Preuss Hongbiao Dong	Imperial College, London University of Manchester University of Leicester

ISIS representatives

Debbie Greenfield	Head, ISIS Instrumentation Division
Andrew Kaye	ISIS User Programme Manager
Philip King	Head, ISIS Spectroscopy and Support Division
Sean Langridge	Head, ISIS Diffraction and Materials Division
Robert McGreevy	Director, ISIS
Steve Wakefield	ISIS Experimental Operations Division

User Satisfaction

All users visiting the facility are asked to complete a satisfaction survey which addresses scientific, technical and administrative aspects of their experience in using ISIS. This feedback helps to ensure a high quality service is maintained and improved where possible.



Beam statistics 2013-14

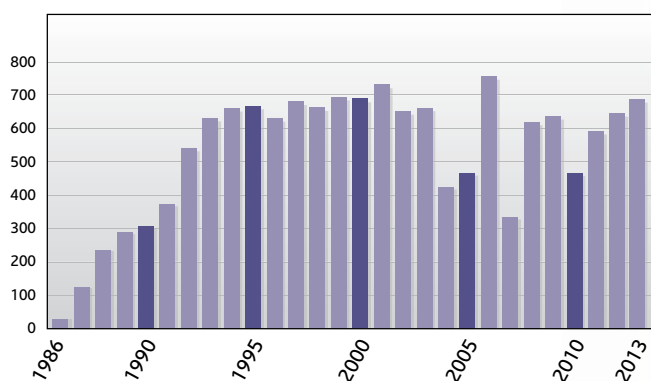
For the period of this report and during scheduled operating cycles, ISIS delivered a total of 694mA.hrs of user proton beam to the muon and neutron targets.

Cycle	13/1	13/2	13/3	13/4	13/5
	14 May – 13 Jun 2013	23 Jul – 9 Aug 2013	17 Sep – 1 Nov 2013	5 Dec – 20 Dec 2013	11 Feb – 4 Apr 2014
Beam on target (hr)	610	374	985	335	1064
Total beam current delivery for both targets (mA-hr)	129.2	77.0	206.8	67.7	213.4
Averaged combined beam current per hour (µA)	211	209	213	202	197

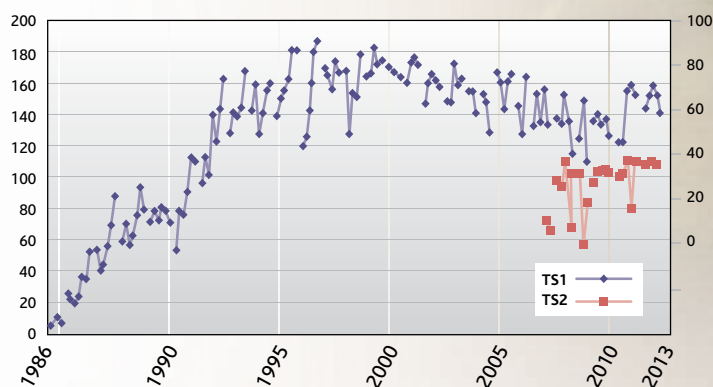
ISIS operational statistics for year 2013-2014.

Year	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
Total integrated current (mAh)	647	409	445	738	317	612	630	459	583	642	694
Average beam current (µA)	177	177	178	179	176	177	208	197	194	203	206

Year-on-year ISIS performance summary for the past 10 years.



ISIS annual integrated current (mAh).



ISIS mean current averaged over a cycle (µA).



Other Statistics

In the 2013-2014 year:

- 801 experiments were run
- 3154 days were delivered to the user programme
- 2736 visits to the facility were made by 1366 individual users, 674 of which were students
- 59 separate companies were involved in ISIS experiments, from large multi-nationals to small hi-tech start-ups
- Over 100 individual Research Council grants supported ISIS proposals
- 446 journal publications came out in 2013 based on ISIS research (see end of this review).

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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

www.stfc.ac.uk/isis

Head office: Polaris House, North Star Avenue, Swindon SN2 1SZ, United Kingdom.

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