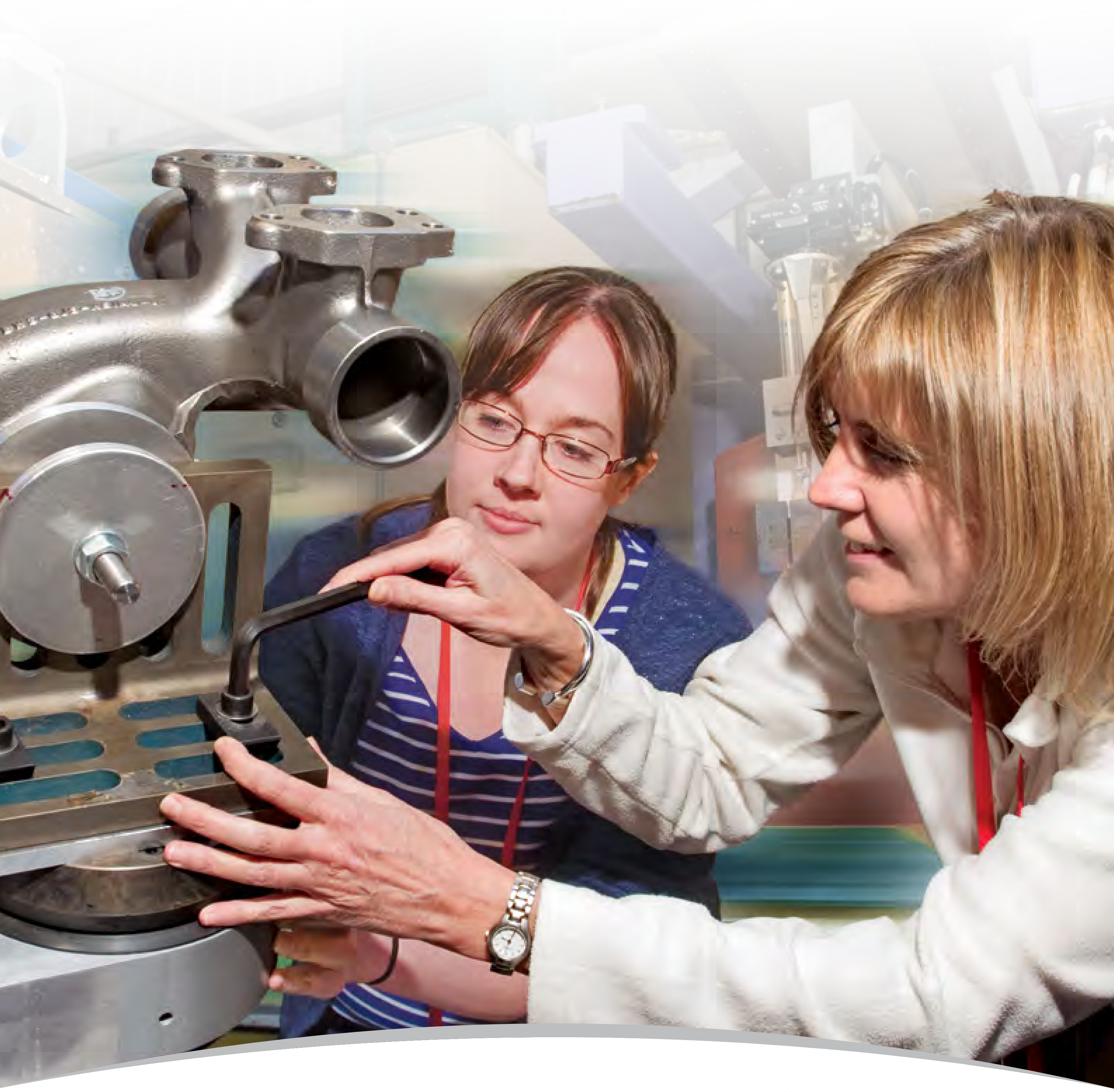
ISIS 2013

neutron and muon source annual review



Science & Technology Facilities Council

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Contents

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2013 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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Visits

Left: *Prof Sir Michael Stirling, Chair of STFC Council, talking with Max Skoda (ISIS) during a visit by STFC Council in January 2013.*

Far left: *Delegations from the Chinese Academy of Sciences, CAS, and RIKEN jointly toured the ISIS facility at STFC's Rutherford Appleton Laboratory on 19th March 2013. Robert McGreevy, ISIS Director with Qiu Huasheng (CAS) and Kenji Oeda, (RIKEN) during a tour of TS2.*

Above: Sir Mark Walport, Government Chief Scientific Advisor, visits ISIS with John Womersley (STFC)

"ISIS is one of the world-leading facilities that makes Harwell such a draw for researchers of all kinds."
Vince Cable MP

Foreword

Below: Members of the MAPS, MARI and TOSCA Instrument Review Panel: front row left to right; David Lennon, Helmut Schober and Richard Catlow.
Back row; Tobias Unruh, Ken Anderson, Hannu Mutka and Bella Lake

Left: Andrew Taylor (STFC), Secretary of State Vince Cable MP and John Womersley (STFC) in TS2.

Having been away from ISIS for a year, working at Oak Ridge National Laboratory in the USA, it is great to get back and find that nothing has changed – which is a good thing! As this annual review clearly shows, ISIS is still a world class facility for neutron scattering and muon spectroscopy. Despite the on-going budget challenges (though we have to acknowledge that science has been relatively well treated by the UK government) the broad-based scientific programme continues to be excellent. Technical development and innovation in the accelerator, targets, instruments, sample environments and software both support and enhance the programme. Experiments are increasingly complex, with ever-faster measurements on ever-smaller samples.

But maybe it is time for some change? In December 2014 ISIS celebrates 30 years of operations. To remain at the forefront for another 30 years change will be necessary – the status quo is not an option. There is plenty of great science that can be done with current capabilities, or with technical improvements that can already be foreseen. Much of this science addresses ‘global challenges’, such as energy, that are not going to disappear. So there is, and will continue to be, significant demand for neutrons and muons. The main current limitation to effective exploitation is capacity – there just aren’t enough sources and instruments available. For example, the ISIS Collaborative Research and Development scheme (see page 36) has been very successful in attracting increasing industrial use of neutrons, but we have very rapidly hit the limit, in terms of available instrument time, of what we can provide in areas such as engineering. Even with the European Spallation Source, there will be decreasing capacity for neutron scattering in Europe in the next decade unless action is taken.

Andy Warhol said, “They always say that time changes things, but you actually have to change them yourself.” So we are developing a new strategy for ISIS. The goal is to double our capacity by 2020, while significantly decreasing our cost per experiment. An upgrade to the first target station target and moderator will be an important element. We also aim to reduce the ‘time to market’ from proposal to publication. A small step in this direction is our recent decision to offer Xpress access on all instruments. I am looking forward to working with our staff and colleagues in STFC and the other UK Research Councils, our user community and international partners including other neutron and muon sources worldwide, to drive forward these changes and secure the future for ISIS.

Robert McGreevy,
Director ISIS

PS I would like to add a personal note of thanks to Uschi Steigenberger, who postponed her retirement and stepped in as Director of ISIS from April to September 2012. Uschi worked tirelessly for the success of ISIS over many years, so we hope she enjoys some well-earned leisure.

An Introduction to **ISIS**

ISIS is a world centre for research in the physical and life sciences at the Rutherford Appleton Laboratory near Oxford in the United Kingdom.

We support a national and international community of more than 3000 scientists for research into subjects ranging from clean energy and the environment, pharmaceuticals and health care, through to nanotechnology and materials engineering, catalysis and polymers, and on to fundamental studies of materials.

ISIS uses neutrons and muons to study how materials work at the atomic level. This enables us to understand every-day materials properties – and so make new ones tailor-made for particular applications.

Why use neutrons and muons?

The neutron is a powerful probe of the atomic-level properties of solids and liquids. Neutrons are able to study both structure and dynamics – where atoms are and how atoms are moving. The neutrons used at ISIS have wavelengths which are comparable to atomic spacings, and so can be used to study structures from the Ångstrom to the micron scale. At the same time, they have energies similar to those of atomic and electronic processes enabling lattice vibrations, molecular motions, diffusion and tunnelling to be explored.

Neutrons scatter from the nucleus of an atom rather than the electron cloud (which x-rays scatter from). This means that light atoms, such as hydrogen, can be seen in the presence of heavier atoms. Neighbouring elements in the periodic table can be distinguished, and different isotopes of the same element can be used to label parts of molecules and enhance the technique's sensitivity. The relatively weak interaction of neutrons with matter makes them a penetrating probe, so that complex sample environment can be used. And neutrons have a magnetic moment, making them suitable for studying magnetic materials.

Muons are an alternative probe of the structure and dynamics of materials. Their applications span a broad range of science areas, and they often provide complementary information to that given by neutrons.

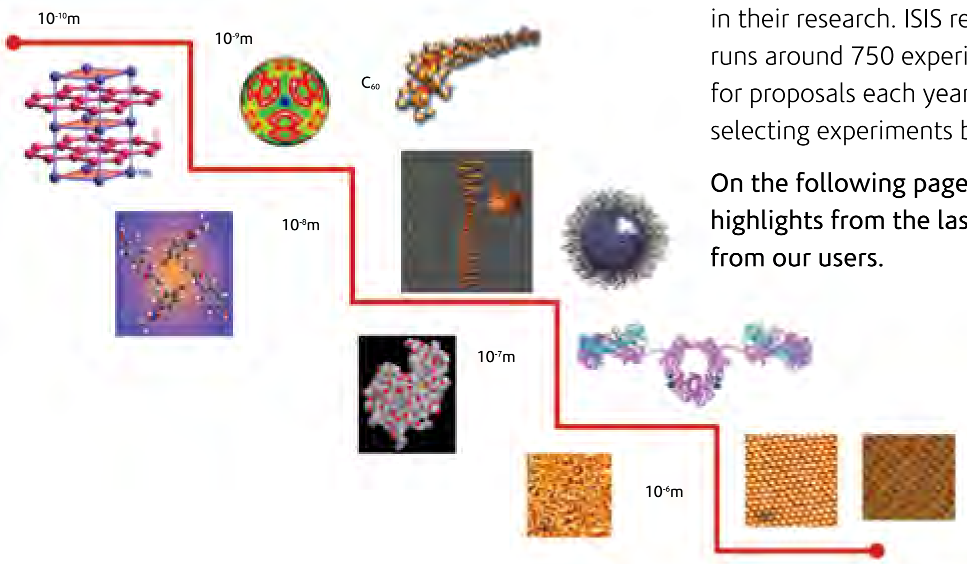
Producing neutrons and muons

Neutrons are produced at ISIS by the 'spallation' process. A heavy metal target is bombarded by an energetic proton beam from a circular, synchrotron accelerator, driving neutrons from the metal nuclei. The neutrons produced in the target are slowed to energies (wavelengths) useful for studying materials by hydrogenous moderators around the target. They are then directed to some 25 instruments, each optimised to explore different atomic-level properties. Muons are produced by the interaction of the proton beam with a thin carbon target and fed to seven experimental areas.

A user facility

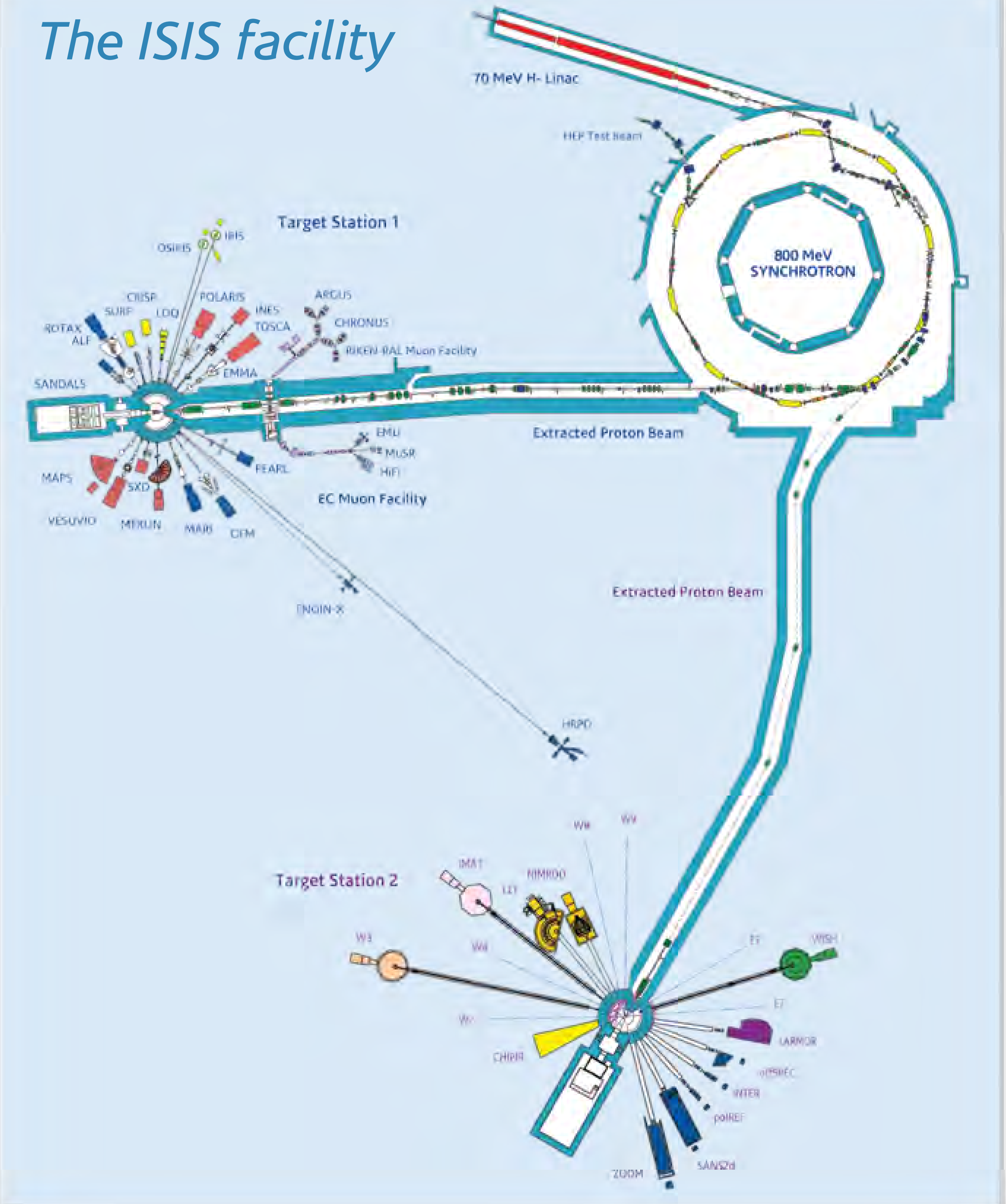
ISIS is a facility dedicated to enabling external researchers – from academia and industry – to use neutrons and muons in their research. ISIS receives around 3000 user visits and runs around 750 experiments per year. It holds two calls for proposals each year, with peer-review panels of experts selecting experiments based on scientific excellence.

On the following pages we described some of the highlights from the last 12 months of excellent science from our users.



Neutrons can be used to study a wide range of length scales – from the Angstrom to the micron level.

The ISIS facility




CIENCE

Biological science

Chemically programmed self-sorting of gelator networks

Instrument: LOQ

KL Morris (Sussex), L Chen, J Raeburn (Liverpool), OR Sellick (Cardiff), P Cotanda (Warwick), A Paul (Cardiff), PC Griffiths (Greenwich), SM King (ISIS), RK O'Reilly (Warwick), LC Serpell (Sussex) and DJ Adams (Liverpool)

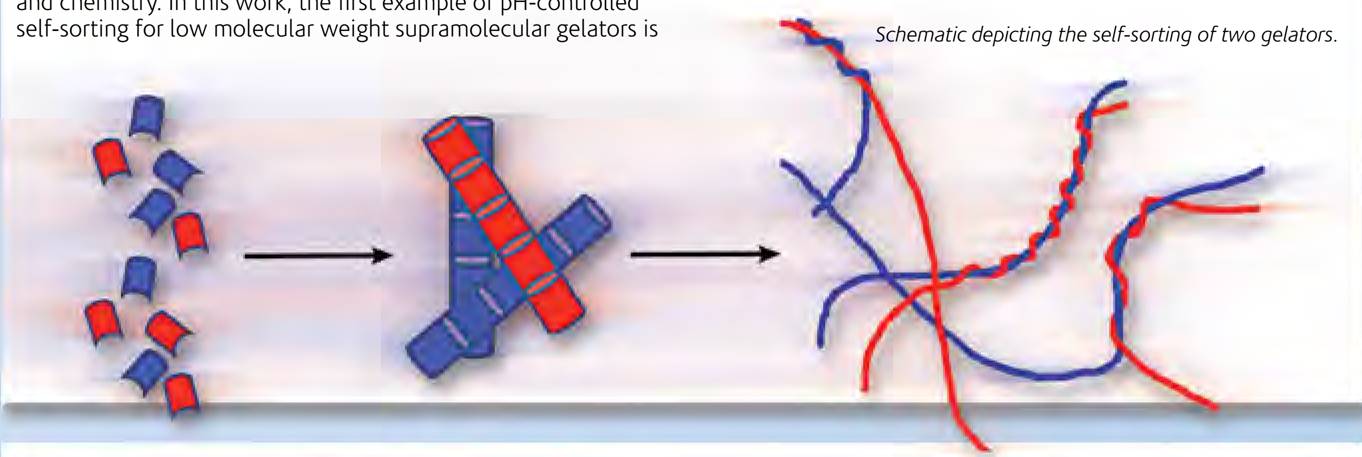
Support for research: EPSRC grant (EP/G012741/1)

Controlling the order and spatial distribution of self-assembly in multi-component supramolecular systems is extremely challenging. When self-assembly occurs in a solution containing two different molecules the molecules can either co-assemble or self-sort, where like-like intermolecular interactions result in the formation of two, co-existing assemblies. However, self-sorting is a real challenge in many self-assembling systems; in water it is especially difficult to pre-design the self-sorting of two molecules with relatively similar molecular structures and chemistry. In this work, the first example of pH-controlled self-sorting for low molecular weight supramolecular gelators is shown. The order of assembly can be controlled, with the pH at which each component assembled being pre-programmed by the acid strength of the gelator. Self-sorting at multiple length scales has been demonstrated by a number of techniques including small angle neutron scattering. This pH-programming method is being used to form new, interesting and complex structures.

Further reading: KL Morris *et al*. Nature Commun. 4 (2013) 1480.

Contact: DJ Adams, d.j.adams@liverpool.ac.uk

Schematic depicting the self-sorting of two gelators.



Bringing things to order

Instrument: SANS2d

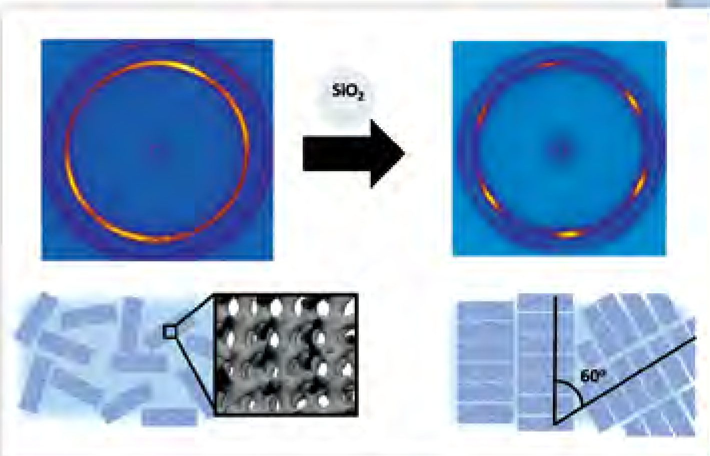
CM Beddoes, JE Bartenstein, K Lange, WH Briscoe (Bristol), R Heenan, S Rogers (ISIS)

Support for research: EPSRC, BCFN, ILL

Amphiphilic (water-loving) molecules (such as lipids) can self-assemble to form nanometer-sized meso-structures of various shapes in aqueous solutions, e.g. lamellar phases with multiple flat sheets and highly curved hexagonal tubular phases. Bicontinuous cubic phases, which contain two continuous but non-connecting water channels separated by the lipid bilayer, twisted so the average curvature on the lipid surface is zero, are particularly interesting. Normally, cubic phase domains are oriented randomly, without any directional preference. It has been shown that the addition of silica nanoparticles (0.126%) can induce long range ordering of the cubic domains of a common lipid (30% monoolein in water). Data from SANS2d show anisotropy persisting on heating to 60°C and cooling. This finding is particularly relevant to soft nanocomposite materials and the fundamentals of nanotoxicity where the interactions between nanoparticles and lipid mesophases are a vital consideration.

Further reading: J Bulpett, WH Briscoe, Soft Matter, submitted (2013).

Contact: WH Briscoe, wuge.briscoe@bristol.ac.uk



Adding silica nanoparticles promotes long range orientation in a bicontinuous gyroid cubic phase of a lipid, seen by the sharpening of the spots in the SANS patterns.

Tackling the Great Wall of *E. Coli*

Instrument: INTER

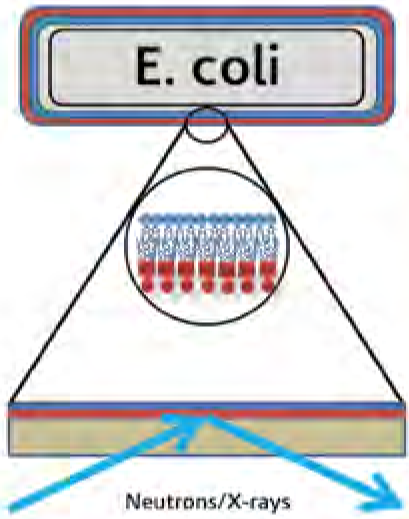
LA Clifton (ISIS) , AP Le Brun, SA Holt, (ANSTO) JH Lakey (Newcastle)

Support for research: Wellcome Trust

E. coli & *Salmonella* food poisoning, bubonic plague, bacterial meningitis, and Legionnaires' disease are all caused by Gram negative bacteria (GNB) which possess a characteristic 'outer' membrane. This outer membrane is a 5 nm thick bilayer with different molecules in each layer making it unusually asymmetric. The outer layer contains a molecule unique to GNB called LPS which presents a formidable barrier and an additional way to develop antibiotic resistance. Neutrons and X-rays can be used to investigate this structure but individual bacteria are too small to give a good signal in either technique. Model outer membranes can be built in the laboratory which can then be tested with antibiotics and other drugs. This study has shown that suitable asymmetric layers necessary for a useful model can be constructed and their molecular structure determined accurately. It is now possible to understand how this barrier to antibiotics is stabilised and how we might overcome it in the clinic.

Further reading: AP Le Brun, *et al*, Biomacromolecules 2013 Jun 10;14(6):2014-22.

Contact: JH Lakey, Jeremy.Lakey@ncl.ac.uk



By creating accurate models of bacterial outer membranes we can make them accessible to structural techniques and understand how they interact with antibiotics.

Damage to lung surfactant following exposure to the environmental pollutant ozone

Instrument: SURF INTER

KC Thompson, JM Hemming, J Szyroka (Birkbeck), AR Rennie (Uppsala), T Arnold (Diamond Light Source), M Skoda (ISIS)

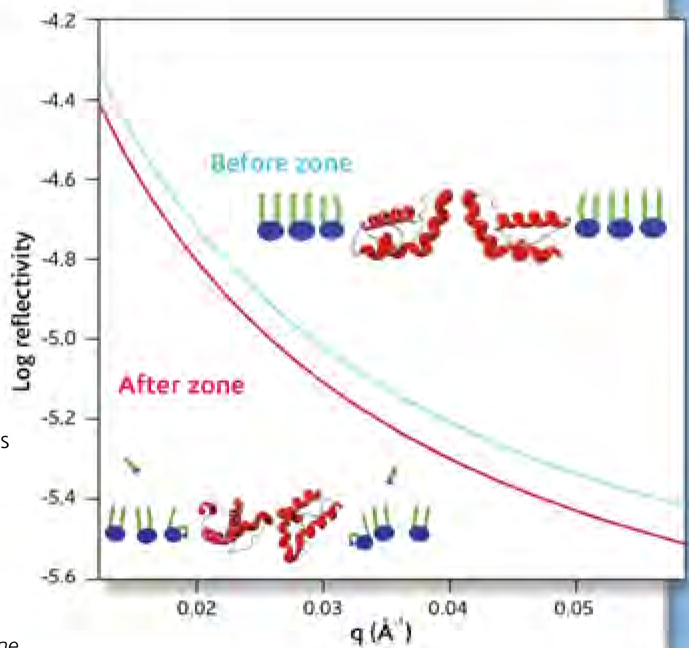
Support for research: Wellcome Trust

The interface of the lung with inhaled air is wet, with the presence of a layer of surfactant containing a mixture of both lipids and proteins on the wet surface, which are essential to maintain a low surface tension. This prevents acute respiratory distress, a potentially fatal condition.

The surfactant layer is directly exposed to atmospheric air and pollutants such as ozone. During episodes of high pollution on sunny days in city centres, ambient ozone levels frequently exceed air-quality limits. These ozone levels are directly linked to significantly increased death rates from respiratory failure. This study has exposed natural pig and sheep lung surfactant to low ozone levels and used neutron and x-ray reflection to follow changes to the structure of the air-water interface. The results show that the surfactant reacts rapidly with the ozone leading to a change in the surface tension, a slight reduction in the amount of material at the interface and a significant thinning of the surfactant layer.

Further reading: KC Thompson *et al.*, Langmuir 29 (2013) 4594.

Contact: KC Thompson, k.thompson@bbk.ac.uk



Neutron reflection profiles before and after lung surfactant is exposed to ozone. Some lipid material is lost from the interface and the damaged film rearranges.

Catalysis

What do you do when the oil runs out?

Instrument: TOSCA, HET

NG Hamilton, IP Silverwood, R Warringham, J Kapitán, L Hecht, and D Lennon (Glasgow), PB Webb, RP Tooze (Sasol UK Ltd), SF Parker (ISIS)

Support for research: University of Glasgow, STFC Centre for Molecular Structure and Dynamics, and Sasol Technology UK Ltd

With the increasing scarcity and rising cost of crude oil, the last few decades have witnessed a resurgence of research activity into Fischer–Tropsch (F-T) catalysis. This process manufactures gasoline and diesel from syngas ($CO+H_2$) using an iron or cobalt-based catalyst. To better understand the active catalyst, a sample was taken from a working F-T reactor at Secunda in South Africa. INS spectroscopy using TOSCA and HET showed a surprisingly well-defined 'molecular-like' spectrum. Simulation of the spectra with models consisting of partially hydrogenated aromatic molecules could account for the molecular-like features, although it could not account for the largely structureless low energy region. A role for a hydrocarbonaceous overlayer in the process chemistry is briefly considered. This is a rare example where it has been possible to gain direct insight into the nature of the overlayer present on a commercial working catalyst.

Further reading: NG Hamilton *et al* Angew. Chem. Int. Ed., 52 (2013) 5608-5611.

Contact: D Lennon, David.Lennon@glasgow.ac.uk


Courtesy of Sasol UK Ltd

A Fischer-Tropsch reactor at Secunda in South Africa.

Probing chemistry and kinetics of heterogeneous catalysts

Instrument: NIMROD

TGA Youngs (ISIS), H Manyar (Belfast), DT Bowron (ISIS), LF Gladden (Cambridge), C Hardacre (Belfast)

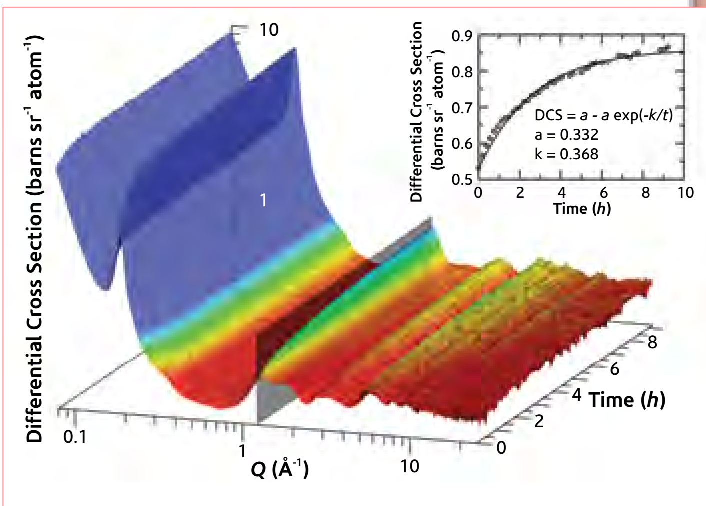
Support for research: EPSRC, Johnson Matthey

Catalysis is big business – estimates suggest that 80% of man-made materials rely on catalysis at some point in their manufacture, and that the industry as a whole is worth in excess of $3 trillion. As such, enabling catalyst design is critical, and to do so it is necessary to first understand them on a fundamental structural level. For liquid-phase heterogeneous catalysts, this means characterisation of the chemical species present and the porous catalyst support, and their interplay on a nanoscopic scale.

NIMROD has been used to study the hydrogenation of benzene and, by employing a reduced pressure of hydrogen, time-resolved data have been collected on the nanometre, molecular, and atomic length scales as the reaction proceeds. From the resulting data several kinetic regimes can be extracted, corresponding to specific processes occurring within the system. This unique study shows that, in principle, the complete kinetics and chemistry of a heterogeneous catalytic process can be obtained with total scattering techniques.

Further reading: TGA Youngs *et al*., Chem. Sci., 2013, 4 (9), 3484 – 3489.

Contact: TGA Youngs, tristan.youngs@stfc.ac.uk and C Hardacre, c.hardacre@qub.ac.uk



Time-resolved F(Q) data for benzene hydrogenation. A slice taken through the data at Q = 1.22 Å⁻¹ reveals the kinetics of changes related to the intermolecular spacing in the liquid.

Boost for carbon capture from new functional materials

Instrument: WISH, TOSCA

S Yang, DP Anderson, R Newby, AJ Blake, M Schröder (Nottingham), J Sun (Peking), AJ Ramirez-Cuesta, SK Callear, WIF. David (ISIS), JE Parker, CC Tang (Diamond Light Source)

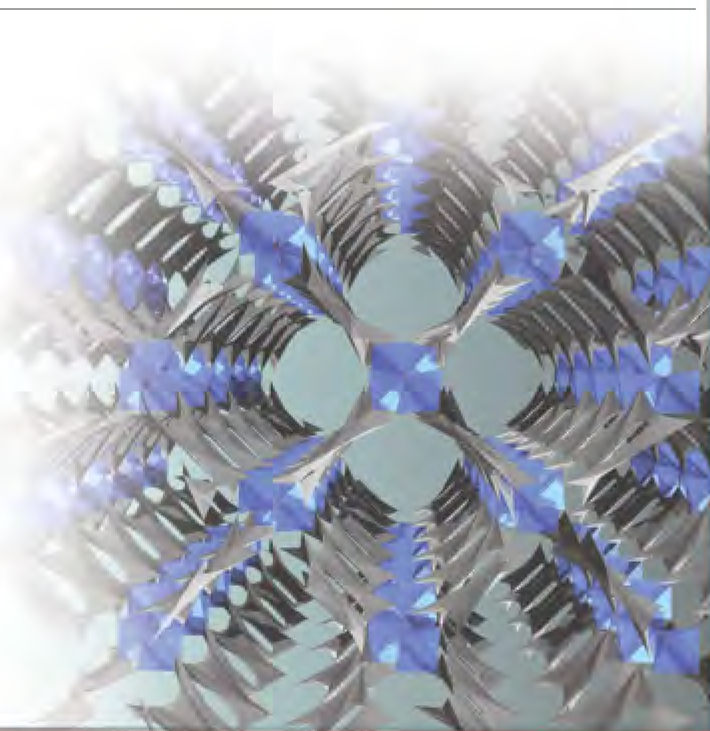
Support for research: Leverhulme Trust, EPSRC, University of Nottingham

Understanding the mechanism by which porous solids trap harmful gases such as CO_2 and SO_2 is essential for the design of new materials for their selective removal. Materials functionalised with amine-groups dominate this area, largely because of their potential to form carbamates, thereby trapping CO_2 covalently. The use of these materials is energy-intensive, however, with significant environmental impact.

Recently a non-amine-containing porous solid (denoted as NOTT-300) has been synthesised, in which hydroxyl groups within pores bind CO_2 and SO_2 selectively. Synchrotron X-ray diffraction and inelastic neutron scattering studies, combined with modelling, reveal that these hydroxyl groups bind CO_2 and SO_2 via the formation of moderate supramolecular and hydrogen bonds. Such weak interactions lead to low isosteric heat of adsorption and therefore zero heating input is required to release captured CO_2 and regenerate NOTT-300. This offers the potential for application of new 'easy-on/easy-off' capture systems for CO_2 and SO_2 that carry fewer economic and environmental penalties.

Further reading: S Yang *et al*., Nature Chem. 4 (2012) 887.

Contact: S Yang, Sihai.Yang@nottingham.ac.uk



View of the extended framework structure for NOTT-300 with one-dimensional channels (aluminium centre: blue; organic ligand: grey)

Battery materials

Muons watch as lithium ions go by

Instrument: EMU, MuSR

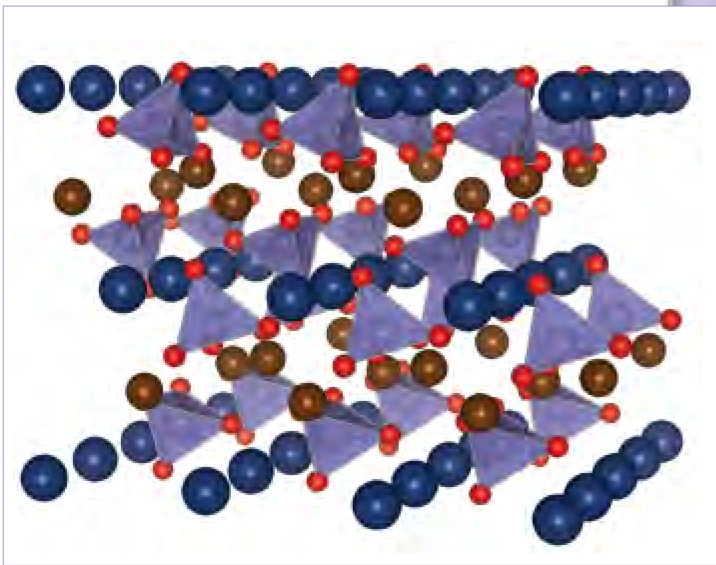
PJ Baker, FL Pratt (ISIS), I Franke, T Lancaster, D Prabhakaran, W Hayes, and SJ Blundell (Oxford)

Support for research: EPSRC

The rate of ionic diffusion in lithium battery materials determines how quickly they can be charged and discharged, but despite being of vital technological importance it can be quite hard to measure. In lithium iron phosphate, measurements of the diffusion rate using different techniques vary over nine orders-of-magnitude. Muons provide a way of measuring the diffusion process over the shortest length scales. A lithium ion hopping along a diffusion channel perturbs the magnetic field that the muon experiences from its environment, allowing the hopping rate to be measured. From this an estimate of the diffusion rate can be obtained. We were able to conclude that in lithium iron phosphate the diffusion rate is quite fast on the short length scale probed by muons, but mesoscopic effects such as the blocking of diffusion channels by defects and grain boundaries must limit the bulk value. This suggests that making nanoparticles of this material could help to overcome these problems.

Further reading: PJ Baker *et al.*, Phys. Rev. B 84 (2011) 174403.

Contact: PJ Baker, peter.baker@stfc.ac.uk



Muons record the rate of lithium ion hopping in $LiFePO_4$.

Nature of the band gap and origin of the conductivity of PbO_2 revealed by theory and experiment

Instrument: POLARIS

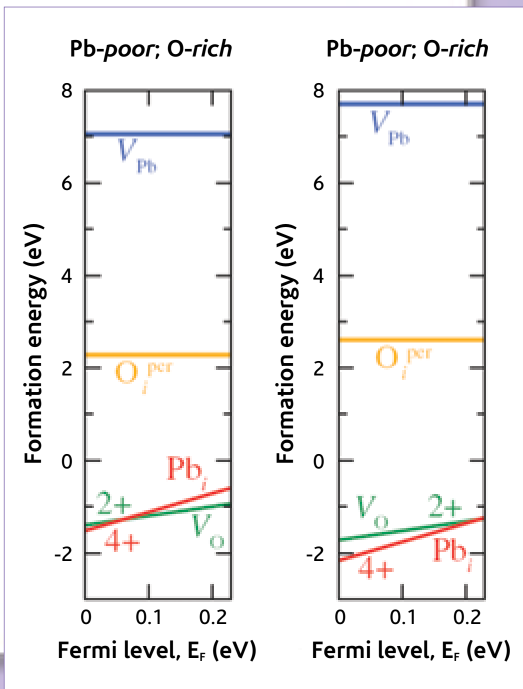
D O Scanlon, A B Kehoe, and G W Watson (Dublin), M O Jones and W I F David (ISIS), D J Payne, R G Egdell, and P P Edwards (Oxford), A Walsh (Bath)

Support for research: University funding

Lead dioxide has been used for over a century in the lead-acid battery. Many fundamental questions concerning PbO_2 remain unanswered, principally: (i) is the bulk material a metal or a semiconductor, and (ii) what is the source of the high levels of conductivity? The electronic structure and defect physics of PbO_2 has been calculated, using a hybrid density functional, and show that it is an *n*-type semiconductor with a small indirect band gap of ~0.2 eV. The origin of electron carriers in the undoped material is found to be oxygen vacancies, which form a donor state resonant in the conduction band. A dipole-forbidden band gap combined with a large carrier induced Moss-Burstein shift results in a large effective optical band gap. The model is supported by neutron diffraction, which reveals that the oxygen sublattice is only 98.4% occupied, thus confirming oxygen substoichiometry as the electron source.

Further reading: A. Walsh *et al.*, Chemical Communications 49, 448-450 (2013).

Contact: GW Watson, watsong@tcd.ie



Formation energies for intrinsic defects in PbO_2 under O-rich (left) and O-poor (right) conditions

Superconductivity

A new family of unconventional superconductors?

Instrument: MuSR

AD Hillier (ISIS), J Quintanilla (ISIS/Kent), B Mazidian, JF Annett (Bristol/ISIS), and R Cywinski (Huddersfield)

Support for research: EPSRC, SEPnet, and STFC

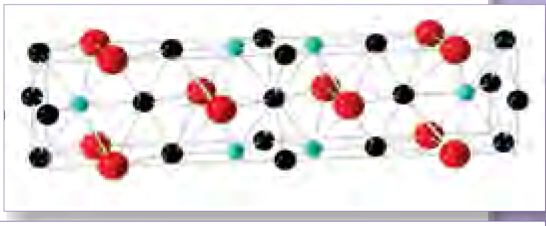
Superconductivity is a state of matter reached by some materials when they are cooled to very low temperatures. In addition to its technological applications, superconductivity is also a useful playground for physicists – for example, the theory predicting the Higgs boson is based on broken-symmetry ideas from superconductivity.

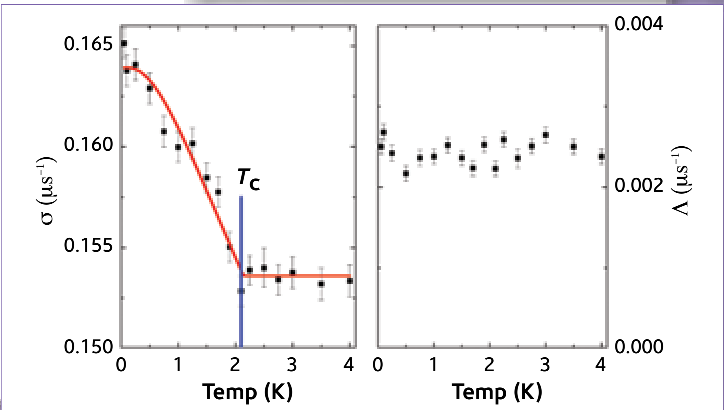
At the heart of superconductivity is Cooper pairing, a phenomenon in which electrons circumvent their mutual repulsion to form pairs. Experimental and theoretical evidence show that in $LaNiC_2$ and $LaNiGa_2$ the structure of the Cooper pairs is highly unusual: electrons whose intrinsic magnetisations point in different directions participate differently in the pairing. This phenomenon, called non-unitary triplet pairing, has only been encountered before in materials whose non-superconducting state is already magnetic. This suggests that a hitherto overlooked coupling between magnetism and superconductivity is behind this, suggesting that a re-examination of the relation between these two important phenomena may be necessary.

Further reading: AD Hillier *et al*., Phys. Rev. Lett. 109.097001 2012.

Contact: AD Hillier, Adrian.hillier@stfc.ac.uk

The crystal structure of $LaNiGa_2$ and the observation of symmetry-breaking fields.





Molecular intercalates of iron-based superconductors

Instrument: GEM, MuSR

M Burrard-Lucas, DG Free, SJ Sedlmaier, JD Wright, SJ Cassidy, AJ Corkett, SJ Blundell, SJ Clarke (Oxford), Y Hara, (Ibaraki), T Lancaster (Durham), PJ Baker (ISIS)

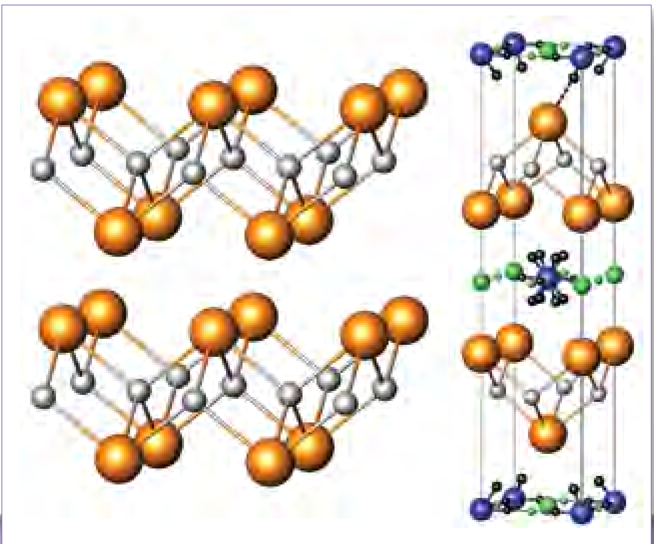
Support for research: EPSRC Grant EP/I017844, Diamond Light Source (Studentship support)

Iron arsenides and selenides are a new class of unconventional high temperature superconductor with layered crystal structures, exhibiting superconductivity at temperatures as high as about 50 K. The interplay between superconductivity and magnetism is sharply dependent on chemical composition or applied pressure. By intercalating ammonia along with lithium and amide molecules between the layers of iron selenide, the superconducting transition temperature can be increased by a factor of 5. The crystal structure and fundamental superconducting properties of this metastable phase have been revealed from a combination of neutron powder diffraction, magnetometry and muon-spin rotation spectroscopy. This study offers the possibility of realising numerous molecular intercalates, and of using substitutions in the intercalate layer or the amount of the intercalate molecule in the compound to control the interplay of magnetism and superconductivity.

Further reading: M Burrard-Lucas *et al*. Nat. Mater. 2013, 12, 15-19.

Contact: SJ Clarke, simon.clarke@chem.ox.ac.uk

Intercalation of lithium and ammonia into iron selenide. The orientationally disordered ammonia molecules are engaged in hydrogen bonding with the selenide ions.



Fundamental chemistry

Theory and experiment moving in harmony

Instrument: SXD

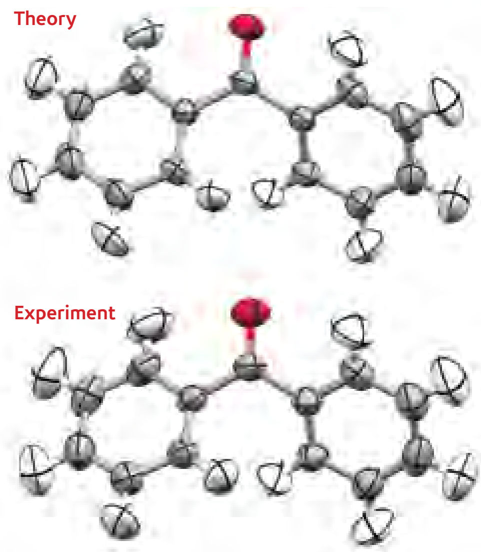
AM Reilly (FHI, Berlin and University of Edinburgh), DA Wann (University of Edinburgh), MJ Gutmann, M Jura (ISIS), CA Morrison and DWH Rankin (University of Edinburgh)

Support for research: University funding (UoE), EPSRC Career acceleration fellowship (DA Wann). Computer resources (HECToR, NSCCS)

Diffraction experiments are often pictured as giving us a static snapshot of crystal structures. In fact diffraction can provide a wealth of information on the vibrations of molecules and hence temperature-dependent phenomena such as proton transfer and phase transformations, which are important in many areas including pharmaceuticals and sensors. Obtaining an accurate description of a crystal structure requires a good representation of this thermal motion. However, many of the most challenging and interesting of experiment studies, such as at high pressure, have limited data and cannot adequately model thermal motion. Can theory help us to perform these difficult experiments? A combined neutron-diffraction and molecular dynamics study of benzophenone has shown how quantum-mechanics based simulations of thermal motion compare well with experiment. This paves the way for routinely using theory to augment the experimental picture of thermal motion in difficult diffraction studies.

Further reading: AM Reilly *et al*., J. Appl. Cryst. 46 (2013) 656.

Contact: AM Reilly, reilly@fhi-berlin.mpg.de



Ellipsoids representing the extent of thermal motion in benzophenone at 300 K from theory and experiment.

Temperature dependent proton dynamics in Li_2NH investigated through inelastic and Compton neutron scattering

Instrument: TOSCA, VESUVIO

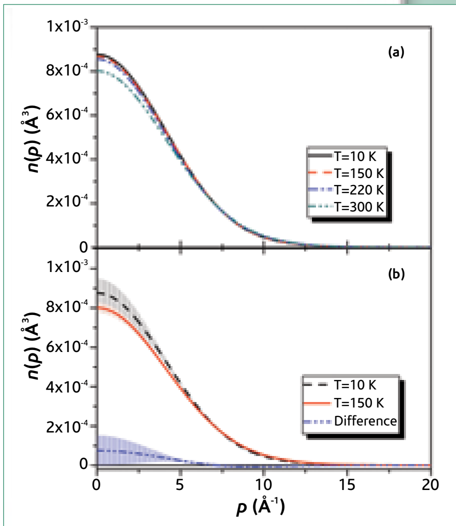
A Pietropaolo (Università degli Studi di Milano-Bicocca, Italy), D Colognesi (ISC-CNR, Italy), M Catti, AC Nale (Università degli Studi di Milano-Bicocca, Italy), MA Adams, AJ Ramirez-Cuesta, J Mayers (ISIS)

Support for research: CNR (Italy) through Cooperation Agreement No. 01/9001 with STFC

Neutron spectroscopic measurements on polycrystalline lithium imide have been performed using inelastic neutron scattering at 20 K, and neutron Compton scattering from 10 K up to room temperature. TOSCA data is used to determine the H-projected density of phonon states up to 100 meV, while the ability of VESUVIO to examine individual elemental species is used to determine the spherically averaged single-particle (i.e., H, Li, and N) momentum distributions and, from this, their mean kinetic energies. Non-Gaussian components of the H momentum distribution are detected at 10 K. However these components do not seem directly connected to the system anharmonicity, being fully compatible with the N-H bond anisotropy. Neutron data are also complemented by lattice dynamics simulations. The trend of single-particle mean kinetic energies in Li_2NH as a function of temperature is not reproduced by simulations, at least as far as H is concerned. Neither its low temperature values nor its temperature trends can be precisely explained in terms of standard phonon calculations, suggesting an interesting complexity to this system.

Further reading: A Pietropaolo *et al*, J. Chem. Phys. 137 (2012) 204309.

Contact: A Pietropaolo, antonino.pietropaolo@enea.it



(a) proton momentum distribution at 10, 150, 220 and 300 K
(b) proton momentum distribution at the two extreme temperatures and their difference.

Chemical reactions in the gas phase: studying the H(Mu)+Br_2 system

Instrument: EMU

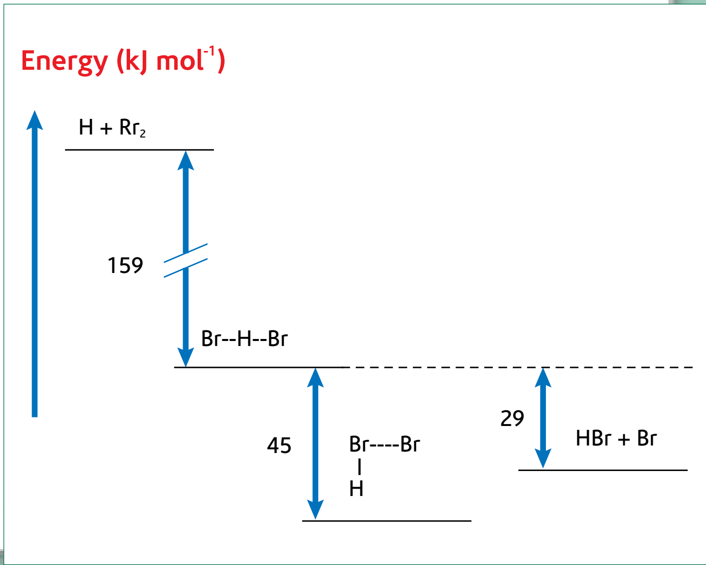
DG Fleming (TRIUMF and British Columbia), SP Cottrell (ISIS), I McKenzie (TRIUMF), RM Macrae (Marian)

Support for research: NSERC (DG Fleming); European Commission, 7th Framework Programme, NMI3

Formation of 'vibrationally bound' Heavy-Light-Heavy quantum systems have been of interest since the early 1980s. Experimentally, studies have focussed on $[I\text{-}H\text{-}I]^-$ but evidence for its existence remains elusive. Muonium (Mu) can be thought of as a light H-atom with the proton replaced by a positive muon. Chemical properties are virtually identical, but with a mass ~1/9th that of H, analogues such as Br-Mu-Br should be much more favourable systems to observe vibrational bonding in. Muon spin relaxation measurements in Br_2/N_2 gas mixtures identified a muoniated radical with an unusually large muon hyperfine coupling constant. *Ab initio* calculations were carried out to investigate the relative energies of product species of the H(Mu)+Br_2 reaction (see Figure) and to calculate coupling constants. While the energetics are consistent with the formation of a strongly bound Br-Mu-Br radical, the large muon coupling appears more consistent with the formation of a Mu···Br_2 van der Waals complex. Further theoretical work is needed to resolve this apparent conundrum for this interesting (but difficult) system.

Further reading: DG Fleming *et. al.*, Phys. Chem. Chem. Phys., 14 (2012) 10953.

Contact: DG Fleming, flem@triumf.ca



Relative energies of the significant species in the H+Br_2 reaction system determined from simple calculations.

Structural disorder and polymorphism in a not-so-simple binary oxide: Ga_2O_3

Instrument: GEM

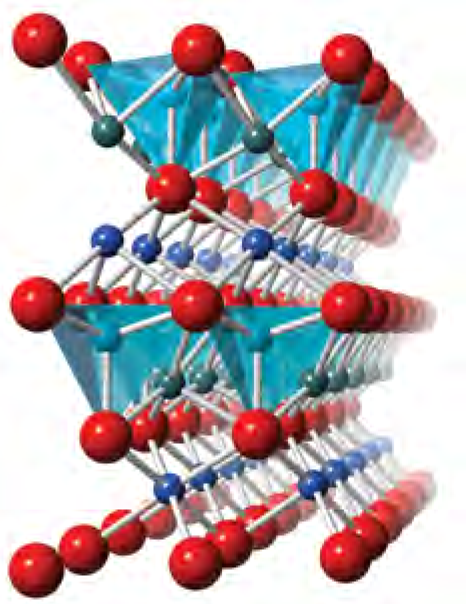
HY Playford, RI Walton (Warwick), AC Hannon, ER Barney (ISIS)

Support for research: STFC CMPC (CMPC08104) and University of Warwick EPSRC Doctoral Training Account

In the past few years gallium oxide, Ga_2O_3, has been the focus of renewed interest for its applications in optics, electronics and catalysis. A deeper understanding of its properties and potential uses is, however, hindered by its complex and poorly understood polymorphism, with uncertainty in the literature as to the existence of some forms. Depending on the synthesis method used, Ga_2O_3 adopts one of several structures and these polymorphs may be structurally disordered and metastable, transforming readily to the β-Ga_2O_3 phase on heating. Total neutron diffraction experiments performed on GEM have allowed the characterisation of several of these disordered polymorphs, including the catalytically active γ-Ga_2O_3, a spinel oxide with locally distorted $[GaO_6]$ polyhedra, and ε-Ga_2O_3, which adopts a layered hexagonal structure. The existence of δ-Ga_2O_3 has been disproved and the existence of orthorhombic κ-Ga_2O_3 (similar to κ-Al_2O_3) determined. This work highlights the importance of probing disordered structures on multiple length scales, even for apparently simple materials.

Further reading: HY Playford *et al.*, Chem. Eur. J. 19 (2013) 2803.

Contact: RI Walton, r.i.walton@warwick.ac.uk



The structure of ε-Ga_2O_3, which contains three crystallographically distinct gallium sites. Gallium shows both distorted octahedral (grey-green and dark blue) and tetrahedral (cyan) coordination.

Magnetism

Spin waves and revised crystal structure of honeycomb iridate Na_2IrO_3

Instrument: MARI

SK Choi, R Coldea, AN Kolmogorov, T Lancaster , SJ Blundell, PG Radaelli (Oxford), II Mazin (Naval Research Laboratory), Y Singh (Indian Institute of Science Education and Research, Mohali), P Gegenwart (Georg-August-Universität Göttingen), KR Choi, SW Cheong (Rutgers), PJ Baker, C Stock, J Taylor (ISIS)

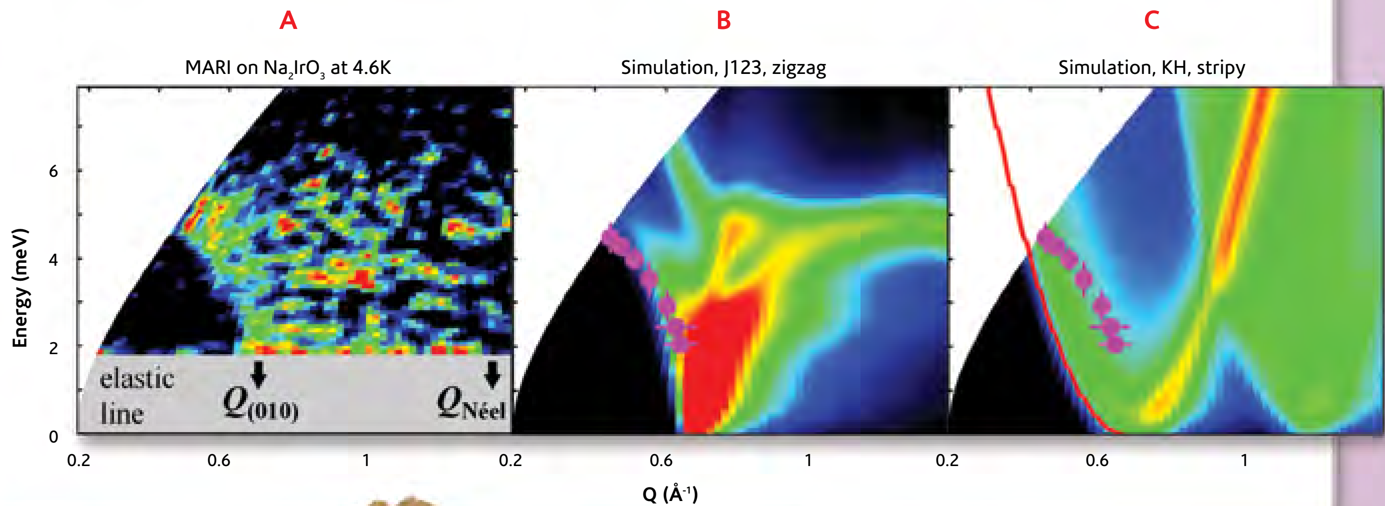
Support for research: EPSRC grant

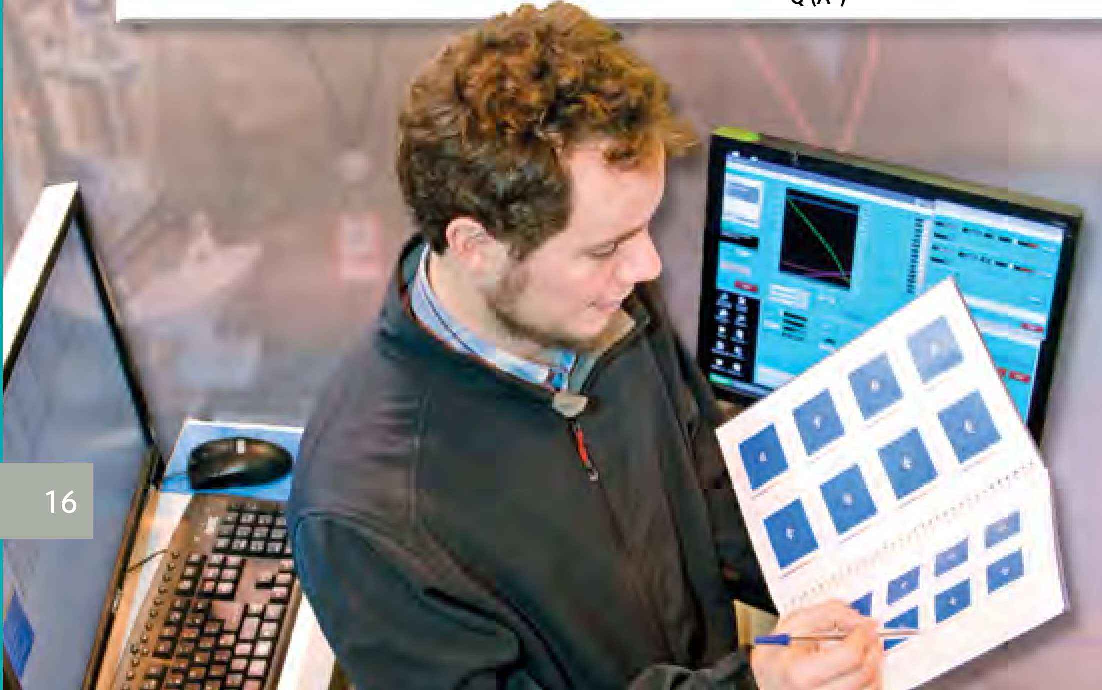
Transition metal oxides of the 5*d* group are currently attracting much attention as candidates to exhibit novel electronic ground states, stabilized by the combined effect of strong spin-orbit coupling and electron correlations. The layered honeycomb material Na_2IrO_3 has been proposed to host novel magnetic states for composite spin-orbital Ir^{4+} j_{eff}=1/2 moments coupled via strongly-frustrated exchanges (the Kitaev model). Using an optimised setup to minimise the very large neutron absorption by Ir nuclei we have successfully observed for the first time dispersive magnetic excitations of Ir magnetic moments. Results provided evidence for a novel zig-zag antiferromagnetic order pattern in the ground state of Na_2IrO_3, stabilized by strong frustration effects from substantial exchanges up to 3rd nearest neighbour couplings. Furthermore, combining single-crystal X-ray diffraction and density functional calculations we have proposed a revised crystal structure model which reveals important departures in the real material from the ideal 90º Ir-O-Ir bonds required for dominant Kitaev physics.

Further reading: SK Choi, R Coldea *et al*., Phys. Rev. Lett. 108 (2012) 127204.

Contact: R Coldea, R.Coldea@physics.ox.ac.uk

A) Inelastic powder neutron scattering data collected on MARI showing a strong spin-wave signal at low energies in good agreement with B) an extended Heisenberg J1-J2-J3 model with zig-zag magnetic order and ruling out a Kitaev-Heisenberg model with stripy order C).





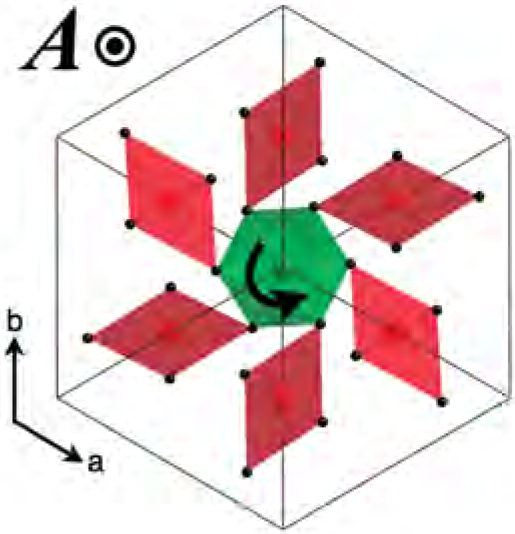
Giant magnetically induced ferroelectricity in multiferroic $CaMn_7O_{12}$

Instrument: WISH

RD Johnson (Oxford), LC Chapon (ILL), DD Khalyavin (ISIS), P Manuel (ISIS), PG Radaelli (Oxford), C Martin (CrisMat, ENSICAEN)

Support for research: EPSRC Grant No. EP/J003557/1, entitled ''New Concepts in Multiferroics and Magnetoelectrics.''

Magnetism and ferroelectricity are widely used properties to store digital information – for example in hard disks and chip-and-pin cards. Usually these two properties are mutually exclusive, but in multiferroics they are coupled, opening the way to faster and more energy-efficient technologies to read and write digital information. Unfortunately all materials so far discovered only work at very low temperatures and their electrical polarisation is very small, making them unsuitable for applications. $CaMn_7O_{12}$, on the other hand, displays 'giant' magnetically induced polarisation persisting up to 90 K – the best performances ever achieved. Intriguingly, the helical magnetic structure, solved through neutron powder diffraction performed at WISH, should not allow for a ferroelectric polarisation at all. However, it has been demonstrated that $CaMn_7O_{12}$ possesses a crystal structure with a special propeller-like "ferroaxial" distortion (see figure), capable of coupling to the magnetic structure and generating electrical polarisation. These results will stimulate the search for other ferroaxial ferroelectrics and even larger electric polarisation.



Further reading: RD Johnson *et al.*, Phys. Rev. Lett. 108 (2012) 067201.

Contact: RD Johnson, r.johnson1@physics.ox.ac.uk

The 'propeller-like' ferroaxial distortion in $CaMn_7O_{12}$, crucial to the development of the giant, magnetically induced ferroelectric polarisation.

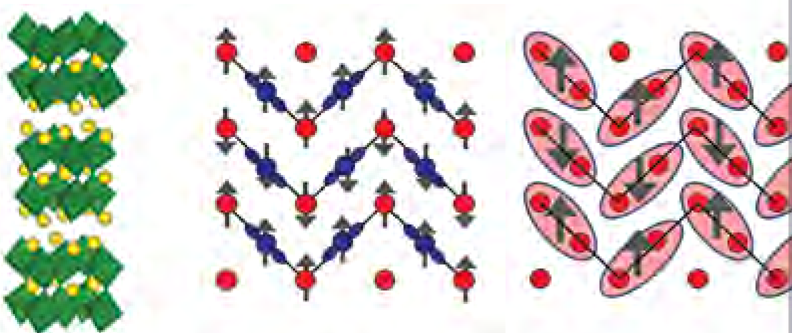
Do Zener polarons exist in a charge ordered manganite?

Instrument: MAPS

GE Johnstone (Oxford), T G Perring (ISIS and UCL), O Sikora (Bristol), D Prabhakaran, AT Boothroyd (Oxford)

Support for research: EPSRC Next Generation Facility Users grant

Certain manganese oxides show colossal magnetoresistance – a reduction of resistance by many orders of magnitude in an applied field of a few Tesla. The phenomenon is most pronounced when the manganite is poised between a ferromagnetic metal and a charge ordered antiferromagnetic insulator. The venerable Goodenough model for the most ubiquitous insulator consists of a stack of sheets with a checkerboard arrangement of Mn^{3+} and Mn^{4+} ions (blue and red ions in the centre panel of the figure). However a more recent and rather controversial picture, the Zener polaron model (right panel), has been proposed in which the magnetic building blocks in the sheets are weakly interacting Mn_2^{7+} dimers. Structural studies to distinguish between these two models have proven ambiguous. The complete spectrum of spin waves measured on MAPS in a naturally layered charge ordered manganite, $Pr(Ca_{0.9}Sr_{0.1})_2Mn_2O_7$, (left panel) unambiguously distinguishes between the two models. The entire measurement is in quantitative agreement with predictions for the Goodenough model, whereas key features of the spin wave dispersion relations and their intensities are inconsistent with alternative Zener polaron models.



***Left**: Crystal structure of $Pr(Ca_{0.9}Sr_{0.1})_2Mn_2O_7$.*
***Centre**: Goodenough model.*
***Right**: Zener polaron model.*

Further reading: G E Johnstone *et al.*, Phys. Rev. Lett. 109 237202 (2012).

Contact: T Perring, toby.perring@stfc.ac.uk

Magnetism

Quantum critical fluctuations in $Sr_3Ru_2O_7$

Instrument: LET

C Lester, T Croft, S M Hayden (Bristol), S Ramos (Diamond Light Source), R S Perry (Edinburgh), EM Forgan (Birmingham), R Bewley ,T Guidi (ISIS)

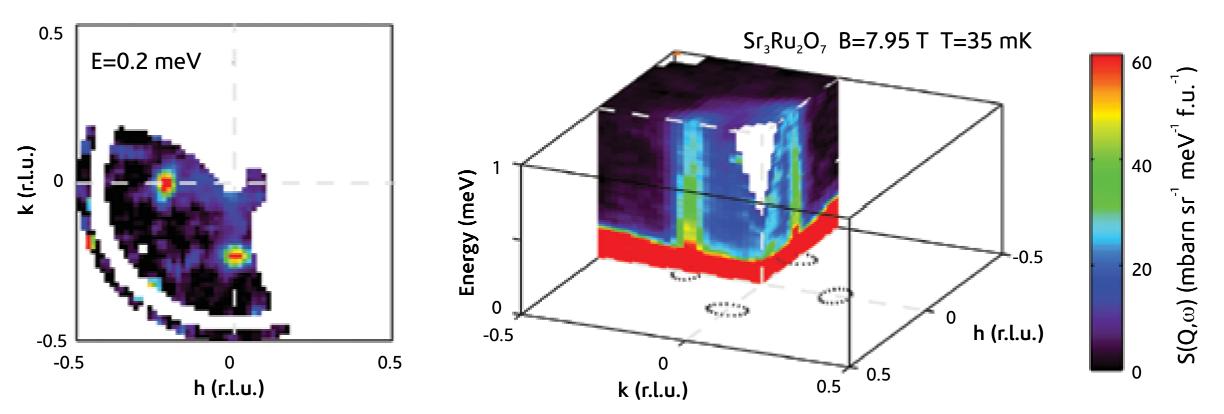
Support for research: EPSRC grant EP/J015423/1

Many novel electronic ground states (such as high temperature superconductivity) form in close proximity to quantum critical points (QCPs), that is, the point where a second order phase transition occurs at zero temperature. By suppressing the second-order metamagnetic transition in $Sr_3Ru_2O_7$ to low temperatures with a magnetic field, the system can be driven into a new and highly unusual electronic ground state. This unusual phase exists below approximately 1 K in the field region $\mu_0 Hc \approx 7.95$ T and is characterised by highly anisotropic transport properties. Low-energy spin excitations within and around the ENP phase of $Sr_3Ru_2O_7$ have been investigated using LET.

This experiment produced spectacular data, showing that the spin excitations are highly localised in wavevector at low energies. As the applied magnetic field is changed the excitations 'soften' (i.e. move to low energy) near the critical field where the unusual phase occurs. This softening of the magnetic excitations in $Sr_3Ru_2O_7$ could provide an explanation for many of the intriguing physical properties of this system.

Further reading: In preparation.

Contact: SM Hayden, s.hayden@bris.ac.uk



Softening the spin excitations in $Sr_3Ru_2O_7$ near $\mu_0 H$=7.95 T at Q=(0.23,0,0), measured using LET

Magnetic field splitting of the spin resonance in $CeCoIn_5$

Instrument: OSIRIS

C Stock (Edinburgh), C Broholm (Johns Hopkins), Y Zhao (Maryland), F Demmel (ISIS), HJ Kang (NIST), K. Rule (HZB), C Petrovic (Brookhaven)

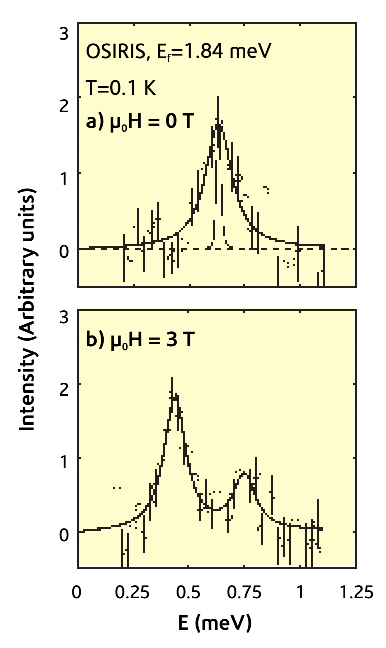
Support for research: STFC, DOE, and NSF

The presence of an underdamped resonance peak in the neutron scattering response has proven to be a strong indication of unconventional superconductivity. Spin resonances have been reported in a series of heavy fermion-, cuprate-, and iron-based superconductors and associated with the gap function undergoing a change in sign. Therefore, neutron scattering can be used to probe the electronic superconducting gap symmetry.

In this experiment, the fine energy resolution of the OSIRIS spectrometer has been used to show that the spin resonance in $CeCoIn_5$ is a doublet. The splitting and subsequent softening of the lower-energy member of the doublet shows that the high field magnetic 'Q-phase' in $CeCoIn_5$ can be interpreted as a Bose condensate of spin excitons.

Further reading: C Stock *et al*. Phys. Rev. Lett. 109, 167207 (2012).

Contact: C. Stock, cstock@ed.ac.uk



(a) A scan through the spin resonance at zero field.
(b) Demonstration of the splitting of the resonance into two peaks under an applied field of 3T.

Self-organized spin motions in a frustrated magnet

Instrument: MERLIN

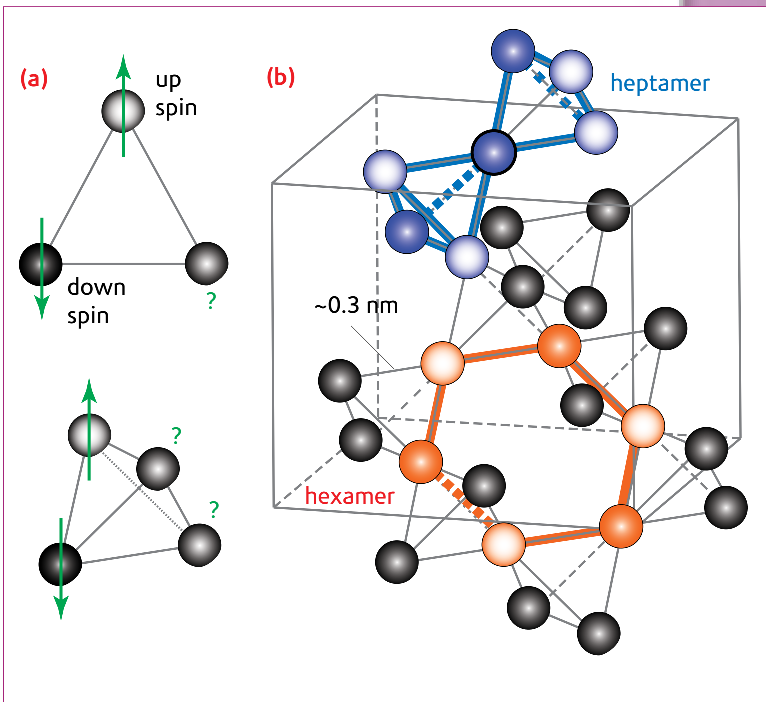
K Tomiyasu (Tohoku), T Yokobori, Y Kousaka (Aoyama-Gakuin), R I Bewley, T Guidi (ISIS)

Support for research: Grants-in-Aid from the MEXT of Japan

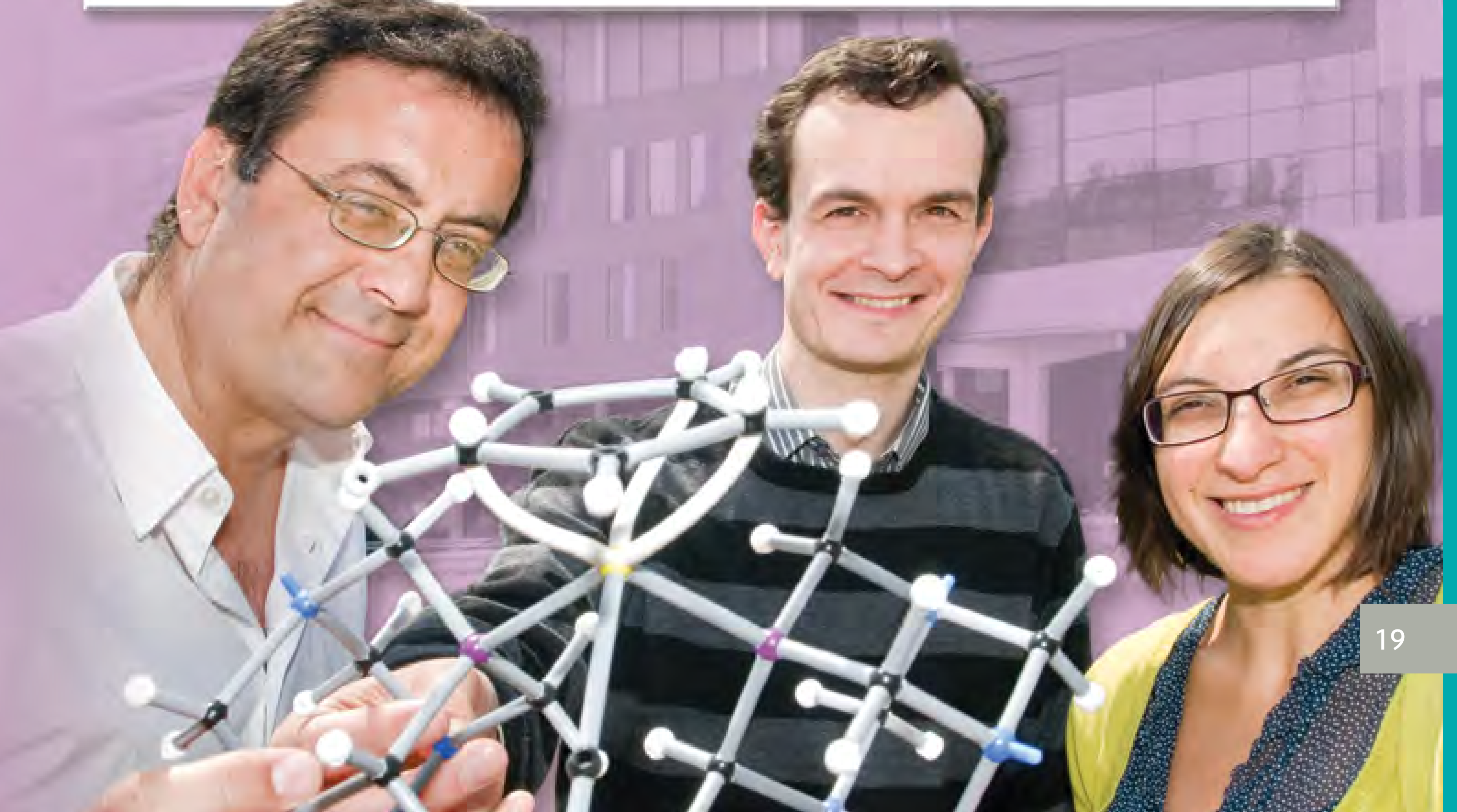
Recently, for a natural mineral of spinel-type magnesiochromite $MgCr_2O_4$, intriguing response properties to stress, sound, and heat were reported. In contrast with normal insulating crystals, with heating from -220°C to even room temperature the lattice hardens, sound speeds up, and thermal conductivity increases continuously. $MgCr_2O_4$ is also a highly frustrated magnet, and is a promising source for studying exotic spin-liquid states and resulting physical properties. In $MgCr_2O_4$ not all spin-vector pairs can be arranged antiparallel (antiferromagnetically) on a triangle and a tetrahedron. Therefore, frustration suppresses normal spin/magnetic ordering and promotes spin-liquid states probably accompanied with spin-lattice coupling. In this study, large-volume and high-quality single crystals (~3 cc) were grown and the overall spin motions were measured by inelastic neutron scattering on MERLIN. The emergence of spin molecules with finite excitation energies and nanometer-scale geometrical figures were observed, which will provide key information for simple description of the intriguing properties and potential application of $MgCr_2O_4$.

Further reading: K Tomiyasu *et al.*, Phys. Rev. Lett. 110 (2013) 077205.

Contact: K Tomiyasu, tomiyasu@m.tohoku.ac.jp



(a) The concept of frustration. (b) Corner-sharing tetrahedral lattice consisting of magnetic Cr^{3+} ions and snapshot of spin molecules in motion in the lattice.



Applied materials

Hydration process of glass ionomer cements for dental restoration

Instrument: IRIS

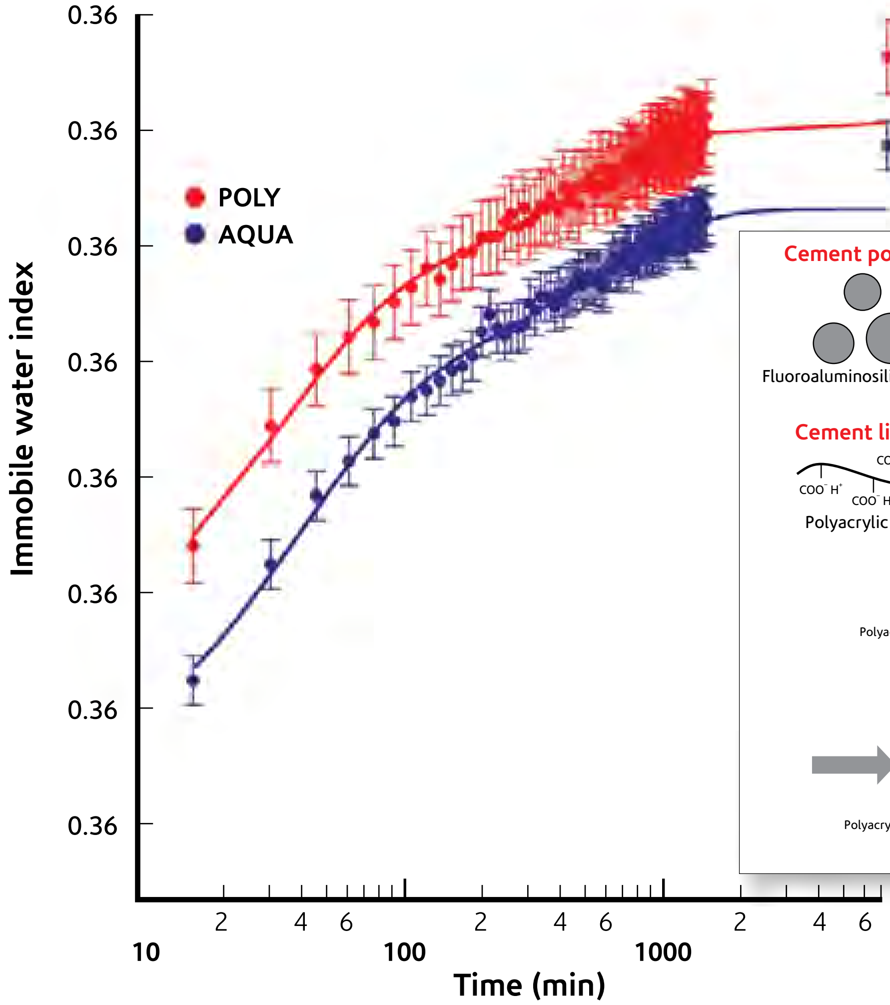
AR Benetti (Department of Odontology, Copenhagen), J Jacobsen (Niels Bohr Institute, Copenhagen and ESS AB), MTF Telling, V Garcia-Sakai (ISIS), HN Bordallo (Niels Bohr Institute, Copenhagen and ESS AB)

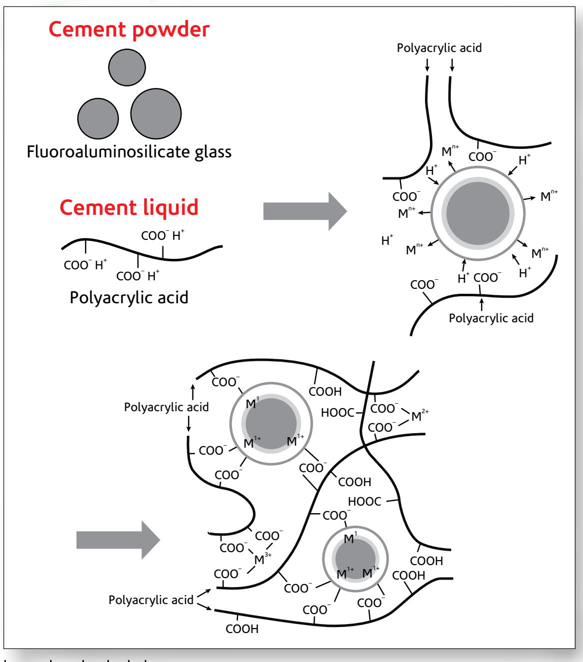
Support for research: Niels Bohr Institute, University of Copenhagen, European Spallation Source, ESS AB

Dental caries (cavities) are a major global health problem. Glass ionomer cements (GIC) offer a clever alternative for preventative dentistry: they contain and release fluoride, show a thermal expansion coefficient similar to that of teeth, and bond chemically to dentin and enamel. Unfortunately their weak mechanical strength currently limits their application. Following the evolution of the elastic signal obtained from quasi-elastic neutron spectra allows the determination of the rate and extent of GIC hydration, and such knowledge may assist in improving GIC mechanical strength. AQUA and POLY cements having different mechanical properties were analysed and shown to exhibit dramatic changes in the immobile hydrogen index (IHI) after 100 minutes. A transition from an initial setting dominated by the fast formation of calcium and sodium polyacrylates, to the slower formation of aluminium polyacrylate was observed. The higher IHI of the POLY cement can be directly related to its greater compressive strength, offering insight for future improvement of these materials.

Further reading: In preparation.

Contact: HN Bordallo, bordallo@nbi.ku.dk





Inset: Davidson CL, Mjor IA, Advances in glass ionomer cements. Quintessence: Chicargo, 1999.

Time evolution of the immobile hydrogen index (IHI) for two GIC. The measured IHI is fitted to a double exponential growth model (full line).

In-situ stress relaxation measurements in welding

Instrument: ENGIN-X

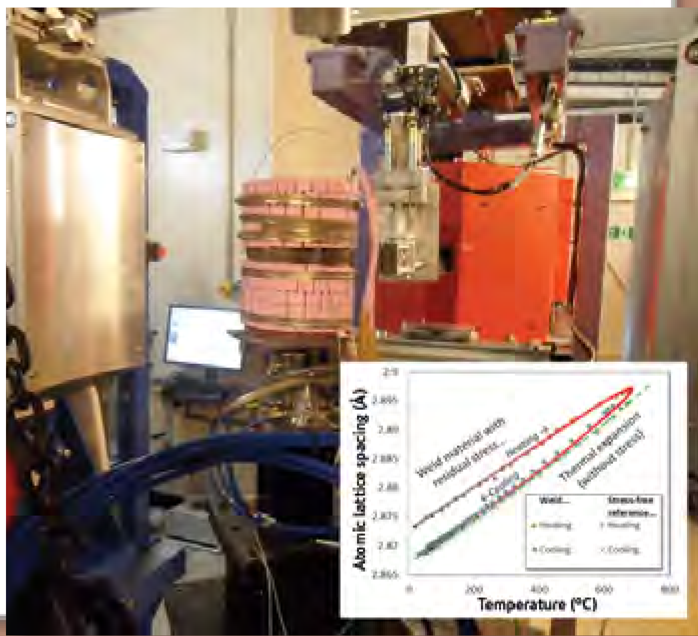
B Chen, A Skouras, YQ Wang, DJ Smith, PEJ Flewitt, M Pavier (Bristol), S Kabra, SY Zhang, JF Kelleher (ISIS)

Support for research: Industry funding for Bo Chen from EDF Energy

Pipes in power stations are usually joined by welding, and often these welds must be heat treated to remove residual stress. ENGIN-X is the only diffraction instrument in the world that can carry out in-situ heat treatment on complex shape engineering objects. By monitoring the change in atomic spacing of a stressed region during heat treatment, and comparing this to a deliberately-created stress free region on the same pipe, it has been possible to directly observe the stress relief process. The stress-free region simply expands and contracts, but the stressed region is seen to change its lattice spacing after around 500°C, becoming more like the stress-free region. This work can help choose the optimum temperature and duration for heat treatments – enough to remove the unwanted stress, but not so much as to cause other less desirable changes.

Further reading: Materials Science and Engineering A (in press).

Contact: B Chen, bo.chen-2@manchester.ac.uk



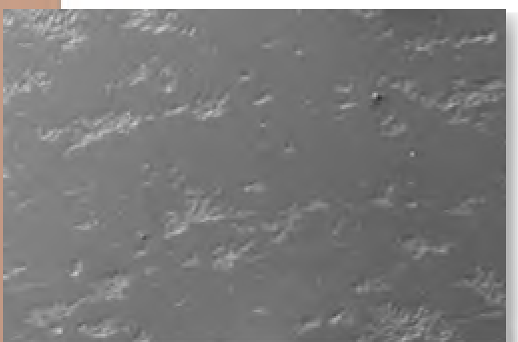
Pipe section inside the ENGIN-X sample area. Heating was applied using the pink blankets while simultaneously measuring the lattice spacing (graph) with the neutron beam.

Unravelling the atomic scale structure of bioactive glasses

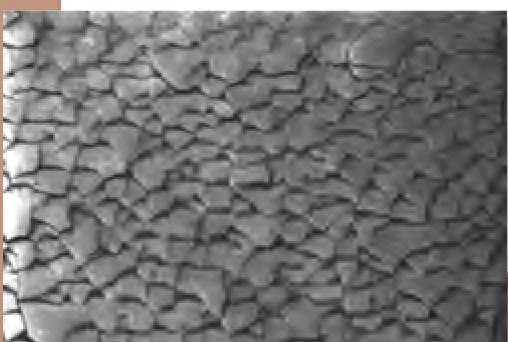
Instrument: GEM

RA Martin (Aston University), HL Twyman (Kent), ER Barney (Nottingham), RM Moss, JM Smith, RJ Newport (Kent)

Support for research: EPSRC grant EP/E050611/1



200 μm



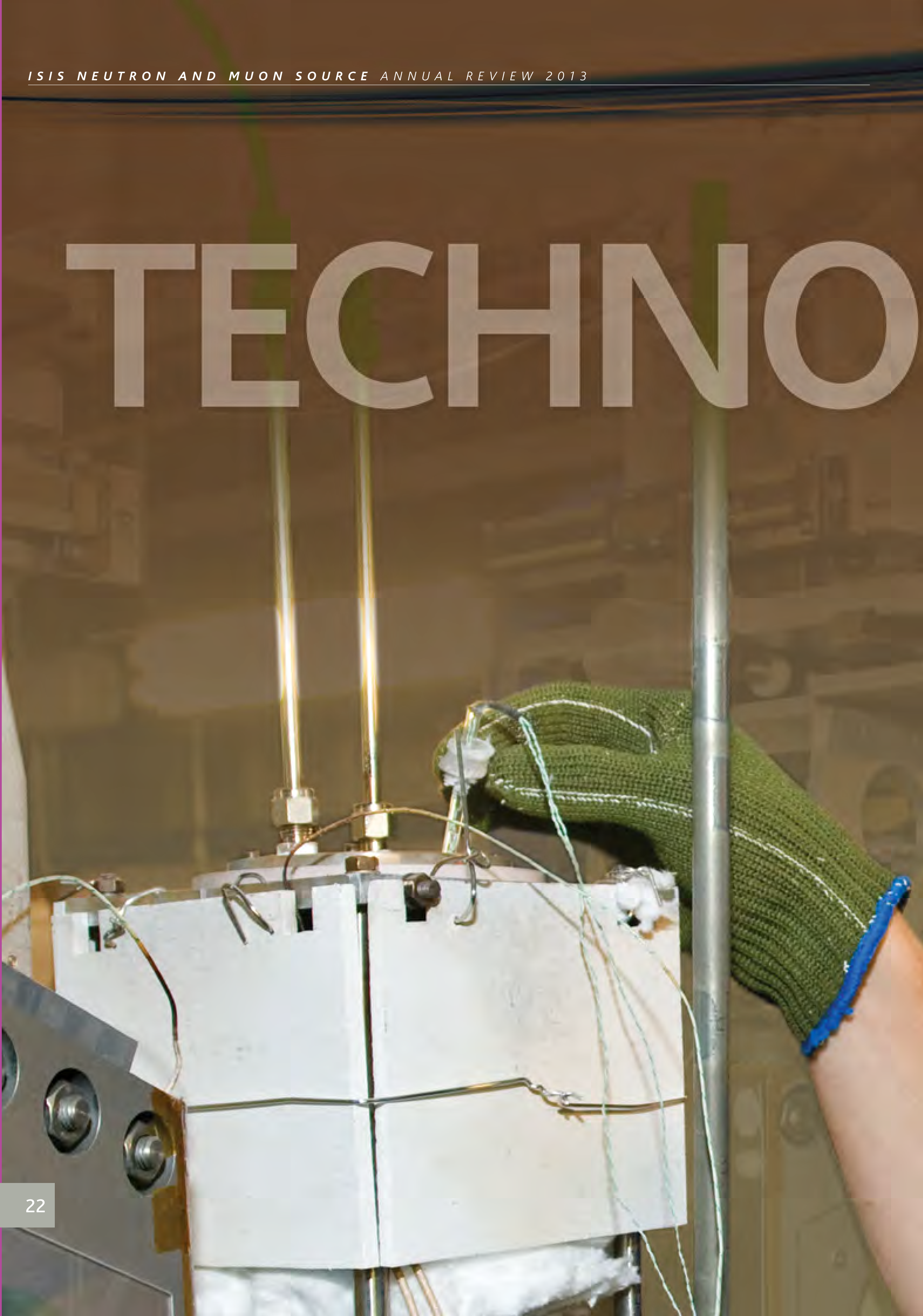
Bioactive glasses have the ability to promote bone regeneration. Consequently they are used for a wide range of biomedical applications including orthopaedic bone grafting, facial reconstruction and periodontal repair. Under physiological conditions these materials dissolve, releasing Ca, P and Si, at a rate which promotes the formation of hydroxyapatite (the mineral component found in teeth and bones). The structural sites present in the glass will be intimately related to dissolution properties in physiological fluids such as plasma and saliva, and hence to the bioactivity of the material. Detailed structural knowledge is therefore a prerequisite for optimising material design. Applying neutron diffraction techniques, conducted using GEM, we have unravelled the structural complexities associated with several bioactive glasses. The diffraction data provided the first direct experimental evidence of two distinct Ca-O nearest-neighbour correlations. These correlations are attributed to calcium ions bonded either to bridging or to non-bridging oxygen atoms.

Further reading: RA Martin *et al.*, J. Mater. Chem. 22 (2012) 22212.

Contact: RA Martin, R.A.Martin@Aston.ac.uk

Scanning Electron Microscopy Images.
***Top**: Bioglass surface.*
***Bottom**: Formation of hydroxyapatite onto the bioglass surface after soaking in a simulated body fluid.*

TECHNO




LOGY

TS2 phase 2 instruments

CHIPIR

The majority of the physical construction of ChipIr is nearing completion ready for the shutter opening next year. The fast neutron collimator has been tested. This will stop neutrons with energies up to 800 MeV and so is quite substantial. Weighing in at 9 tonnes, the multi-layered disk-shaped device will perform the primary collimation of the beam that will eventually provide a flexible beam size ranging from 2mm^2 to 1m^2. This will allow users to test the cosmic-ray neutron resilience of their devices all the way from individual chips up to full system level.

IMAT

The IMAT building extension on the side of the TS-2 hall has been completed this year. It has been designed to enable engineering components of up to 1.5 tonnes to be studied. The larger part of the 44 m long supermirror guide will be put in place in summer 2013. From spring 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.

Top: Inside the ChipIr hutch the sample tables, provided as a contribution in kind from Italy, have been installed.

Left: The IMAT extension building

LARMOR

Many Larmor components have now been installed. Optical beamline parts have now either been delivered or are on order. The large, moving detector bench will be installed early in 2014 ready for the installation of the detectors and monitors. Commissioning is due to start during early 2014, with further Small Angle Neutron Scattering (SANS) components being installed during the commissioning phase. The collaboration with Delft University to deliver the Spin Echo SANS (SESANS) and Larmor diffraction systems continues to progress with the intention to make SESANS available during 2015. During the long shutdown in 2014, the TS-2 reflector will be modified to provide Larmor with the correct moderator view. User operations are then planned from late 2015.

ZOOM

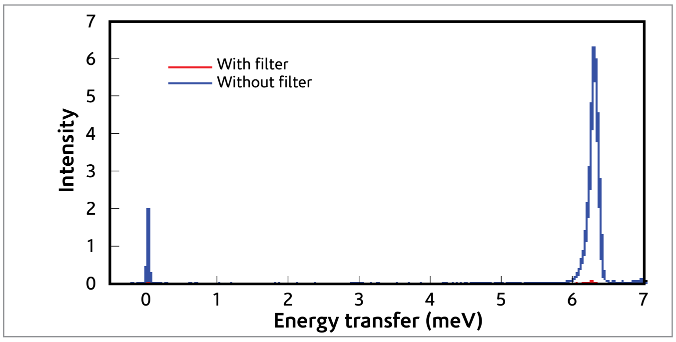
ZOOM will be a flexible small angle neutron scattering (SANS) beamline capable of polarised and grazing incidence SANS. Construction is currently on hold but design activities continue along with installation of some key components. The vacuum tank has been delivered and will be installed on a sloping rail system required to suit the vertical supermirror bender filter. The detector motion system inside the tank is also in final test. The sample stack and polariser and analyser have also been delivered, with further components being provided by the ISIS partnership with Italy also due shortly.

***Above**: The inside of the Larmor blockhouse. The raised floor contains a granite section that will be used to allow the large detector bench to rotate around the sample position from 0 to 135 degrees on an air-pad system.*

Further instrument developments

A new beryllium filter for OSIRIS

A new beryllium filter is now operational on the OSIRIS spectrometer. The filter suppresses higher-order reflections from the graphite analyser and provides a much cleaner spectrum for high-resolution applications using the graphite 002 reflection. It also opens up the possibility of accessing spectral features at energy transfers up to 20 meV, and to probe these with outstanding resolution. To access a wider momentum transfer range with the graphite 004 reflection, the filter can be moved in and out of the beam with a motor-controlled system. First tests with the filter in place have been performed successfully.



Reduction of higher order reflections with the Be filter in place.

New jaws and more for WISH

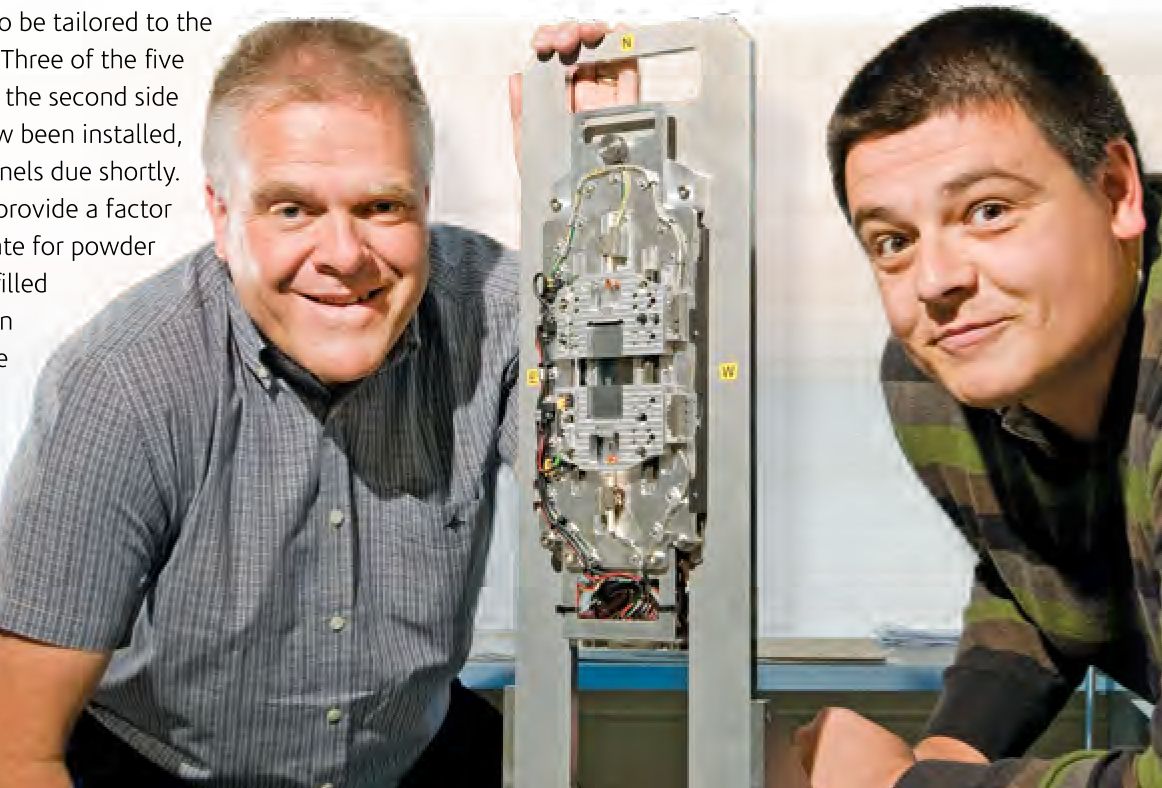
The ongoing programme of developments on WISH has continued during the past year. This includes a set of adjustable jaws in front of the sample position, to allow the size of the neutron beam to be tailored to the size of individual samples. Three of the five panels of ^{3}He detectors on the second side of the instrument have now been installed, with the remaining two panels due shortly. Once completed, this will provide a factor of two increase in count rate for powder diffraction studies. Argon filled tanks to reduce attenuation of the scattered beam have been constructed and will be installed between the sample tank and detectors once all the detector panels are in place.

Upgraded POLARIS back in full swing

The POLARIS powder diffractometer resumed full user operation at the end of May 2012 following its major upgrade (funded by the STFC Facilities Development scheme and with significant contributions from international partners in Sweden and Spain). The first publications containing diffraction data from the new instrument have now appeared. The final piece of hardware, the novel ^{10}B coated radial collimator assembly (see right), was installed in July and has significantly reduced the background scattering when using complex sample environment devices. This will be of particular benefit to the programme of developments of in-situ reaction cells for hydrothermal and microwave synthesis and electrochemical cells for time-resolved studies of battery materials.

The novel ^{10}B-coated radial collimator assembly before installation on Polaris

***Below**: The jaws on WISH have significantly reduced the background for experiments with bulky sample environments such as high pressure cells and cryomagnets.*



Muon beamline upgrade

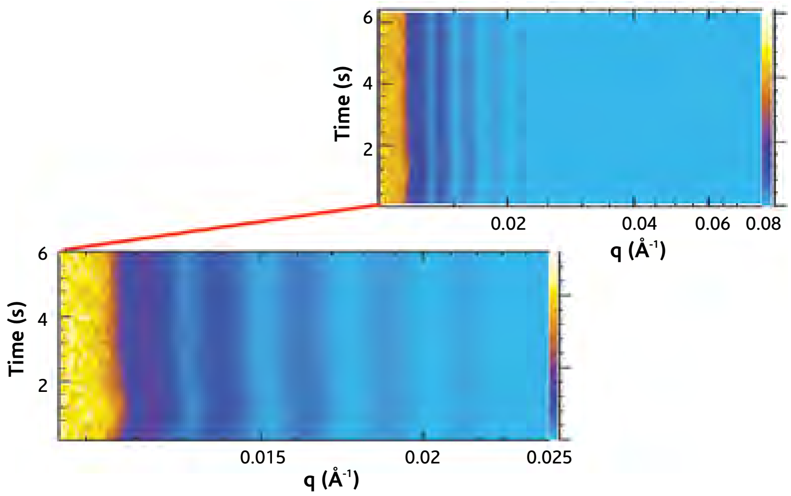
We have now begun the project to upgrade the south side muon beamlines. We will replace all the primary beamline quadrupole magnets, plus a number of other components. The new quadrupoles are designed specifically for the transport of our muon beam and will give us a muon flux increase of 2-3. The new quadrupoles are currently in construction with installation planned for 2014/15. In addition the three South side muon instruments have received new data acquisition electronics leading to a doubling of their data rates.

Exciting muons on HIFI

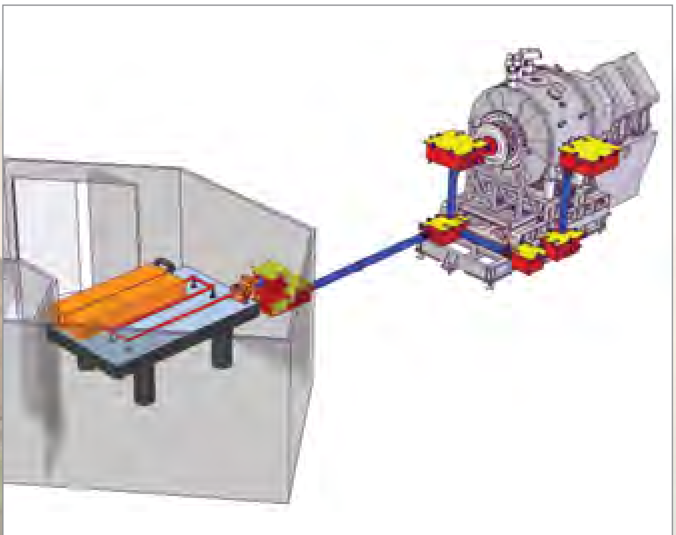
Dr Alan Drew from Queen Mary University of London has been awarded a European Research Council grant of €1.5M to develop the HiFi muon spectrometer. This five year project enables us to build a unique facility by installing a powerful laser system on to the existing HIFI instrument – the ability to perform muon experiments enhanced by a laser in magnetic fields as high as 5T is not available anywhere else. This will allow us to obtain a direct microscopic understanding of the electron dynamics in biological molecules, such as peptides and proteins. This research has potential impact in fields ranging from green energy production to biology and medicine.

Improvements to INTER

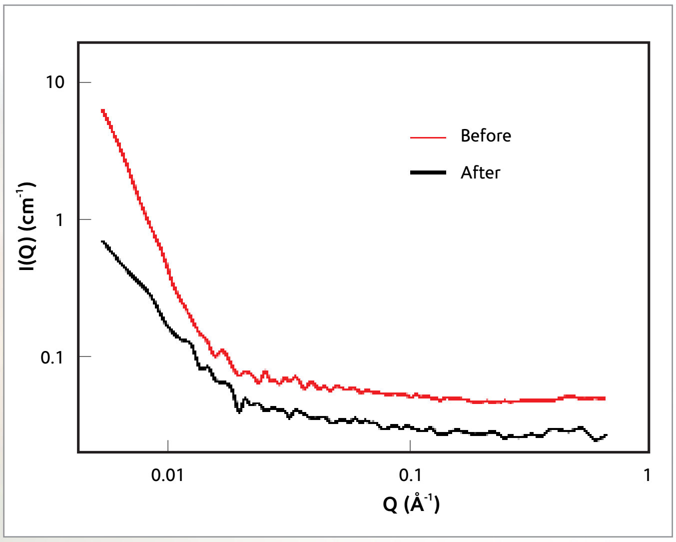
The front-end cloche has been installed and tested on Inter. The cloche allows the upstream optics section of the beam line to be filled with inert gas leading to an increase in neutron flux at long wavelengths. Improvements to data acquisition and control electronics have made available stroboscopic type data collection. Recent electrochemistry experiments have exploited these new capabilities and we can now collect data in 0.2 second time slices.



***Above**: Example of stroboscopic measurement on Inter. Time slices are 200 milliseconds for cycled Polymer redox system.*



***Above**: HIFI with the new laser system installed.*



***Above**: Significant improvements to the background on SANS2D have been achieved through modifications to both the collimation and beam defining apertures in the front end of the instrument. Shown above is the 'empty beam' profile for a typical SANS2D configuration both before and after replacement of all B4C and BN apertures with Cd and the widening of collimation sections at strategic points along the beamline.*

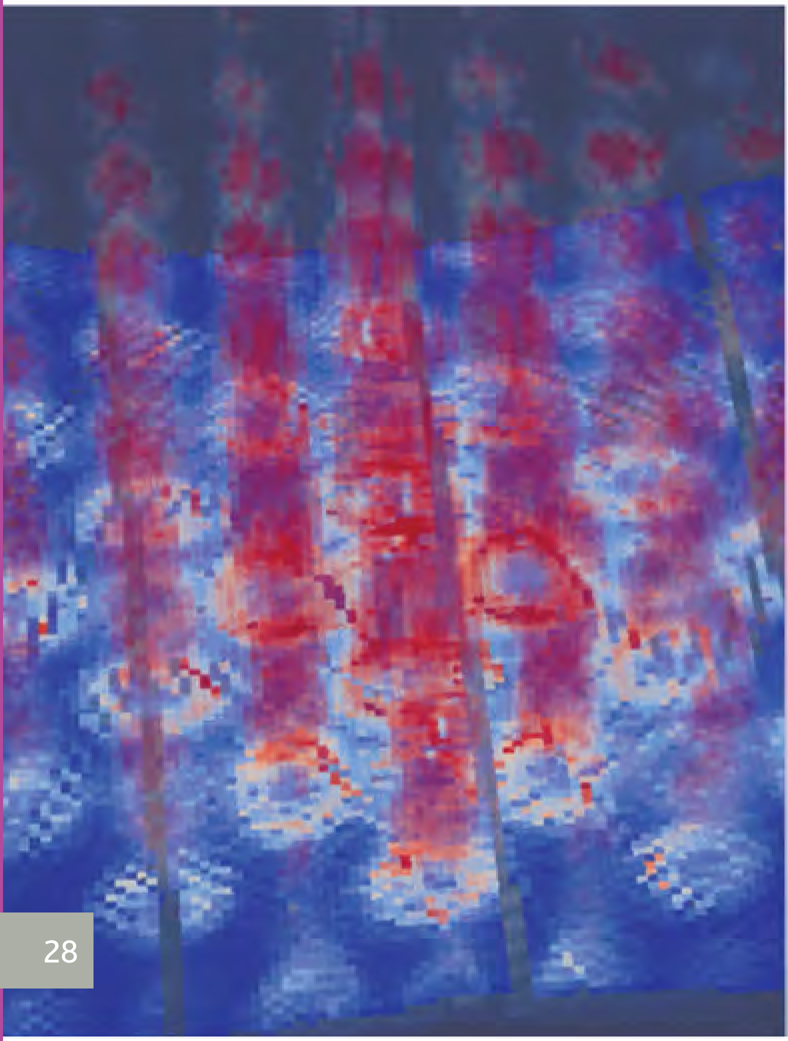
Computing and data acquisition

Mantid: the next dimension

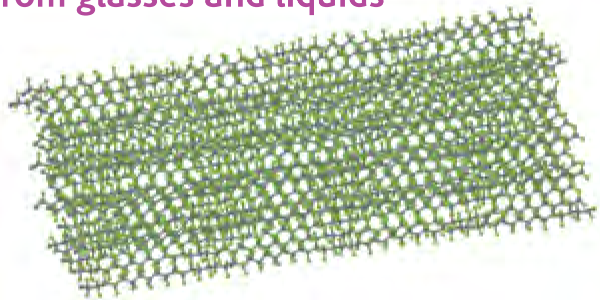
The Mantid project is the largest collaborative software development for neutron scattering data today, focused on delivering professional-quality state of the art data analysis and visualisation software. This collaboration between ISIS, Tessella and Oakridge National Laboratory is also supported by developers from ILL, PSI, ESS and the Los Alamos National Laboratory.

The magnitude of the development has been recognised by software company Kitware. Kitware worked with the team to adapt their Paraview programme to accommodate the requirements of neutron scientists allowing them to view their data in 3D glory! 3D visualisation of data is essential for the state of the art instruments installed on TS1 & TS2, allowing users to visualise large data volumes for both single crystal diffraction and inelastic neutron scattering.

Simulated data of Strontrium-122 model convolved with the instrument resolution of MERLIN



Computer simulation for interpreting total scattering data from glasses and liquids



Teflon as determined from EPSR simulations. This shows the helical structure of these polymers which gives rise to a periodicity along the axis of the polymer.

Computer simulation of neutron and X-ray scattering data is big business within the disordered materials and crystallography groups, and is a field in which ISIS has taken a world lead. It has become widely used as a tool for understanding total scattering data from liquids, glasses and crystalline materials since the late 1980s. The technique of empirical potential structure refinement (EPSR) was introduced in 1996 as an extension of the existing Reverse Monte Carlo (RMC) method. Recent work by Alan Soper has investigated the extent to which the EPSR technique can provide unique interpretations of radiation total scattering experiments on disordered materials.

The study looked at two cases where data is readily available for both X-ray and neutron scattering with isotope substitution; water and dimethylsulphoxide (DMSO). Neutron scattering data were collected on NIMROD at ISIS, and X-ray data from the X-ray diffractometer located near NIMROD. The study demonstrated how powerful the EPSR technique is in providing insight into the local organisation of materials, but also into how uniquely a given data set defines the structure. It can also determine whether existing models for the interatomic potential are correct, whether measurement uncertainties have led to problems in the data, and the extent to which the structure can vary and yet still be consistent with the given data set. Whilst this work focused on small molecule systems, work is underway looking at fluids in confined media and polymeric systems – this will be reported on in the near future.

***Further reading**: A Soper, Molecular Simulation 38 (2012): 14-15, 1171-1185*

Support laboratories

Increased computational power on the SCARF-RAL cluster

The SCARF cluster is a computing resource run at RAL for scientific use. ISIS has provided 512 new nodes for SCARF this year which are available for ISIS users, so that now more than 1000 nodes can be accessed at any one time. These new capabilities are being exploited to run large first-principles calculations for comparison with neutron-scattering experiments, as well as Monte-Carlo simulations for instrument design and optimization.

First flux lattice phase measurement via SANS at ISIS

This year saw the first flux lattice phase measurement made via SANS at ISIS. Ted Forgan from the University of Birmingham used a 17T cryomagnet, built with EPSRC funding, to study the flux line lattice of YBCO. This is the highest DC magnetic field recorded for an experiment at ISIS.

New catalysis infrastructure at ISIS

As part of ongoing collaborative efforts between the group of Dr David Lennon (Univ. Glasgow), and the ISIS Sample Environment and Molecular Spectroscopy Groups, the ISIS-Glasgow gas panel has been upgraded into a compact, mobile unit. The panel enables the preparation of samples needed for studies of catalysts with neutrons. There is also a dedicated residual-gas analyser to characterise the exit stream. In parallel, a range of cells has been developed to carry out chemical reactions from room temperature to nearly 1000 K, and at any pressure up to 20 bar.

Developments in the Support Labs

This year we have increased the capability of the facilities available in the Support Labs. The X-ray Diffractometer in the ISIS Materials Characterisation Laboratory has been upgraded with new sample stages allowing data to be collected at temperatures as high as 1500 K and as low as 12 K. This instrument has already saved many days of wasted beamtime helping users pre-screen samples for neutron and muon experiments.

We have also built a new instrumentation lab in the Target Station 2 Hall. This lab now houses a new HPLC Mass Spectrometer and a new variable temperature and pressure Differential Scanning Calorimeter (DSC).

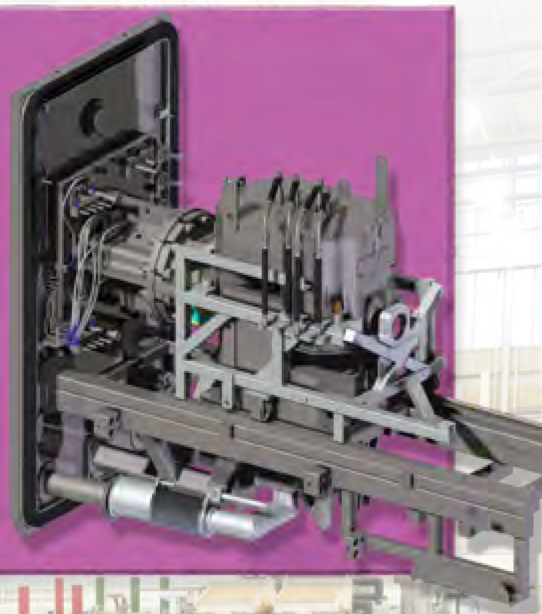
The ISIS Biolabs have benefited from considerable investment too, with a new analytical suite set up in the Target Station 2 Biolab. The new facilities available include a FT-IR Spectrometer, a Dynamic Light Scattering instrument and a Quartz Crystal Microbalance.

Accelerator and targets

TS1 upgrade

Target station 1 (TS1) has been serving the neutron community for 25 years, during which time there have been significant technological advances. Using our operational expertise combined with advanced computational methods, the ISIS team is looking to optimise the design of TS1, with the goal of at least doubling the neutron flux, as well as considering flexibility for future moderator developments.

This year has seen a detailed model of the existing TS1 target and moderators developed and simulated, and the start of possibilities for its upgrade being developed. Over the next six months or so, a wide variety of different target and moderator configurations will be simulated with the aim of providing an increase in neutron flux to all TS1 instruments. ISIS is aiming to install the new target and moderator systems around 2018.



Above: Oliver Newell with the first kicker K1 in R78 workshop.

New kicker magnets

There are many components within the ISIS accelerator that need to function faultlessly to enable the delivery of beam to target. The extract kicker magnets have some of the most demanding requirements of all the equipment in the accelerator systems. Operating at 5000 Amperes and at 40 kiloVolts, the magnets rise from zero to reach their maximum field in around 200 nanoseconds; and they do it 50 times every second. Having been in operation since 1994, the present magnets are estimated to have completed around 15 billion cycles. The first of three new kicker magnets for the synchrotron has been built on site at RAL to replace the existing ones.

Main magnet power supply upgrade programme

In September the order was placed for a replacement 1.44MW DC power supply to replace the existing obsolete supply which feeds the main magnets in the ISIS synchrotron. When installed in 2014 this power supply will improve the stability of the sine wave current used to drive the 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 programme.

From concept to reality: the new power supply along with its associated electrical substation and demineralised cooling water system will be housed in the extension to R6A which was completed in August 2012.

Accelerator and targets

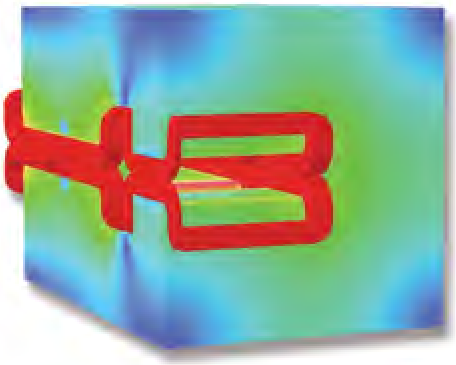
Synchrotron steering magnets and trim quadrupole magnets power supplies

In January the programme to replace the power supplies for the synchrotron vertical and horizontal steering magnets and the trim quad magnets was completed. The new power supplies are capable of a higher current output and of delivering a programmed current waveform with a slew rate of 300,000 Amps per second, which is twice the slew rate of the existing units.

***Right**: Steve Gray making adjustments to the newly installed trim quad power supplies.*

New injection dipole magnet and power supply

Design work has started on the replacement injection dipole magnets and power supply which will allow for injection of the beam from a possible replacement linear accelerator in the future. The pulsed power supply for the injection dipole has a design specification of a maximum pulse current of 26,000 Amps with a rise and fall time of 100 μs and will allow improved injection of the beam into the synchrotron.



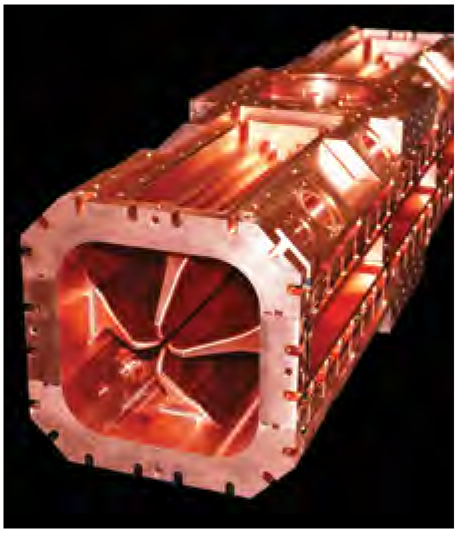
Computer modelling of the Injection Dipole Magnet

Upgrade to R55 electrical distribution system

R55 Electrical distribution system was based on four 1.25MVA dual packaged substations which were installed when ISIS was originally built. These have reached the end of their working life and are currently in the process of being replaced with upgraded dual 1.5MVA packaged substations. To date two of the four substations have been replaced with a further two replacements planned for 2013 and 2014. When complete the new substations will allow for higher capacity and more flexibility in the ISIS TS1 hall along with more reliable operation of the system.

Linac R&D

The first metre of the Front End Test Stand (FETS) RFQ. The remaining three metres of RFQ are also almost complete. Completion of the manufacture of the RFQ is a major milestone for the FETS project. The FETS project aims to develop technologies for the next generation of high power proton accelerators.



EMMA

Work is underway to develop EMMA (Equipment, Materials and Mechanics Analyser), making use of the previously de-commissioned HET beamline. EMMA is an instrumentation beamline which is to be used internally to test shielding materials, detectors, data acquisition electronics, instrument software and control, Fermi chopper controls and other beamline equipment. EMMA has recently begun to provide material testing capability using a test rig located in the chopper pit. Installation of new wax tanks is set to dramatically increase EMMA's capabilities by providing a shielded environment in which detectors can be tested.

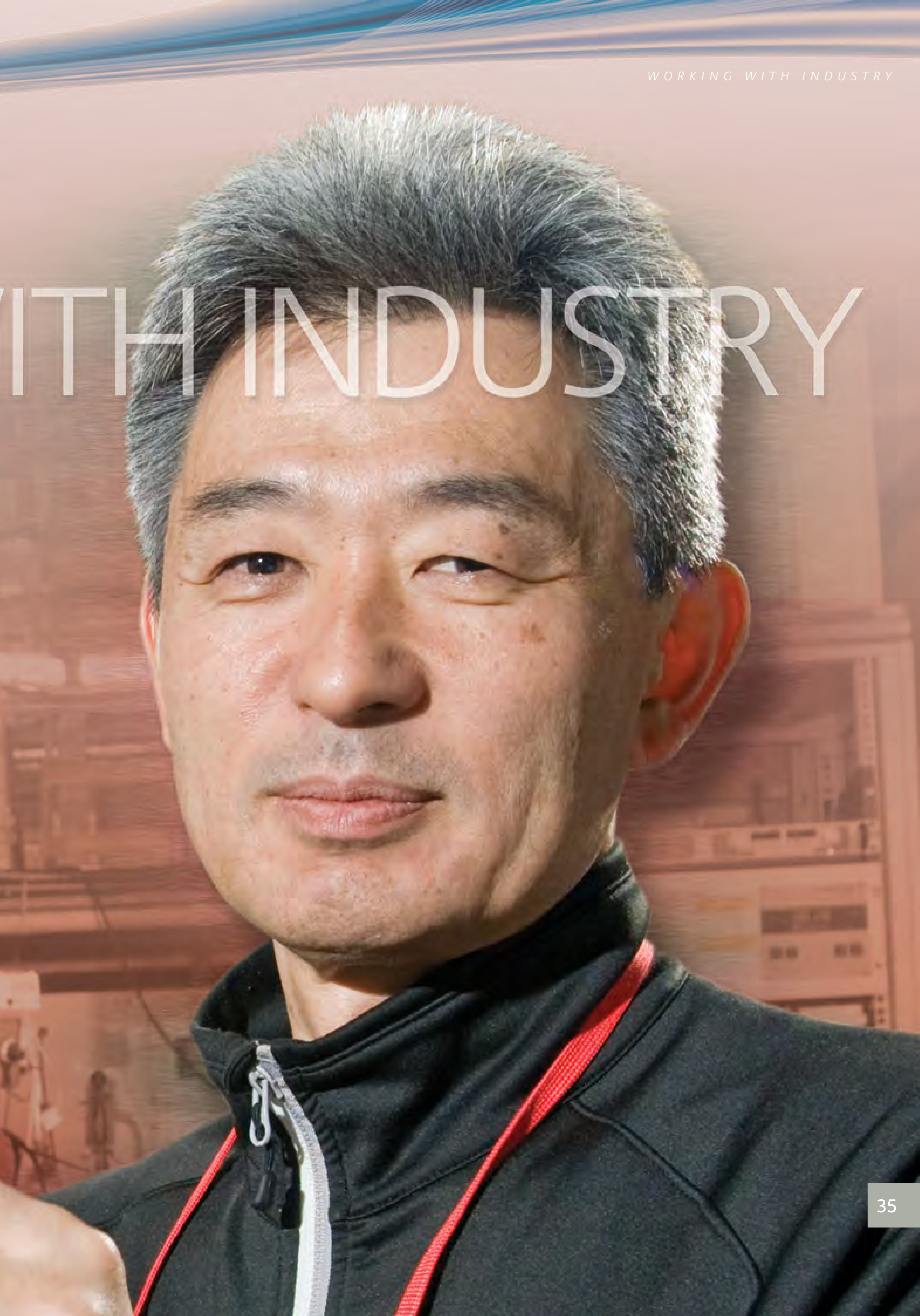
TS2 reflector

The upgraded TS2 reflector is due for installation in the long shutdown starting in August 2014. It has a special cut-out pointing at ChipIR to allow the new instrument to have a more direct view of the target and hence a stream of high energy neutrons. The groove has also been extended to give Larmor a full view of the coupled moderator.

The reflector was delivered to ISIS in May 2013. It will now be assembled on the dummy target rig to allow cooling water pipes to be fitted.

***Right**: Leslie Jones unpacks the new TS2 Phase II Beryllium Reflector components*

WORKING W


ITH INDUSTRY

Industry and innovation

ISIS works closely with industry, with 61 companies using the facility over the past year, ranging from large multinationals to hi-tech start-ups. Sectors include chemicals and plastics, healthcare, transport, automotive, aerospace, manufacturing and the energy industry.

The ISIS Collaborative R&D programme was set up in 2011 to provide a new access mechanism to ISIS specifically tailored for industry. It aims to widen the use of ISIS by industry in order to further increase the economic benefit that ISIS contributes to the United Kingdom.

The scheme provides industry with the opportunity to:

- ***explore how neutrons can add to their research***
- ***use ISIS expertise to plan experiments, collect and analyse data***
- ***use a fully confidential service with the option to buy depending on the results.***

Case study: TWI Ltd

The outcome of a study carried out by engineering consultancy TWI and ISIS has important implications for the oil, gas and nuclear industries.

Pipelines used to carry fluids must be robust and able to withstand production and installation. Leading engineering consultancy TWI have been using Engin-X at ISIS to assess how pipes used in the offshore oil and gas industry are affected by installation processes introducing high plastic strain. The results give an insight into how residual stresses introduced by pipeline welding change after strains imposed during installation, and what this means for the structural integrity of the pipe.

“This study has important implications for the oil and gas industry and these findings have been submitted to the R6 panel, a group of industrialists and academics working on the development of the UK nuclear industry’s fracture integrity assessment procedure. Ultimately the work will also influence the standards on fracture mechanics used by the oil and gas industry.”

Dr Elvin Eren and **Dr Isabel Hadley**, TWI Ltd.

Below: *Dr Eren with the steel pipe studied on Engin-X.*

Case study:
The Linde Group launches revolutionary carbon nanotube ink with help from ISIS

The Linde Group, a world-leading gases and engineering company, has launched SEER^{e-} Ink, a revolutionary ink based on carbon nanotubes for use in flat screen TVs, touchscreens and solar cells. The team behind the research used the LOQ instrument at ISIS to gain vital information on the structure of the ink.

"SEER^{e-} Ink doesn't use harsh processing techniques, meaning the nanotubes maintain their length and can be used to create excellent quality transparent conductive films. ISIS played a vital role in confirming that the process of reducing nanotubes in liquid ammonia really worked."

Siân Fogden,
Linde Nanomaterials

Case Study:
Letting the train take the strain

An academic and industrial collaboration has used Engin-X to understand the stresses and strains within train wheels.

Every five years or so, every wheel on every train in the UK has to be replaced. In everyday use the wheels are subjected to stresses and strains that can cause cracks to develop, particularly in the wheel rims. A group from the University of Huddersfield has been using Engin-X at ISIS to study new and used train wheels to understand how cracks begin and spread. Their work is funded by a consortium including the Rail Safety and Standards Board, the Association of Train Operating Companies, Siemens, Lucchini, and EPSRC.

"We are always willing to support Universities in genuine new research such as this. We have extensive facilities in Italy but we don't have anything like ENGIN-X at ISIS. Collaboration between industry and academia can be beneficial and lead to improvements in safety and processes."

Sean Barson,
Lucchini UK

EDUCATION AND

OUTREACH

Inspiring the next generation

ISIS places a strong emphasis on communicating the excitement of our science and inspiring the next generation of scientists. We regularly welcome members of the public, especially students, to see what goes on and meet our scientists and engineers. Staff also visit local schools and take part in science fairs and activities aimed at encouraging students to engage with science and recognise the core role it plays in our society. Finally we provide training for science teachers, giving them first-hand knowledge of our cutting edge research to take back to the classroom.

Public access day

"It was absolutely fascinating to come back to the site and see how science has moved on after so many years."

ISIS opened its doors to the public for a day as part of the site-wide Public Access Day, giving visitors a fantastic opportunity to see what goes on 'behind the scenes' at ISIS. Visitors particularly welcomed the opportunity to talk to real scientists and engineers about their work. ISIS scientist Christ Frost provided some practical demonstrations, bringing to life superconductivity research at the facility by floating a magnet above a nitrogen-cooled superconductor.

Teacher Training School

The huge variety and breadth of the science carried out at ISIS became the focus for a Teacher Training Day in April when 23 trainee teachers from the University of Oxford's Department of Education heard from scientists at ISIS on topics ranging from spider's silk, catalysis and magnetism to the latest in hydrogen storage and the effects of cosmic rays. This was all wrapped up with an explanation of how the ISIS accelerators work, a tour of the experimental areas and the chance to look at demonstrations of some of the physics involved in producing and using neutrons. A hugely educational and enjoyable day for all involved.

"Our PGCE students really value this opportunity to visit an international research laboratory, as they learn more about current research across the sciences and the resources and events available for them to enrich the learning of their pupils."

Judith Hillier, lecturer in physics education, University of Oxford.

Equipping the scientists and engineers of the future

In addition to our public engagement activities we recognise the need to equip scientists and engineers with the skills they need to continue research at ISIS, now and in the future. We also take on both apprentices and work experience students.

We support a diverse programme of events from masterclasses for A-level students to highly specialised workshops and international conferences. In the past year over 640 students took part in user experiments at ISIS, and the highly successful Neutron Training School aims to increase this number further.

Neutron Training School

24 PhD and postdoctoral researchers attended the neutron training course in March 2013. Led by ISIS scientists the course focuses on practical aspects of neutron scattering, with students gaining hands-on experience of a host of instruments that they will use in their future research programmes.

"These four weeks have been a really great experience; before coming here I thought I might like to go into research but my time here has really confirmed this for me. I've learnt so much."

Rachel Lau, work experience student

Facts and figures

- *641 students took part in user experiments at ISIS*
- *400 A-level students visited as part of the Particle Physics Masterclass*
- *ISIS supported 10 apprentices, and 16 sandwich students and summer placements*

Particle Physics Masterclass was a hit

Between 26th February and 1st March 2013, around 400 Physics A-level students toured around ISIS target stations as part of the Particle Physics Masterclass. In addition to a series of lectures on current topics in particle physics they were guided through the target stations and around the instruments by volunteers from all across ISIS.

Conferences and workshops

Denim 2012

17-19 September 2012

ISIS hosted the first Design and Engineering of Neutron Instruments Meeting (DENIM 2012). The workshop brought together over 50 multi-discipline engineers from neutron facilities worldwide for two and a half days, providing a forum for discussing the techniques, successes and areas for improvement of instrument design. The event included presentations by facilities and suppliers, tours of ISIS and proved a fantastic networking opportunity for all involved. The success of this event has prompted other facilities to host future DENIM meetings, with Oak Ridge National Laboratory set to host DENIM 2013 in October.

Frontiers of Muon Spectroscopy

17-18 September 2012

Held at St Hugh's College, Oxford this meeting celebrated 25 years of μSR at ISIS and marked the recent retirement of Prof Steve Cox, one of the pioneers of the muon technique at ISIS.

Steve Cox (ISIS) with Roger Lichti (Texas Tech) at the Frontiers in Muon Spectroscopy meeting.

Frontiers in Molecular Spectroscopy

14-16 November 2012

Attendees at the Frontiers in Chemical Spectroscopy meeting, which included talks, posters, and a discussion session.

The international symposium Advances and Frontiers in Chemical Spectroscopy with Neutrons, was held at The Cosener's House, Abingdon to discuss the state-of-the art and explore the future of chemical spectroscopy with neutrons. The meeting also celebrated the scientific careers of Jerry Mayers and John Tomkinson, who recently retired after many years at ISIS. Around eighty attendees from all over the world showcased the scientific diversity of neutron spectroscopy, including stimulating discussions on computational modelling, future instrumentation, and sample environment.

NOBUGS2012

24-26 November 2012

Fostering computing collaboration between Large User Facilities, over 140 IT professionals from around the world met at RAL to discuss software development practices, data acquisition and control, data analysis, data management and much more. The conference highlighted successful collaborations that have been created over the years, developments from around the world and offered a series of workshops.

Disordered Materials User Meeting

6 February 2013

This meeting was held at Cosener's House in Abingdon from the 5th to the 8th February 2013, and attracted 40 delegates from the UK and Europe. A data analysis and simulation workshop was held immediately after, and was attended by 25 members of the disordered materials community.

Proton Accelerators for Science and Innovation (PASI) Meeting

3 April 2013

The second Proton Accelerators for Science and Innovation three-day workshop was held at RAL in April, hosted by ISIS. The meeting brought together over a hundred leading members of the proton beam user, developer, and 'consumer' communities from the UK and the US to review and discuss ways in which greater cooperation can substantially strengthen domestic programmes. Particular emphasis was placed on how appropriate development of collaborative projects would allow benefits to the science, health-care, energy, and security agendas to be delivered more rapidly.

2013 Neutron and Muon User Meeting (NMUM)

8-9 April 2013

The 2013 NMUM meeting was held over two days in Warwick and attracted 150 ISIS and ILL users. The meeting enabled users to hear about and discuss latest developments at the facility, and there was a student poster session with poster prizes.

Spintronics Meeting

18 April 2013

On the 18-19 April 2013 leading researchers from Korea and the UK met to discuss the latest developments in spintronics and advanced materials research. The workshop, jointly funded by ISIS, the Korea Institute of Science and Technology, Diamond, and Samsung UK, was part of a series of meetings to explore opportunities for

Prof. Christopher Marrows, University of Leeds, Prof. You Chun-Yeoul, Inha University, Dr. Choi Jun-Woo, Korea Institute of Science and Technology, and Prof. Choe Sug-Bong, Seoul National University enjoying the ISIS model during a break in the workshop.

Conferences and workshops

collaboration between the UK and Korean researchers. The meeting covered a wide range of research from spintronic logic, antiferromagnetic semiconductors to spin torque oscillators. We are already looking to further extend this successful workshop series given the extensive scientific overlap and the direct relevance of neutron and muon techniques to this topic.

EPICS 2013 Spring Collaboration Meeting

29 April-3 May 2013

EPICS is a control system which ISIS will use in the future for its instrument control systems. 120 participants interested in the use of EPICS in a variety of areas from accelerators to experiment beamlines to telescopes, providing training, workshops, presentations and discussions on its use at the Spring Meeting held at RAL.

The UK's first Quantum Design Physical Property Measurement System (PPMS) Workshop

8-9 May 2013

The UK's first Quantum Design Physical Property Measurement System (PPMS) Workshop was held at ISIS in May 2013 and well attended by both staff and users.

Theoretical and Experimental Magnetism Meeting (TEMM)

4 July 2013

The eleventh Theoretical and Experimental Magnetism Meeting (TEMM) was held at the Cosener's House Abingdon, UK from July 4-5 2013. This meeting has become a highlight in both the UK and European scientific calendar for those in the field of magnetism, attracting 80 registered participants. The meeting presented an excellent opportunity to hear and discuss with leading experts from all over the world on topics of current research in magnetism such as exotic superconductivity, heavy fermion systems, manganites, multiferroics, ferroelectrics, low-dimensional and frustrated magnetism, skyrmions and quantum phase transitions.

International Conference on Neutron Scattering (ICNS) 2013

8-12 July 2013

Edinburgh hosted the 2013 International Conference on Neutron Scattering (ICNS). ISIS was well represented in both the invited and contributed talks, covering both the technology and applications of neutron scattering.

Dynamics of Molecules and Materials II (DMM-II)

July 2013

DMM-II was held at the University of Glasgow in July 2013 to highlight existing capabilities in broadband inelastic neutron scattering for molecular spectroscopy. The workshop covered current scientific trends and highlighted an increasing need for complementarity across different neutron instruments and other techniques.

Seminars

ISIS hosts a regular programme of scientific seminars given by ISIS staff and international researchers on a wide range of scientific topics.

April 2012

Dr. Javier Almeida
Institute of Theoretical Physics, Ulm Germany
Optical spectroscopy applied to the new topics of quantum biology (electronic energy transfer in photosynthetic protein-pigment complexes)

May 2012

Dr. Ferruccio Renzoni
Department of Physics and Astronomy, University College London
Control of atomic motion with ac fields: from the ratchet effect to vibrational mechanics

Dr. Ludovic Jaubert
Okinawa Institute of Science and Technology (OIST) Japan
Spin ice dynamics and spin liquid Curie law

September 2012

Dr. David Singh
Oak Ridge National Laboratory
Superconductivity near magnetism

Prof. Walter Kohn
Nobel prize in Chemistry in 1998
Electronic near-sightedness and density functional theory

October 2012

Dr. Una Karahasanovic
Royal Holloway University of London
Quantum order-by-disorder near quantum criticality and the secret of partial order in MnSi

Dr. Rachel Evans
Trinity College Dublin, Ireland
Structure-property correlation in conjugated polyelectrolyte hierarchical assemblies: a route to nanostructured thin films and modulated emission

Dr Klaus Koepernik
Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research, Dresden, Germany
Surface sensitivity: how reliable are photo emission and tunneling scanning probes in Iron pnictide superconductors

November 2012

Dr. Fernando Bresme
Imperial College London and Department of Chemistry, Norwegian University of Science and Technology
Interfacial structure of soft interfaces without thermal fluctuations

Prof. Angelos Michaelides
University College London, UK
Towards accurate and reliable simulations of physical and chemical processes at surfaces

January 2013

Dr Martin Lueders, L.Petit, Z.Szotek and W.M. Temmerman
The Band Theory Group in Daresbury
A first principles approach to correlated materials

Prof. John Chalker
University of Oxford
Static and dynamic correlations in geometrically frustrated magnets, probed via neutron scattering from ZnCr2O4 and MgCr2O4.

Dr S. Mukhopadhyay
ISIS
Vibrational spectroscopy of organic ferroelectric croconic acid: combined investigations using experiments and density functional theory

February 2013

Prof. Martin Long
University of Birmingham
Controversial issues in pyrochlores

March 2013

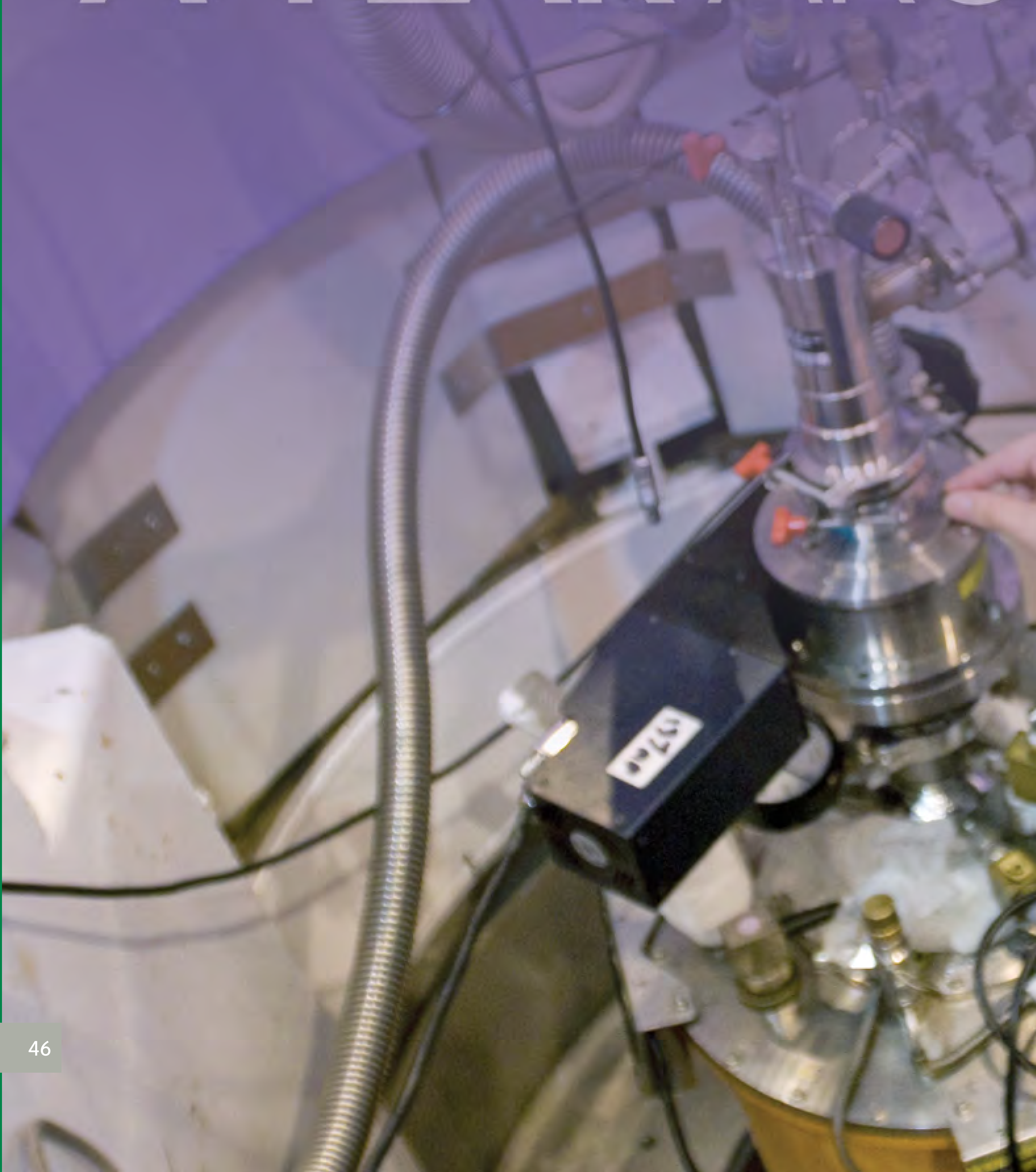
Dr. Giovanni Sordi
Royal Holloway University of London
Mott physics in cuprates: insights from cluster dynamical mean-field theory

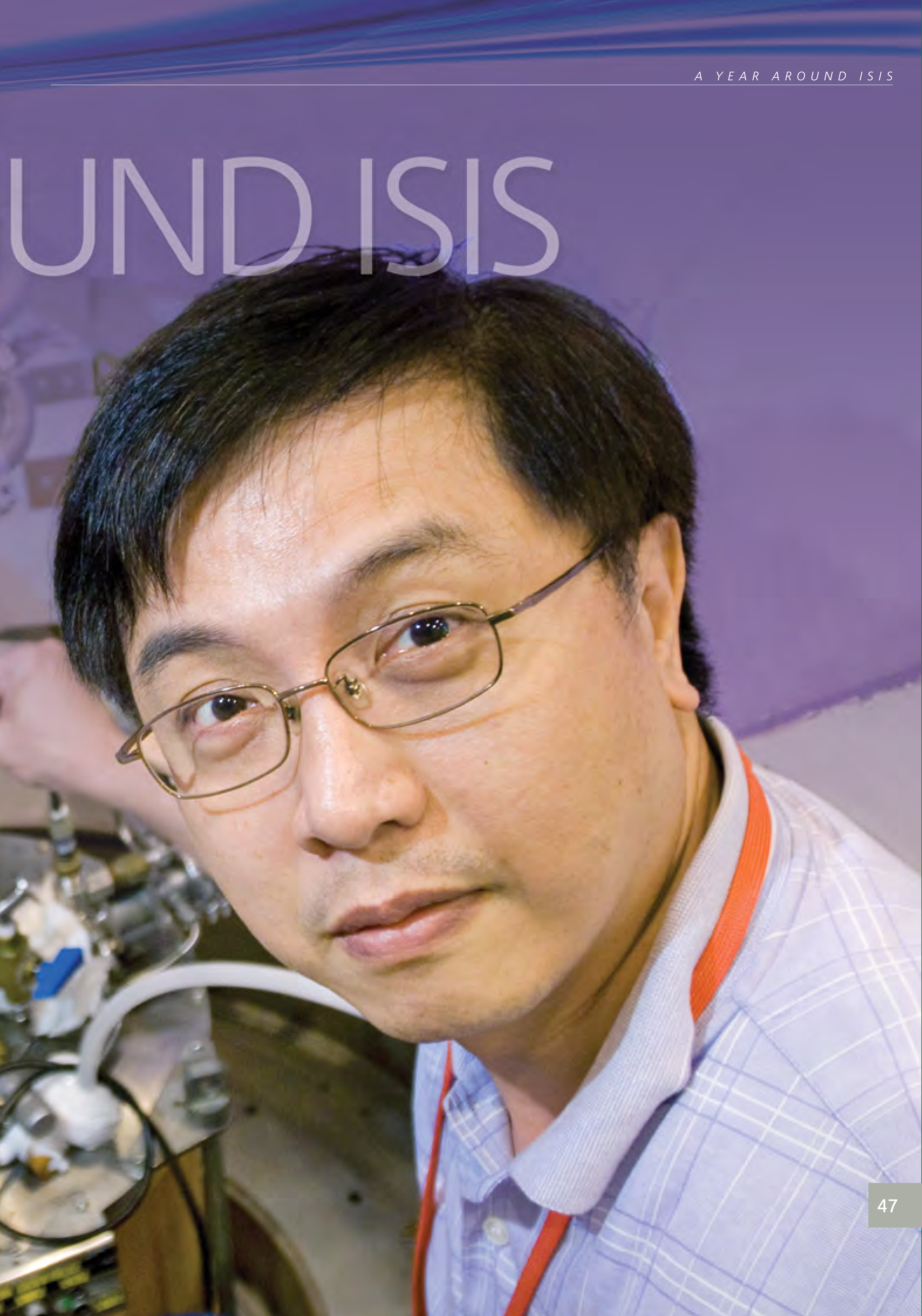
April 2013

Dr. Kostya Trachenko
Queen Mary University of London
New understanding of liquid heat capacity and dynamic crossovers in the supercritical state

Dr. Aldo Isidori
University of Frankfurt
Rotationally-invariant slave-bosons for strongly correlated superconductors

A YEAR ARO




UND ISIS

A year around ISIS

Italian president of CNR visits ISIS

Prof. Nicolais, the President of the Italian National Research Council (the CNR) visited ISIS in October 2012. The aim of the visit was to celebrate over twenty years of successful collaborations between ISIS and CNR. During this visit Prof. Nicolais visited ISIS instruments that CNR has supported including Chipir, IMAT, LET, Nimrod, Vesuvio, Prisma, Tosca and INES.

Crisp supports Australian colleagues

Over 2012 CRISP hosted part of the Australia's ANSTO reflectometry programme. Problems with the cold source at the OPAL reactor lead to a plea for beam time from ISIS. ANSTO provided an instrument scientist and a technician to run experiments.

Willis prize goes to work on gas storage

Dr Sihai Yang, Leverhulme Early Career Fellow at the University of Nottingham, was awarded the B T M Willis Prize for 2013 by the Institute of Physics and the Royal Society of Chemistry Neutron Scattering Group. The award recognises Dr Yang's outstanding research in the application of neutron scattering science to understand gas storage and separation properties of porous materials. Sihai was presented with his award at the UK Neutron and Muon User Meeting 2013 held on 8th April.

Dr Sihai Yang (right) receiving the B T M Willis Prize for research excellence at the UK Neutron and Muon User Meeting 2013. This work isdescribed in the highlight on page 11.

RIKEN and the Chinese Academy of Science visit

In March staff from the RIKEN Global Relations office brought colleagues from the international department of the Chinese Academy of Sciences to visit the RIKEN-RAL muon facility at ISIS. The facility has been a long-term collaboration between ISIS and RIKEN lasting 30 years, and the RIKEN staff were keen to show off this significant international activity to their Chinese colleagues.

BBC films new documentary in the ISIS Second Target Station

The BBC chose ISIS to be one of their filming locations for a new documentary on the sun for BBC2. The producer and director Matt Barrett commented on how professional the facility looked and admitted he had never seen anything like ISIS in the UK: "ISIS is an impressive facility, and I assumed these things only existed in the States".

So long, Farewell, Auf Wiedersehen…

Uschi Steigenberger

Uschi Steigenberger retired from ISIS in August 2012. Uschi was acting Director following Andrew Taylor's move to STFC Executive Director for National Laboratories. Before this she was Head of ISIS Operations and Head of the Spectroscopy and Support Division. Here, Robert McGreevy is presenting her with a history of her time at ISIS.

David Findlay

After 10 years at the helm David Findlay has retired as Head of the Accelerator Division. He will continue to maintain a presence at ISIS on a part-time basis.

Jeff Penfold

Jeff Penfold pioneered the use of scattering techniques, particularly SANS and neutron reflectivity for the study of soft condensed matter in solution, surfactants and polymers adsorbed at interfaces and surfactants under shear. Jeff joined Harwell before going to study Physics at Brunel University. In 1971 he was appointed Scientific Officer in the Neutron Beam Research Unit at the Rutherford Laboratory. From 1977 to 1979 he was seconded to the Institut Laue-Langevin, Grenoble then returned to lead the Large Scale Structures group from 1980 to 2003. In 2001 he was appointed as Project Scientist for the successful Target Station 2 project at ISIS. In 2000 he was appointed Visiting Professor at University of Bristol, and since 2002 he has been Visiting Professor in Physical and Theoretical Chemistry at the University of Oxford. He was a senior research fellow at ISIS until his retirement.

FACTS AND

FIGURES

Facility Access Panels

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	Molecular 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 2012

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

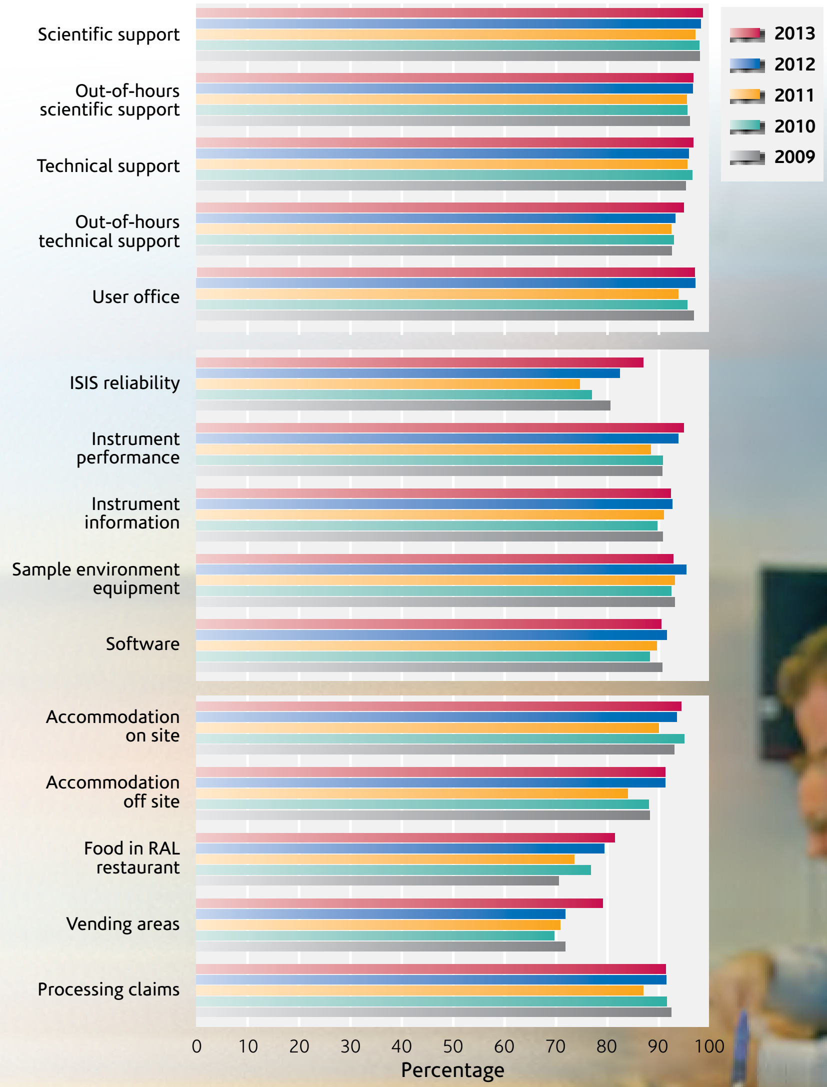
Chair	Jon Goff	Royal Holloway University of London
IUG1 Crystallography	Anthony Powell Peter Slater	Herriot Watt University University of Birmingham
IUG2 Liquids & amorphous	John Holbrey Beau Webber	Queen's University of Belfast University of Kent
IUG3 Large Scale Structures	Jeremy Lakey Ali Zarbaksh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

ISIS representatives

Robert McGreevy	ISIS Director
Zoe Bowden	Head ISIS Experiment Operations Division
Debbie Greenfield	Head ISIS Instrumentation Division
Philip King	Head ISIS Spectroscopy and Support Division
Sean Langridge	Head ISIS Diffraction Division
Andrew Kaye	ISIS User Programme Manager
Christy Kinane	Recording Secretary

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 2012-13

For the period of this report and during scheduled operating cycles, ISIS delivered a total of 642mA.hrs of user proton beam to the muon and neutron targets.

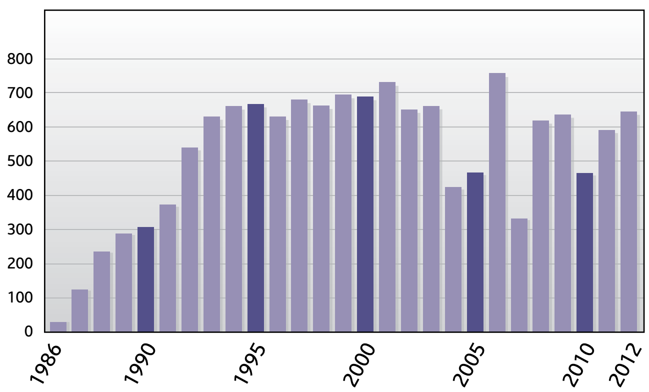
Cycle	12/1	12/2	12/3	12/4	12/5
	15 May – 15 Jun 2013	10 Jul –10 Aug 2013	1 Oct –1 Nov 2013	20 Nov – 21 Dec 2013	19 Feb –29 Mar 2013
Beam on target (hr)	557	501	660	658	795
Total beam current delivery for both targets (mA-hr)	109.2	102.9	136.8	125.9	167.3
Averaged beam current per hour (μA) for targets 1 and 2 combined	170.0	182.5	198.6	193.4	193.6

ISIS operational statistics for year 2012-2013.

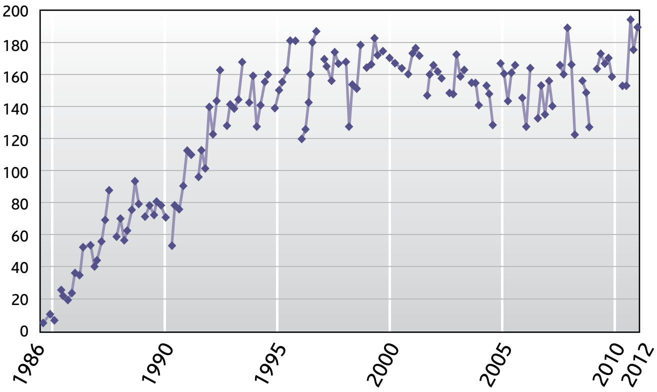
Year	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012
Total scheduled days[1]	156	165	106	119	190	86	163	156	116	138	145
Total integrated current (mAh)	612	647	409	445	738	317	612	630	459	583	642
Average beam current (for beam on target) (μA)	178	177	177	178	179	176	177	208	197	194	203

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

[1] This is the total days available from the accelerator, before instrument calibration and commissioning time, and instrument and accelerator down-time, are taken into account. The days available for the user programme are therefore less than this figure – 120 days were delivered to the user programme in 12/13, averaged across the fully-scheduled instruments.



The ISIS integrated beam current year-on-year



Average ISIS beam current per cycle.

Other Statistics

In the 2012-2013 year:

- 755 experiments were run
- 3029 days were delivered to the user programme
- 3152 visits to the facility were made by 1370 individual users, 641 of which were students
- 61 separate companies were involved in ISIS experiments, from large multi-nationals to smaller, national companies. These represent a variety of industrial areas, including chemicals/plastics, healthcare, transport, automotive, aerospace, manufacturing, energy/oil and other high-tech companies
- 91 individual EPSRC grants supported ISIS proposals from UK users
- at least 419 publications came out in 2012 from ISIS work (see end of this review).

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