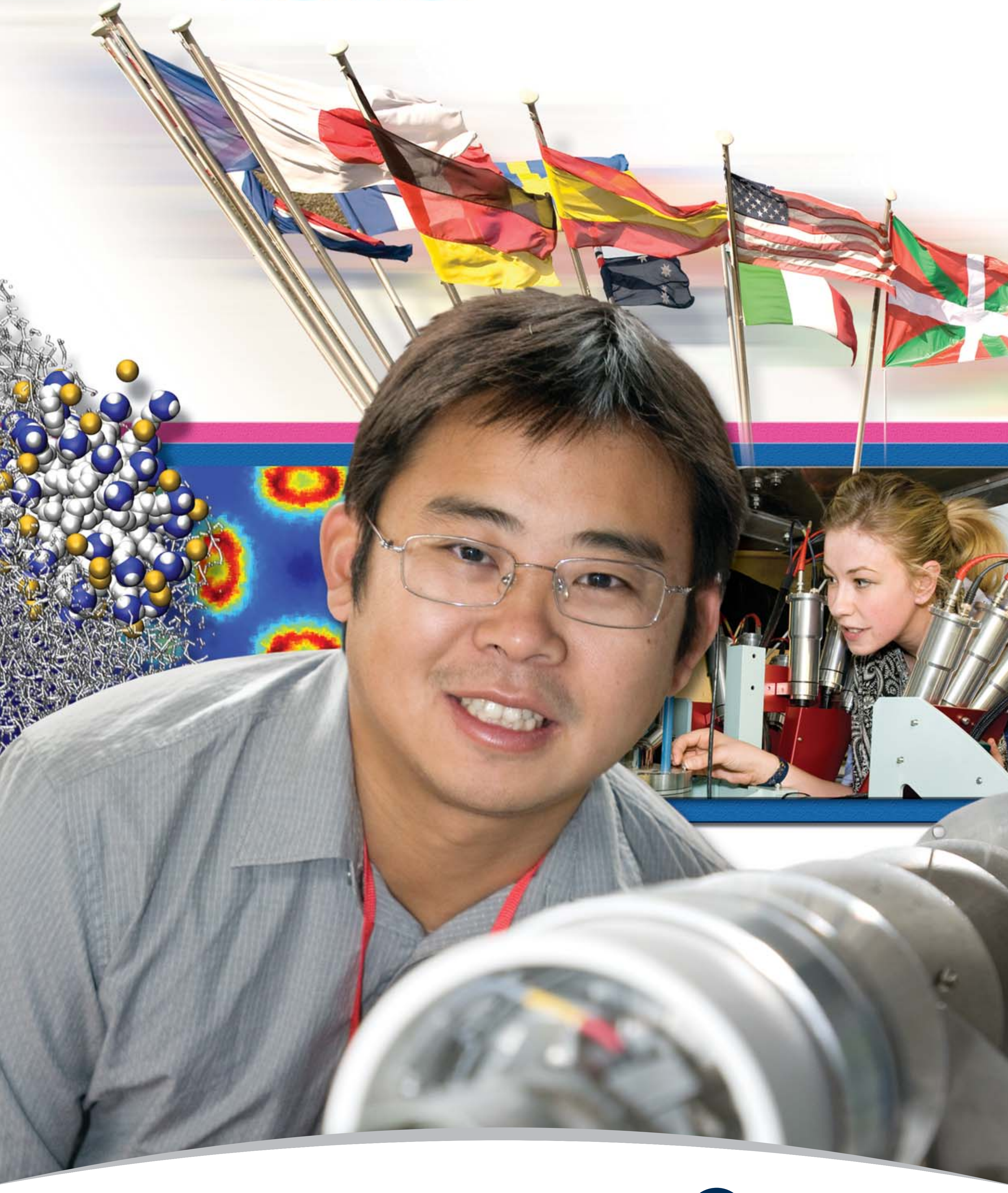
ISIS

Pulsed Neutron and Muon Source
Review of the Year 2012



Science & Technology
Facilities Council

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September 2012

ISIS 2012

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2012 details the work of the facility over the past year, including accounts of science highlights, descriptions of major instrument and accelerator developments and the facility's publications for the past year.

CONTENTS

***Below**: The Large Facilities Steering Group of Research Councils UK toured ISIS in February. Left to right: Lesley Thompson (EPSRC), Jennifer Scratcher (secretariat, STFC), Anne Marie Coriat (MRC), Richard Wade (STFC), Colin Miles (BBSRC), Michael Schultz (NERC), Anna Curzon (Wellcome Trust).*

***Below**: Martin Donnelly, Permanent Secretary at the Department for Business, Innovation and Skills, visited ISIS in May. Here he is being shown the Offspec reflectometer on the Second Target Station by Sean Langridge (ISIS).*

***Right**: Members of the STFC Science Board inside the ISIS Second Target Station building in February. Science Board is STFC's principal scientific advisory committee.*

Top row, left to right: Tony Ryan (Sheffield), Martin Dove (Queen Mary London), Shiela Rowan (Glasgow), Matt Griffin (Cardiff), Bob Warwick (Leicester), Alison Davenport (Birmingham), Peter Butler (Liverpool), Steven Rose (Imperial College London), John Butterworth (University College London), Neville Greaves (Aberystwyth).

Bottom row, left to right: Jenny Hiscock (STFC), Andrew Taylor (STFC), Olwyn Byron (Glasgow), Alan Heavens (Edinburgh), Alfons Weber (Oxford),George Lafferty (Manchester), Bob Newport (Kent), Janet Seed (STFC), Victoria Wright (STFC).

***Below**: Representatives from UK Research Councils visited ISIS in October 2011. Here, Tony Peatfield (MRC), Paul Boyle (ESRC), Rick Rylance (AHRC and RCUK Chair), John Womersley (STFC) and David Delpy (EPSRC) are about to see the ISIS Second Target Station.*

FOREWORD

For the first time since 1992 the Foreword to the ISIS Annual Review is not written by Andrew Taylor. In April 2012 Andrew stepped down as Director of ISIS to take on new responsibilities as STFC's Executive Director for the National Laboratories. In the nearly twenty years of his stewardship of ISIS Andrew has been a charismatic and inspirational leader, shaping the development of the facility in response to evolving and emerging science challenges. We wish him all the best in his new role.

The ISIS science programme remains as strong and diverse as ever, from the understanding of industrial catalysis processes, to the study of animal cryopreservation mechanisms, to revealing how antibacterial proteins attack bacteria, to fundamental studies of magnetic systems that test our theoretical understanding to the limits. In this context, we congratulate ISIS users Stephen Bramwell (UCL) and Alan Tennant (HZB, Berlin), Claudio Castelnovo from the ISIS Theory group and university colleagues on the award of the Europhysics Prize 2012 for the prediction and experimental observation of magnetic monopoles in spin ice.

We are always proud to be working with international partners to take forward ISIS science and instrumentation. In May this year we welcomed Professor Lars Kloo from the Swedish Research Council and colleagues from the Swedish research community to celebrate the Sweden – ISIS partnership. Sweden, together with Spain, contributed significantly to the upgrade of the Polaris diffractometer which was commissioned earlier this year and is already producing exciting new science. We were also very pleased that our colleagues at the Technical University in Delft have secured a €4M grant from the Dutch research organisation NWO for the development of neutron spin manipulation techniques on Larmor, one of the four phase 2 instruments under construction on the Second Target Station.

Our interactions with industrial partners working on commercially relevant science problems have grown this year. ISIS introduced the Industrial Collaborative R&D scheme to provide a new route for industry to gain access to the facility. The uptake has been impressive, with a variety of companies benefiting from the use of neutrons. At the other end of the supply chain, ISIS works with local businesses on new technologies that meet the facility's needs whilst also developing the technical capabilities of the business.

In addition to the impact that ISIS creates through its science, the facility also plays a significant role in the training of young people. Pages 34 and 35 describe how ISIS contributes to the skills of PhD students, vacation students, sandwich course students, apprentices and graduates.

The forthcoming year will continue to see challenges for ISIS, particularly in the current economic climate. Our strong commitment is to continue to deliver exciting new, high impact science in partnership with our user community.

Uschi Steigenberger

Uschi Steigenberger,
Director, ISIS

Above left: *New STFC council member Ian Taylor visited ISIS in September.*

Above centre: *Prof Sir David Wallace and Prof John Toland (Isaac Newton Institute for Mathematical Sciences, Cambridge) discussing ISIS science with Toby Perring (ISIS).*

Above right: *Loiuse Tillman (left) and Susan Morrell (centre) from EPSRC discussing ISIS science with Toby Perring (ISIS).*

Left: *Indian nuclear researchers visiting ISIS in March, with Andrew Taylor and Uschi Steigenberger.*

Below: *John Dodds, Head of Innovation at the Department for Business, Innovation and Skills, with Stephen Voller, CEO, Cella Energy Ltd, an ISIS spin-out company, and Barbara Ghinelli, ISIC.*

Above left: *Senior managers from Siemens Healthcare visited the ONIAC facility, a particle accelerator test facility built at ISIS for Siemens research.*

Above centre: *Lars Kloo (Swedish Research Council and Stockholm) toasting the ISIS – Sweden partnership with Uschi Steigenberger (ISIS).*

Above right: *Scientists from South Korea visited ISIS in March. Present were representatives from the Institute of Basic Science, Seoul National University, the Korean Embassy in London and the British Embassy, Seoul.*

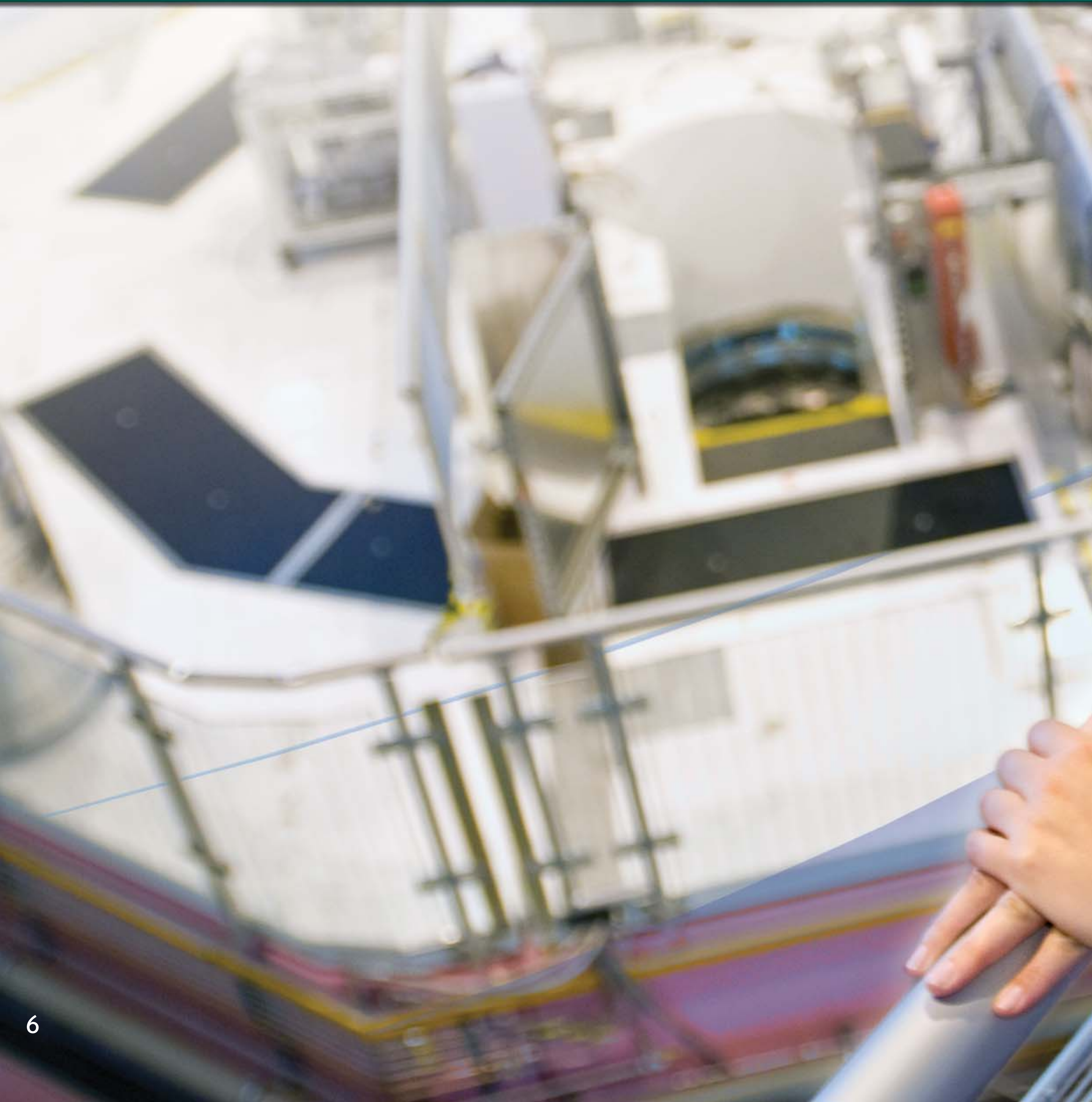
Left: *Researchers from BP visited ISIS in March. They are seen here in the Second Target Station foyer with ISIS staff members.*

A YEAR **AROUND ISIS**

Right: *Members of the Chinese Academy of Sciences visited ISIS in April. Hosting the visit was Andrew Taylor, Executive Director, STFC National Laboratories and ISIS instrument scientist Shu Yan Zhang.*

The advanced facilities provided by ISIS enable world-class research to be performed by scientists from around the world together with facility staff. Academic and industrial applications of the intense neutron and muon beams encompass a very broad range of science areas. Presented in the following pages are brief summaries of recent science highlights.

HIGHLIGHTS OF **ISIS SCIENCE**



Using neutrons to understand cryoprotection

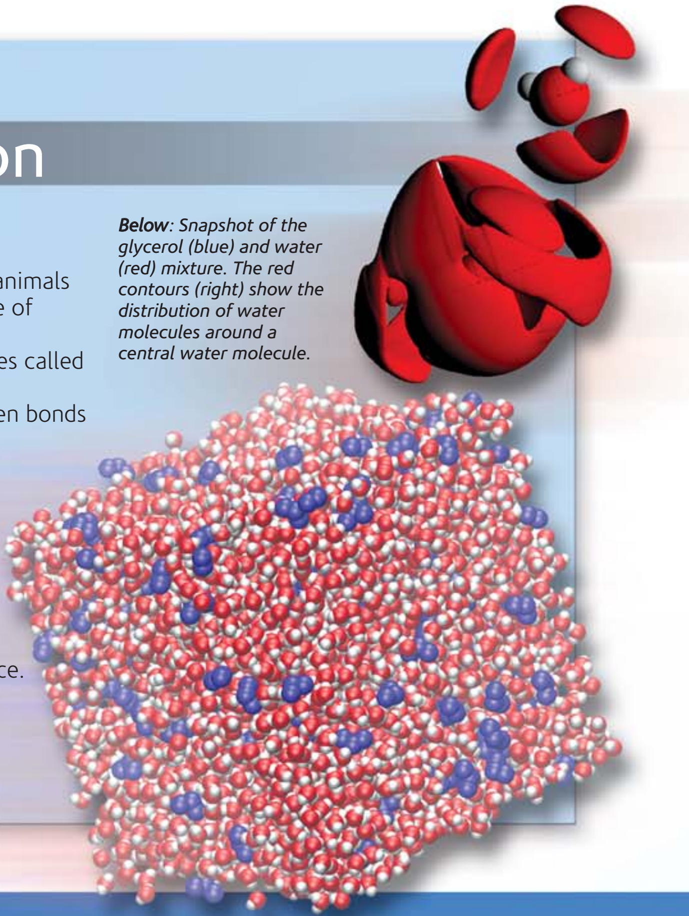
JJ Towey, L Dougan (University of Leeds)

Support for research: EPSRC grant EP/H020616/1

The ability to survive after exposure to low temperatures is important for animals that live in regions of extreme cold. This process is also used in the storage of samples for scientific research, in the food industry as well as for in-vitro fertilisation (IVF). This capability is achieved with the use of small molecules called cryoprotectants, such as glycerol. The method that glycerol uses is not yet understood but one key hypothesis is that it lowers the number of hydrogen bonds formed by water molecules preventing the formation of ice.

To test this hypothesis, we used a combination of neutron diffraction experiments and computer modelling. We found that the number of hydrogen bonds per water molecule is not affected by the addition of glycerol. Instead, we found that water and glycerol mix very efficiently, stopping groups of water molecules from forming clusters. We also found that the water structure looks very similar to pressurised water. This suggests that glycerol acts as a cryoprotectant by compressing the water and preventing large groups of water molecules getting together to form ice.

Below: Snapshot of the glycerol (blue) and water (red) mixture. The red contours (right) show the distribution of water molecules around a central water molecule.



Contact: Dr L Dougan, L.Dougan@leeds.ac.uk
Further reading: JJ Towey et al., J. Phys. Chem. B 116 (2012) 1633; J. Phys. Chem. B 115 (2011) 7799; Phys. Chem. Chem. Phys. 12 (2011) 939

SOFT MATTER *AND BIOMOLECU*

Finding the bacterial Achilles' heel

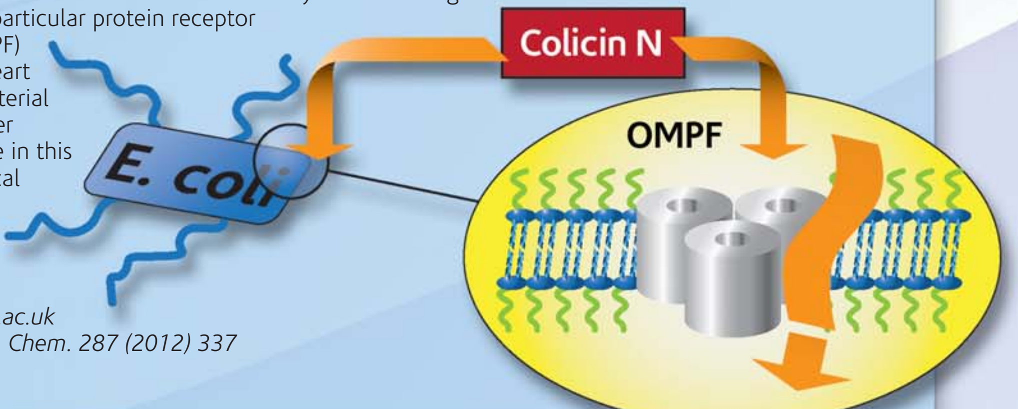
CL Johnson, AS Solovyova, H Ridley, JH Lakey, (Newcastle University), LA Clifton, JRP Webster, CJ Kinane (ISIS), P Callow (ILL), KL Weiss (ORNL), AP Le Brun, SA Holt (ANSTO)

Support for research: The Wellcome Trust

In the search for new antibiotics, we are studying the toxic molecules deployed by bacteria against each other in their battle for resources. Colicins are proteins used by *Escherichia coli* to kill closely related competing bacteria. They have the amazing ability to evade the host defences which consist of a robust and normally impenetrable outer membrane.

To follow the journey of the colicin across this barrier, which is only 5 nm thick (~30,000 times thinner than a sheet of A4 paper), we needed special techniques and neutron scattering gave us critical insights. By recreating the bacterial outer membrane in the laboratory and reflecting neutrons from its surface, we were able to show that a particular protein receptor called Outer membrane protein F (OMPF) allowed the colicin to penetrate the heart of the membrane. This may be the bacterial Achilles' heel – a weak spot in the outer membrane barrier. Neutrons are unique in this ability to see through complex biological structures and differentiate between their components.

The E. coli outer membrane is a complex mixture of lipids and proteins. Neutron scattering showed that colicin N penetrates at the OmpF-Lipid boundary.



Contact: Prof J Lakey, jeremy.lakey@ncl.ac.uk
Further reading: LA Clifton et al., J. Biol. Chem. 287 (2012) 337

Early-stage kinetics of amyloid aggregate formation

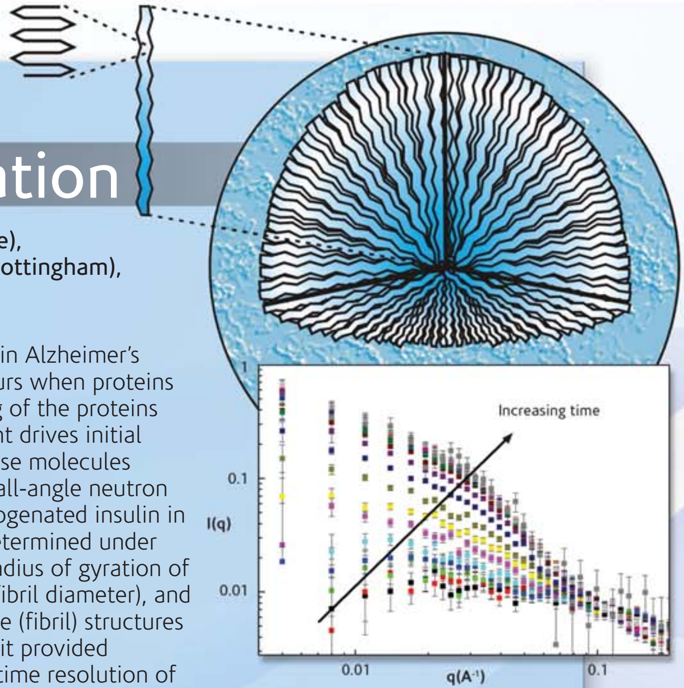
MI Smith (University of Nottingham), V Fodera (University of Cambridge), AJ Parnell (University of Sheffield), JS Sharp, CJ Roberts (University of Nottingham), AM Donald (University of Cambridge), S Rogers (ISIS)

Support for research: EPSRC Grant EP/H004939/1

Amyloid fibrils and spherulites are protein aggregates that are implicated in Alzheimer's disease, Parkinson's disease, and Type-II diabetes. Amyloid formation occurs when proteins denature under certain protein-specific solution conditions. The unfolding of the proteins and exposure of hydrophobic molecular cores to the aqueous environment drives initial aggregation. Internal structural rearrangements can then occur within these molecules resulting in the formation of ß-sheet-rich fibrils. This experiment used small-angle neutron scattering (SANS) to study the early-stage kinetics of aggregation of hydrogenated insulin in D_2O-based solvents. Changes in the size and shape of aggregates were determined under conditions where fibrils and spherulites form. The results show that the radius of gyration of scatterers varies from ~1.5 nm (protein-molecule dimensions) to ~7 nm (fibril diameter), and that the shape of the growing aggregates changes from spheres to rod-like (fibril) structures on time scales of a few hours. SANS was an excellent technique because it provided information about aggregates over a broad range of length scales with a time resolution of minutes, and eliminated potential concerns regarding radiation damage to the samples.

Contact: *Dr JS Sharp, james.sharp@nottingham.ac.uk*

Further reading: *MI Smith et al., Colloid Surface B 89 (2012) 216; Soft Matter 8 (2012) 3751*



Top: *Amyloid spherulites are formed when ß-sheet-rich amyloid fibrils grow radially from a central core.*

Bottom: *SANS data taken during aggregation.*

ULAR SCIENCE

Understanding the dynamics of everyday-use surfactant micelles

VK Sharma, S Mitra, PA Hassan, R Mukhopadhyay (BARC, India), V Garcia Sakai (ISIS)

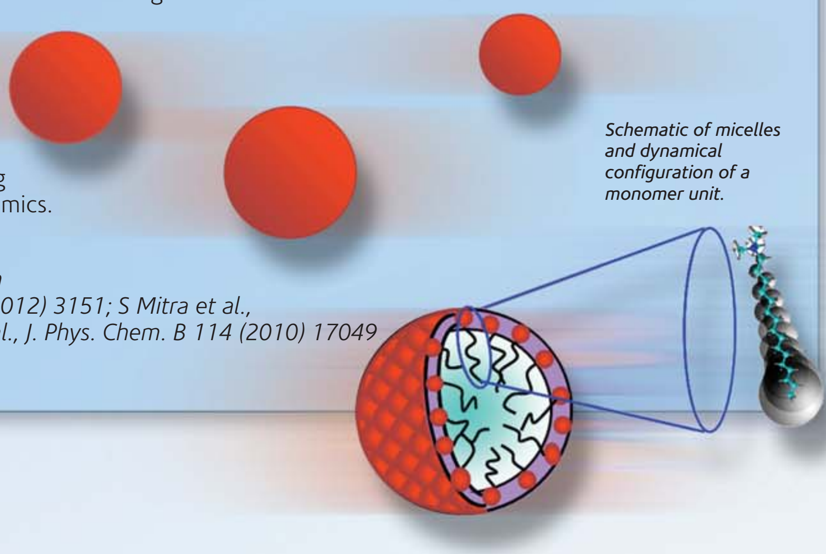
Support for research: Indian government

Amphiphilic molecules (molecules with both water-loving and fat-loving parts) in aqueous solution undergo self-association under specific conditions to form aggregates such as micelles. The local dynamics of such assemblies are important in order to understand, for example, the mechanism of release of soluble drugs or mass transport across membranes. Measurements on Iris on two commonly-used micelle-forming surfactants, anionic sodium dodecyl sulfate (SDS) and cationic cetyltrimethyl-ammonium bromide (CTAB), have revealed the structure-dynamics correlation of surfactant molecules in these assemblies.

The global motion of the micelles follows well-established diffusion laws in solution, with CTAB being slower than SDS micelles due to their size difference. The dynamics of different segments of surfactant molecules within a micelle is adequately described with a model which accounts for the dynamics of head groups and hydrophobic alkyl chains separately. Flexibility of the alkyl chain occurs in a form where the hydrogen atoms move within a spherical volume; size and associated diffusivity increase linearly from head towards tail. Increasing chain length hinders both internal and global dynamics.

Contact: *Dr R Mukhopadhyay, mukhop@barc.gov.in*

Further Reading: *VK Sharma et al., Soft Matter 8 (2012) 3151; S Mitra et al., J. Phys. Chem. B 115 (2011) 9732; VK Sharma et al., J. Phys. Chem. B 114 (2010) 17049*



Schematic of micelles and dynamical configuration of a monomer unit.

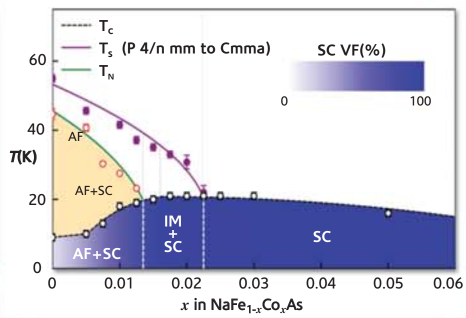
Destroying magnetism and promoting superconductivity with cobalt substitution in iron-based superconductors

JD Wright, T Lancaster, I Franke, AJ Steele, JS Möller, MJ Pitcher, AJ Corkett, DR Parker, DG Free, SJ Clarke, and SJ Blundell (University of Oxford) FL Pratt, PJ Baker (ISIS)

Support for research: EPSRC grant EP/G067481/1

Muons have been used to map out the phase diagram of the iron-based superconductors LiFeAs and NaFeAs in which Co substitutes for Fe. These experiments have shown the subtle interplay of structure, magnetism and superconductivity. In NaFeAs, substituting Fe by Co weakens an ordered magnetic state through a suppression of the transition temperature and a reduction in the size of the ordered moment. Upon further substitution of Fe by Co the high sensitivity of the muon as a local magnetic probe reveals a magnetically disordered phase, in which the size of the moment continues to decrease and falls to zero around the same point at which the magnetically-driven structural distortion is no longer resolvable. Both the magnetism and the structural distortion are weakened as the robust superconducting state is established. In LiFeAs even the unsubstituted compound shows a robust superconducting state. In both compounds the superfluid stiffness, a parameter used to characterize a superconductor's behaviour, tracks the superconducting transition temperature, but in LiFeAs the superfluid stiffness is markedly enhanced.

Contact: *Prof SJ Blundell, s.blundell@physics.ox.ac.uk*
Further reading: *JD Wright et al., Phys. Rev. B 85 (2012) 054503; MJ Pitcher et al., J. Am. Chem. Soc. 132 (2010) 10467*



The phase diagram of $NaFe_{1-x}Co_xAs$ showing regions of antiferromagnetism (AF), superconductivity (SC), and inhomogeneous magnetism (IM), as well as their regions of co-existence.

MANY-BODY *PHYSICS*

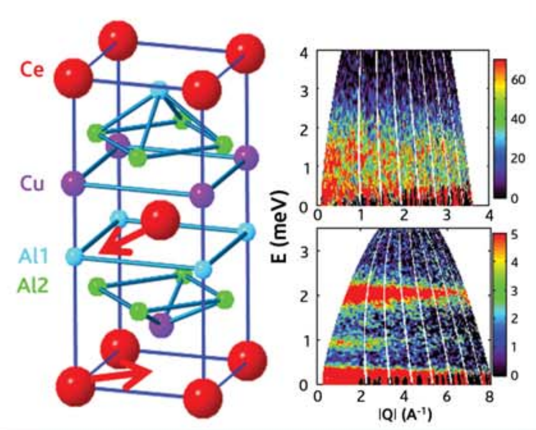
Vibron quasi-bound state in the non-centrosymmetric tetragonal heavy-fermion compound $CeCuAl_3$

D T Adroja (ISIS), A del Moral, C de la Fuente (Zaragoza University), A Fraile, E A Goremychkin, J W Taylor, A D Hillier and F Fernandez-Alonso (ISIS)

Support for research: STFC

Magnetic materials can exhibit behaviour associated with their atomic spins, charges, and atomic positions in the crystal lattice. In the latter case, elementary excitations can arise from crystal electric fields around atoms (CEFs) as well as from the vibrational motions of the atoms (i.e. phonons). Both types of excitations have very similar energy scales, but they are in general considered not to interact with each other. Although when they do interact, superconductivity can arise, the interplay between CEF and phonons is still a largely open question. To fill this gap in our current understanding, we have investigated the magnetic compound $CeCuAl_3$ using inelastic neutron scattering. In the temperature range where magnetic ordering does not exist, our results show three magnetic excitations that cannot be explained by current theoretical models. To analyse these data, we have extended previous theoretical models to include the particular form of the $CeCuAl_3$ crystal structure. This extension provides an excellent explanation of the three observed magnetic excitations. The present study also highlights the increasing importance of understanding the interplay between magnetic and vibrational dynamics in magnetic materials of technological relevance.

Contact: *Dr DT Adroja, devashibhai.adroja@stfc.ac.uk*
Further reading: *DT Adroja et al, Phys. Rev. Lett. 108, 216402 (2012)*



Unit cell of $CeCuAl_3$. The arrows represent the active longitudinal optic phonon modes. (right) Contour plots of the INS data, energy transfer, and momentum transfer at 5 K.

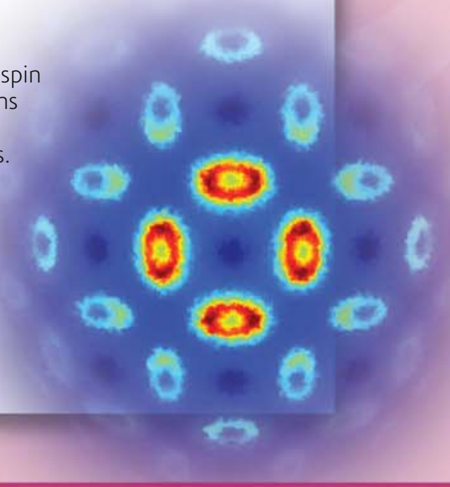
Nature of magnetic excitations in in superconducting $BaFe_{1.9}Ni_{0.1}As_2$

M Liu, L Harriger (University of Tennessee), H Luo, M Wang (Institute of Physics, Beijing), R Ewings, T Guidi (ISIS), H Park, K Haule, G Kotliar (Rutgers University), S M Hayden (University of Bristol), P Dai (University of Tennessee)
Support for research: US National Science Foundation, Ministry of Science and Technology China 973 Programs, National Natural Science Foundation of China, US Department of Energy, American Chemical Society Petroleum Research Fund, Alfred P. Sloan Foundation

Iron and magnetism have a long and rich history, dating back to the days when the ancients realized that lodestone, a naturally magnetized mineral, could attract a piece of iron. However, the story of magnetism and iron still has some new chapters to come, as magnetism may be the glue that binds electrons together in Cooper pairs which lead to superconductivity.

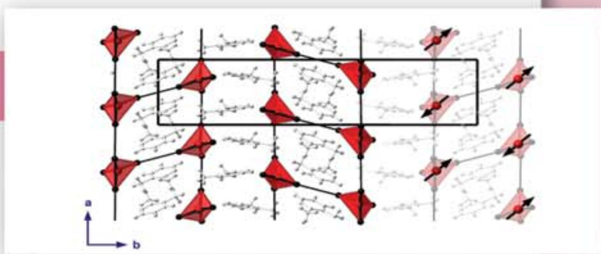
To understand the origin of this magnetism, we measured the intensity of magnetic excitations or spin waves in electron-doped superconducting $BaFe_{1.9}Ni_{0.1}As_2$ and compared the results with excitations in antiferromagnetic non-superconducting $BaFe_2As_2$. Such measurements can help determine the effect of electron-doping which induces superconductivity to spin waves in the parent compounds. Surprisingly, we find electron-doping only affects spin excitations below 100 meV while the total size of the magnetic moment and the energy distribution do not change much. It shows that the magnetic moments in both materials are similar to insulating copper oxides, an indicator of the importance of strong electron correlations in high temperature superconductivity.

Contact: *Dr P Dai, pdai@utk.edu*
Further reading: *M Liu et al., Nature Physics 8, 376–381 (2012)*



Spin excitations in $BaFe_{1.9}Ni_{0.1}As_2$

Full excitation spectrum of a spin-ladder



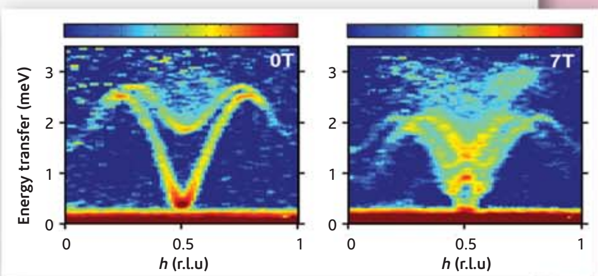
D Schmidiger, A Zheludev (ETH Zürich, Switzerland) T Guidi, R Bewley (ISIS)
Support for research: Schweizerische Nationalfonds SNF, Project 23171

One-dimensional spin systems – systems in which the atomic magnetic moments interact with neighbours primarily along a single direction only – offer access to exciting physics very different from the higher-dimensional counterparts. Due to the reduced dimensionality, quantum fluctuations inhibit magnetic ordering even at zero temperature. These systems remain in a non-magnetic spin-liquid or an exotic nearly ordered Luttinger-liquid ground state.

Antiferromagnetic Heisenberg spin ladders belong to the simplest model 1D magnetic systems. In zero field, they feature a spin-liquid ground state while a large enough magnetic field induces a transition to a Luttinger-liquid state.

Luckily, nature provides us with materials in which spin-ladder systems are realized due to a particular arrangement of magnetic ions. We investigated an exceptionally clean spin-ladder material, $(C_7D_{10}N)_2CuBr_4$ (DIMPY). Using the Let spectrometer, we observed a fundamental change in the excitation spectrum by moving from the spin-liquid into the Luttinger-liquid regime. Our results are in full agreement with state-of-the-art numerical calculations and emphasise that both due to remarkable developments in neutron instrumentation and spectacular capabilities of supercomputers, the spin-ladder problem can nowadays be tackled on a fully quantitative level.

Contact: *D Schmidiger, schmdavi@phys.ethz.ch*
Further reading: *D Schmidiger et al., Phys. Rev. Lett. 108 (2012) 167201*



Top: *DIMPY crystal structure. Large organic molecules effectively separate individual spin-ladders.*

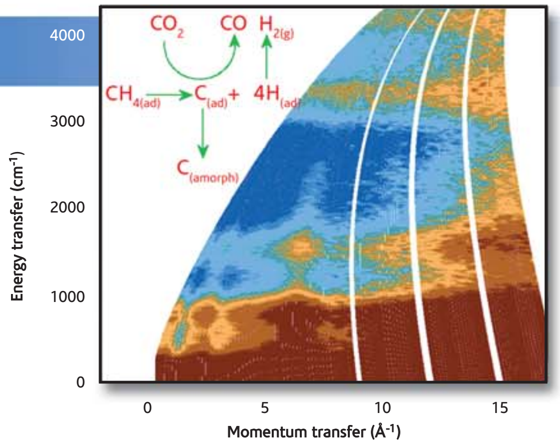
Bottom: *measured excitation spectrum in the spin liquid (left) and Luttinger-liquid (right) phase.*

Dry reforming of methane – a use for CO_2?

D Lennon, I P Silverwood, N G Hamilton, A R McFarlane, J Kapitán, L Hecht, (Glasgow University), E L Norris, R M Ormerod, (Keele University), C D Frost, S F Parker (ISIS)

Support for research: EPSRC grant EP/E028861/1

Hydrogen is produced industrially by reacting methane and steam (steam reforming) at high temperature typically over a nickel-alumina catalyst. It can also be produced by using carbon dioxide (dry reforming) instead of steam. This is an environmentally very attractive route because it provides an economic use for carbon dioxide.



INS data of a Ni/Al_2O_3 catalyst after dry reforming of methane. The inset shows the associated reaction scheme.

Our studies of this process showed that most of the carbon dioxide is converted to the useful reactant carbon monoxide and a small proportion is reduced to amorphous carbon that was retained on the catalyst. An array of techniques that included reaction testing, temperature-programmed oxidation and inelastic neutron scattering (INS) spectroscopy showed that the catalyst is very efficient at cycling hydrogen as very little was present in the carbon overlayer that builds-up on the catalyst surface. Uniquely, INS is able to both quantify the amount of hydrogen present in the carbon and to show that most of it is bonded to aliphatic, sp^3, carbons.

Contact: *Dr D Lennon, David.Lennon@glasgow.ac.uk*
Further reading: *IP Silverwood et al., Phys. Chem. Chem. Phys. 14 (2012) 15214-15225*

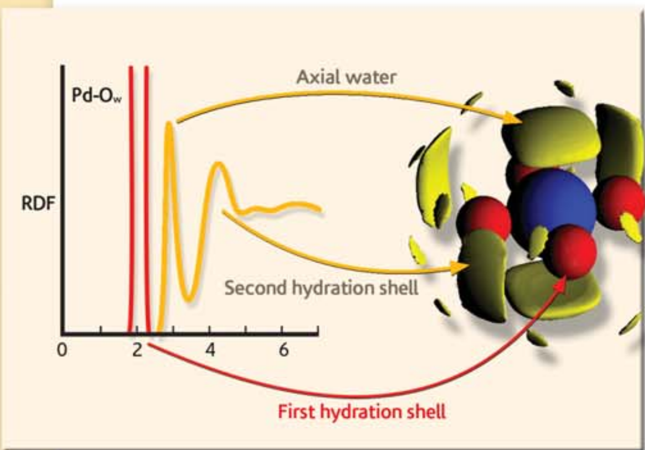
CHEMISTRY *AND CATALYSIS*

Axial structure of the Pd(II) aqua ion in solution

DT Bowron (ISIS), EC Beret (University of Seville), E Martin-Zamora (University of Seville), AK Soper (ISIS) and E Sánchez Marcos (University of Seville)

Support for research: University of Seville and ISIS

The solution chemistry of Pt(II) and Pd(II) cations has attracted much attention because of their relevance in catalytic processes and pharmacological activity in cancer treatments. The square-planar ligand arrangement adopted by these transition-metal cations has drawn attention to their axial coordination which is intimately related to their reactivity. Prior experimental and theoretical techniques provide competing structural pictures of this region. Our work has investigated the Pd(II) aqua ion in perchloric acid solution by a multi-technique approach to resolve the controversy. The approach made use of neutron diffraction, X-ray diffraction, EXAFS and a Monte Carlo structure refinement technique. The Pd-O(water) radial distribution function derived from this study shows, between the first and second hydration shells, a well-defined peak which corresponds to water molecules in the axial region. An unexpected discovery about this axial coordination is the competition between water and perchlorate anions to occupy this region and highlights the importance of considering the counterion in chemical reactions with these salts.



Spatial representation of the hydration structure of the square planar Pd(II) aqua ion highlighting the chemically important axial hydration region.

Contact: *Dr DT Bowron, daniel.bowron@stfc.ac.uk*
Further reading: *DT Bowron et al, Journal of the American Chemical Society 134 (2012) 962-967*

Dimethylamine borane dehydrogenation chemistry

CY Tang, N Phillips, JI Bates, AL Thompson, S Aldridge (University of Oxford), MJ Gutmann (ISIS)

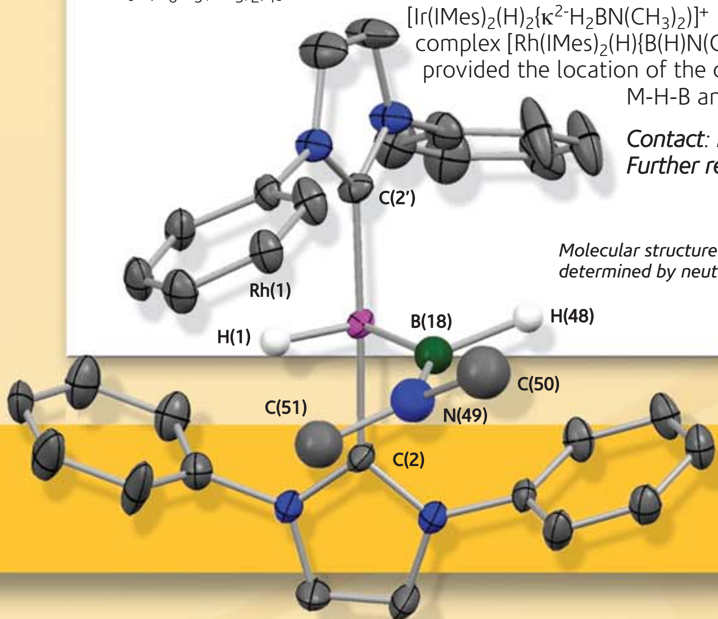
Support for research: EPSRC grant EP/F01600X/1

The metal-catalysed dehydrogenation of saturated bonds represents a powerful approach to producing both synthetically valuable functional groups (e.g. alkenes from alkanes) and to novel polymeric materials. In the case of saturated C-C bonds, such processes can be carried out either with or without a sacrificial hydrogen acceptor. The isoelectronic B-N containing systems have been investigated explicitly as in situ sources of free H_2.

We have investigated the rhodium / iridium catalyzed dehydrogenation of dimethylamine borane. Thus, the reaction of $(CH_3)_2NH{\cdot}BH_3$, with $M(IMes)_2(H)_2Cl$ (M = Rh, Ir, IMes = N,N'-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene) in the presence of $Na[B\{C_6H_3(CF_3)_2\}_4]$ leads to the isolation of the 18-electron aminoborane adduct $[Ir(IMes)_2(H)_2\{\kappa^{2}\text{-}H_2BN(CH_3)_2\}]^+$ and the remarkable 14-electron rhodium aminoboryl complex $[Rh(IMes)_2(H)\{B(H)N(CH_3)_2\}]^+$. Single crystal neutron diffraction studies have provided the location of the crucial hydrogen atom positions in amino functionalized M-H-B and M-B-H species formed under catalytic conditions.

Contact: *Prof S Aldridge, Simon.Aldridge@chem.ox.ac.uk*

Further reading: *CY Tang et al., Chem. Comm. 48 (2012) 8096-8098*



Molecular structure of the cationic component of $[Rh(IMes)_2(H)\{B(H)NMe_2\}]$ $[B\{C_6H_3(CF_3)_2\}_4]$ as determined by neutron diffraction.

How water dissolves in protic ionic liquids

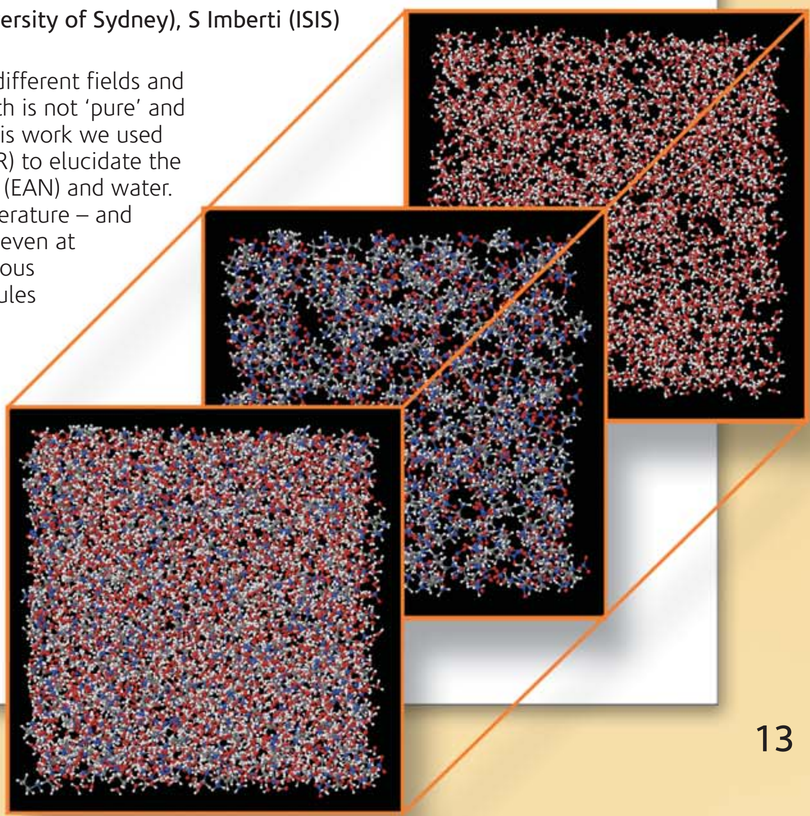
R Hayes, R Atkin (University of Newcastle), GG Warr (University of Sydney), S Imberti (ISIS)

Support for research: ARC grant DP0986194

Scientific interest in water is broad and deep, uniting many different fields and disciplines. However more than 99% of water found on Earth is not 'pure' and instead contains significant quantities of dissolved salt. In this work we used neutron diffraction (Sandals) and computer simulations (EPSR) to elucidate the structure of salty water: mixtures of ethylammonium nitrate (EAN) and water. EAN is an ionic liquid (IL) – a salt that is liquid at room temperature – and is miscible in water in all proportions. Our results show that even at high salt content, EAN/water forms a pronounced, bicontinuous nanostructured fluid. The local arrangement of water molecules and EAN ions in this solution is strikingly similar to the pure liquids because of self-assembly akin to surfactant mesophases but on much smaller length scales. Our study paves the way for new, environmentally friendly nanostructured fluids that retain key solvent properties of ILs and water, but at lower overall cost.

Contact: *Assoc Prof Rob Atkin, Rob.Atkin@newcastle.edu.au*

Further reading: *Hayes et al. Angewandte Chemie Int. Ed. 51 (2012) 7468-7471*



Snapshot of EAN + H_2O bicontinuous bulk structure, with EAN and water-only domains highlighted. (C=grey, H=white, N=blue, O=red)

Colossal negative thermal expansion in $BiNiO_3$

M Azuma, WT Chen, H Seki, M Czapski, O Smirnova, K Oka, S Ishiwata, Y Shimakawa (Kyoto University), M Mizumaki, N Kawamura (Japan Synchrotron Radiation Research Institute), T Watanuki (Japan Atomic Energy Agency), N Ishimatsu (Hiroshima University), MG Tucker (ISIS), JP Attfield (University of Edinburgh)

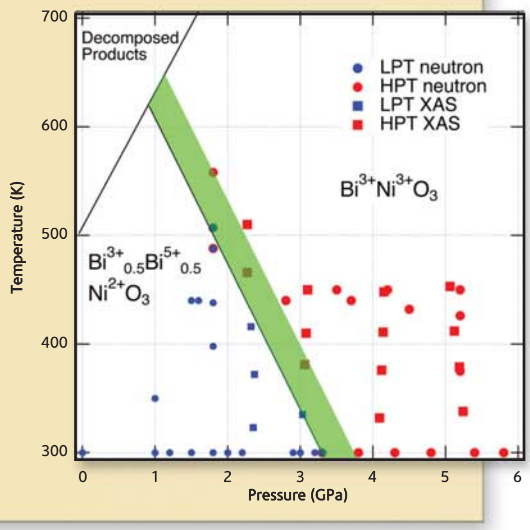
Support for research: Japan Science and Technology Agency and EPSRC Strategic Japan-UK Cooperative Programme

The unusual property of negative thermal expansion (NTE) may be used to fabricate composites with zero or other controlled thermal expansion values. Colossal NTE effects have been discovered in perovskite type oxides showing intervalence transitions. $BiNiO_3$ undergoes a remarkable Bi-Ni charge transfer under pressure, accompanied by a broad insulator-to-metal transition and a substantial (3%) volume decrease. High pressure and temperature neutron powder diffraction studies and complementary X-ray absorption experiments have been used to map out the phase diagram, which shows that the transition has a negative temperature-pressure slope. This enables the same structural change and accompanying volume reduction to be observed by heating $BiNiO_3$ at a moderate pressure. Chemical substitution of lanthanum for bismuth has been used to shift the charge transfer transition to ambient pressure and a ceramic pellet of this material shows colossal NTE when heated above room temperature.

Contact: *Prof JP Attfield, j.p.attfield@ed.ac.uk*

Further reading: *M Azuma et al., Nature Comm. 3 (2011) 347*

Pressure-temperature (PT) phase diagram for $BiNiO_3$ showing the broad transition from the low PT ($Bi^{3+}_{0.5}Bi^{5+}_{0.5}Ni^{2+}O_3$) to the high PT ($Bi^{3+}Ni^{3+}O_3$) form where negative expansion occurs.



CONDENSED MATTER AND FUN

Muons probe hydrogen interactions with defective graphene

M Riccò, D Pontiroli, M Mazzani, M Choucair (Università di Parma), J A Stride (University of New South Wales, Australia), O V Yazyev (Institute of Ecole Polytechnique Fédérale de Lausanne, Switzerland)

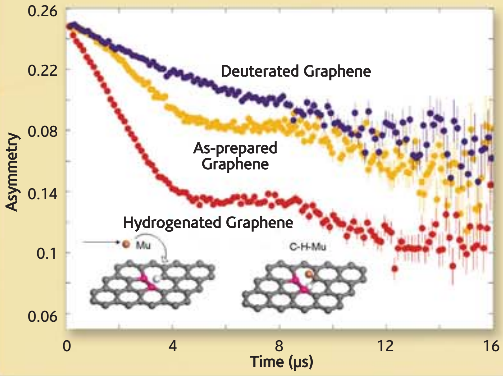
Support for research: Swiss National Science Foundation HyCarBo project (grant No. CRSII2-130509) and grants No. PBELP2-123086 and PP002-133552.

The reactivity and magnetic behaviour of graphene, whose extraordinary properties inspired the 2010 Nobel prize in Physics, can be modified if defects such as vacancies (missing carbon atoms) are present. The chemically produced graphene investigated here is known to possess this type of defect.

The µSR technique can probe graphene's properties by following the spin evolution of implanted muons that, in graphene, form muonium, which behaves like hydrogen. The observation of muon spin precession is usually associated with long range magnetic order, whose onset, according to theoretical predictions, could be attributed to the presence of defects in graphene. However, treatment with hydrogen and deuterium showed that the precession which we observed was caused by the nuclear dipolar interaction of the muon with a hydrogen already present in the vacancy and not due to a local field of a magnetic material. This result disproves defect-induced magnetism in graphene, but suggests that defects in graphene possess an extraordinary efficiency for trapping hydrogen.

Contact: *Prof M Riccò, Mauro.Ricco@fis.unipr.it*

Further reading: *M Riccò et al., Nano Letters 11 (2011) 4919*



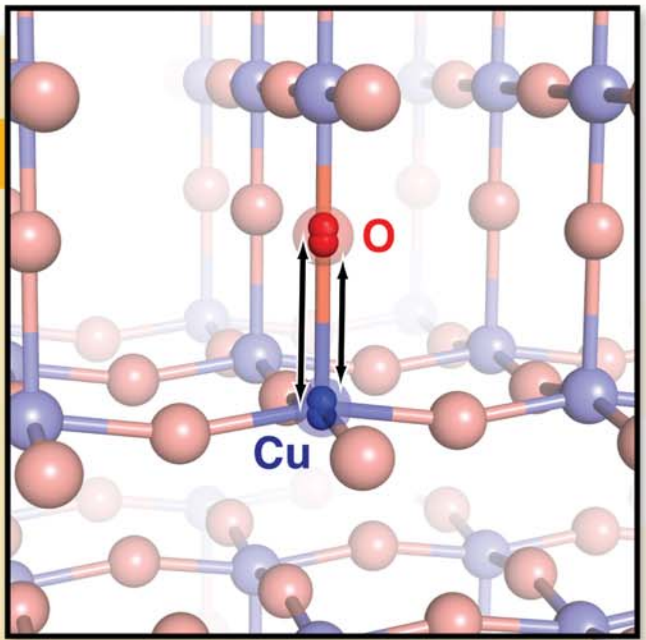
Muon spin precession in defective graphene disappears after treatment with deuterium, confirming its nuclear dipolar origin. Inset: formation of the CHMu group responsible for the precession.

Hidden distortions in YBCO superconductor

C A Young, E Dixon, M A Hayward, A L Goodwin (University of Oxford), M G Tucker, D A Keen (ISIS)

Support for research: EPSRC Grant EP/G004528/2

The ceramic oxide $YBa_2Cu_3O_{6.93}$ (YBCO) is arguably the most widely-studied of the high-temperature superconductors – a family of materials capable of conducting electricity with zero resistance. While the mechanism responsible for superconductivity in YBCO remains unknown, the consensus is that conduction takes place within square-grid-like CuO_2 layers. Perhaps the longest-standing debate concerning the structural chemistry of YBCO centres on the interaction between these Cu atoms and axial O atoms involved in joining the layers together. EXAFS measurements indicate two different Cu-O bond lengths, whereas diffraction indicates all Cu-O bonds are equivalent. Distinguishing the two cases is important in order to understand charge localisation within the layers. Using neutron total scattering measurements and reverse Monte Carlo refinement, we show there are indeed two separate Cu-O bond lengths, but correlations between Cu and O displacements give rise to an apparent single Cu-O bond length in the average crystal structure.



Correlations between Cu and O displacements conceal the existence of two distinct axial Cu–O bonds in YBCO, each potentially associated with different Cu charge states.

Contact: *Dr AL Goodwin, andrew.goodwin@chem.ox.ac.uk*
Further reading: *CA Young et al., Z. Krist. 227 (2012) 280*

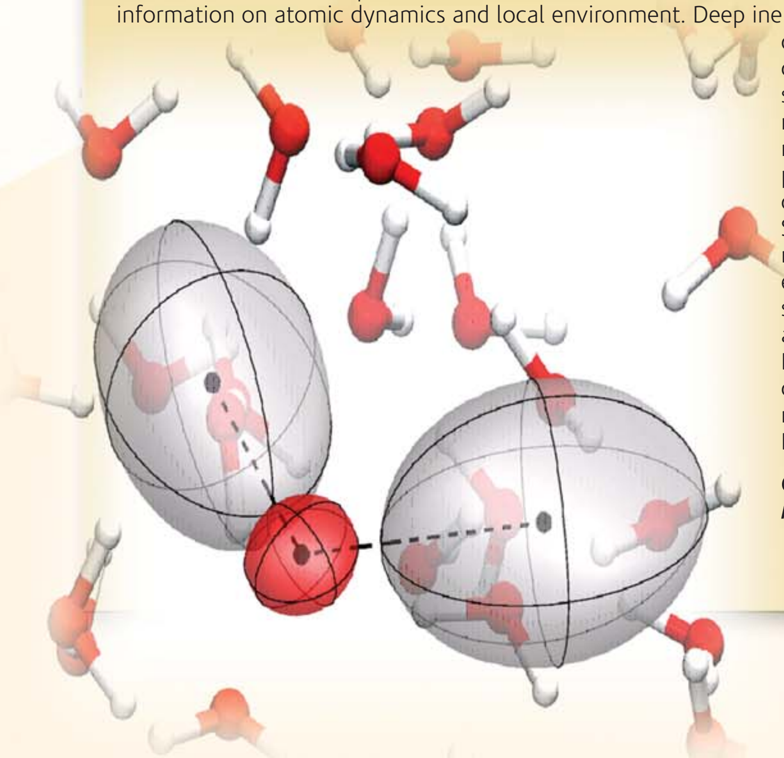
NDAMENTAL SCIENCE

The quantum nature of oxygen in heavy water

G Romanelli, R Senesi, C Andreani (University of Rome Tor Vergata and CNR-IPCF), M Ceriotti (University of Oxford)

Support for research: CNR-STFC Agreement No. 06/20018 concerning the collaboration in scientific research at ISIS.

Because of its intrinsic quantum nature, the momentum distribution (MD) of light nuclei conveys a great deal of information on atomic dynamics and local environment. Deep inelastic neutron scattering experiments can measure this quantity with great precision. Most recently, atomistic computer simulations are beginning to provide new and significant insights into the understanding of heavy nuclei in hydrogen-bonded systems. The study of heavier nuclei, although challenging because of their less pronounced quantum nature, promises a more comprehensive picture of the underlying physics. Simultaneous measurements of the MD of both D and O nuclei in D_2O on Vesuvio demonstrate that both O and D exhibit significant quantum behaviour. Further, computer simulations highlight the fact that the O atom possesses an anisotropic MD. Do the O and D dynamics reflect the D/H reduced-mass effect? Joint neutron experiments and computer simulations provide the answer: D and O nuclei have lower and higher kinetic energy values in D_2O than H and O nuclei in H_2O, respectively.



Contact: *Dr G Romanelli, Giovanni.romanelli@uniroma2.it*
Further reading: *M Ceriotti et al., Phys. Rev. Lett. 109 (2012) 100604*

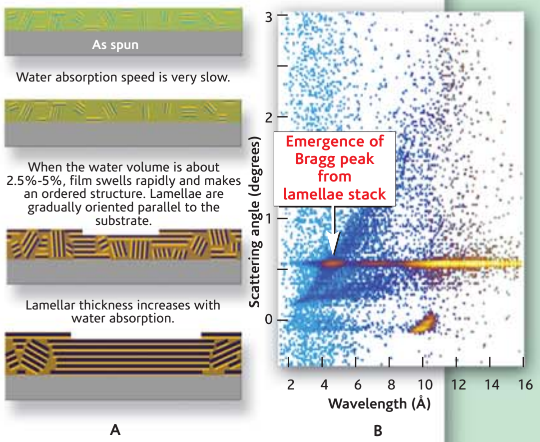
Hydration and ordering of lamellar block copolymer films prior to the formation of polymer vesicles

Y Kamata, AJ Parnell, RAL Jones (University of Sheffield), AJC Dennison, R Barker, P Gutfreund (ILL), MWA Skoda (ISIS), S Mai (University of Sheffield)
Support for research: EPSRC grant EP/E046215/1

Vesicles are microscopic sacs that enclose a volume with a molecularly thin membrane. The membranes generally self-assemble from molecules with a mixed hydrophilic (water-loving) – hydrophobic (water-hating) or amphiphilic character. Biological vesicles are important for cell function and are principally formed from lipids. Block copolymers that mimic lipid amphiphilicity can also self-assemble into vesicles.

Polymersomes – vesicles based on self-assembled bilayers composed of amphiphilic copolymers – are good candidates for molecular delivery systems. Hydrophilic molecules can be enclosed within the aqueous core, to be released by a trigger which disrupts the vesicle's wall. Their wall thicknesses and compositions can be tuned to control the diffusion of molecular species in and out of the vesicle. We used the Inter reflectometer to study the initial stages of the formation of the lamellar structure – which is the precursor of the polymersomes - by rehydration of spin-cast thin films in real time. When the water volume is 2.5-5%, the film swells rapidly and makes an ordered structure. Lamellae become gradually oriented parallel to the substrate.

Contact: *Y Kamata, Yohei_Kamata@kuraray.co.jp*
Further reading: *AJ Parnell et al., Faraday Discuss. 143 (2009) 29*



Formation of lamellar structures by rehydration of a block copolymer thin film. These structures act as precursors to polymer-vesicle formation – see 'A'.

NANO *AND SUPRAMOLECULAR*

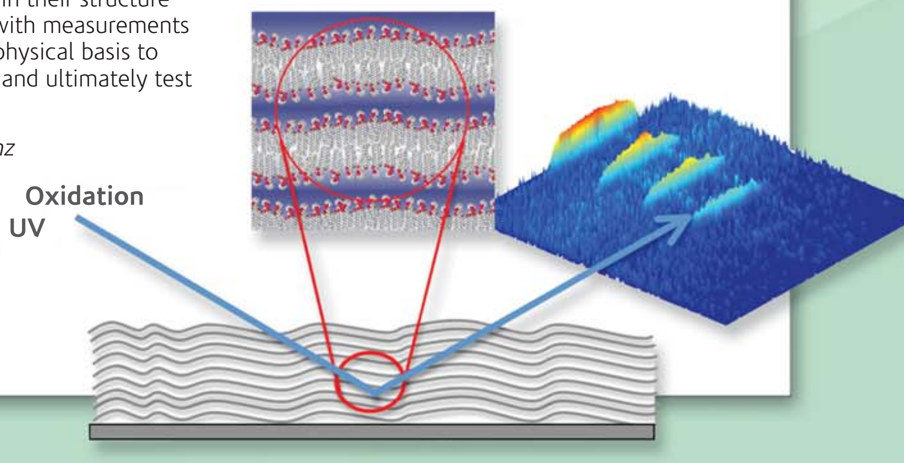
Understanding oxidative stress in cellular membranes – red wine for long life?

JJ Knobloch, DJ McGillivray (University of Auckland, New Zealand), AJ Nelson (ANSTO, Australia), RM Dalgliesh (ISIS)
Support for research: The Royal Society of New Zealand Marsden Fund; the Australian Institute of Nuclear Science and Engineering.

The human body is continuously fighting a wide range of oxidative stresses, from free radicals caused by UV light or pollution, to toxins from poor diet. Oxidative damage causes changes to the structure of cellular membranes, compromising their integrity as a diffusion barrier – this phenomenon has been widely linked to a range of aging problems, including Parkinson's, Alzheimer's, and heart disease. As a consequence, there is a multi-million dollar industry in antioxidant supplements promoting youth, energy, and immunity – promises based unfortunately on limited physical knowledge.

We have used the wide momentum-transfer range available on Offspec for the first time to study aligned phospholipid bilayer membrane stacks, which are crystalline in one-dimension and give rise to diffraction peaks. These membranes mimic cellular membranes, and are very sensitive to subtle changes in their structure after damage by oxidation. By correlating this study with measurements of membrane function, we are working to provide a physical basis to understand the complex biology of oxidative stress – and ultimately test the hypothesis that red wine leads to a long life!

Contact: *Dr D McGillivray, d.mcgillivray@auckland.ac.nz*
Further reading: *JJ Knobloch et al., in preparation*



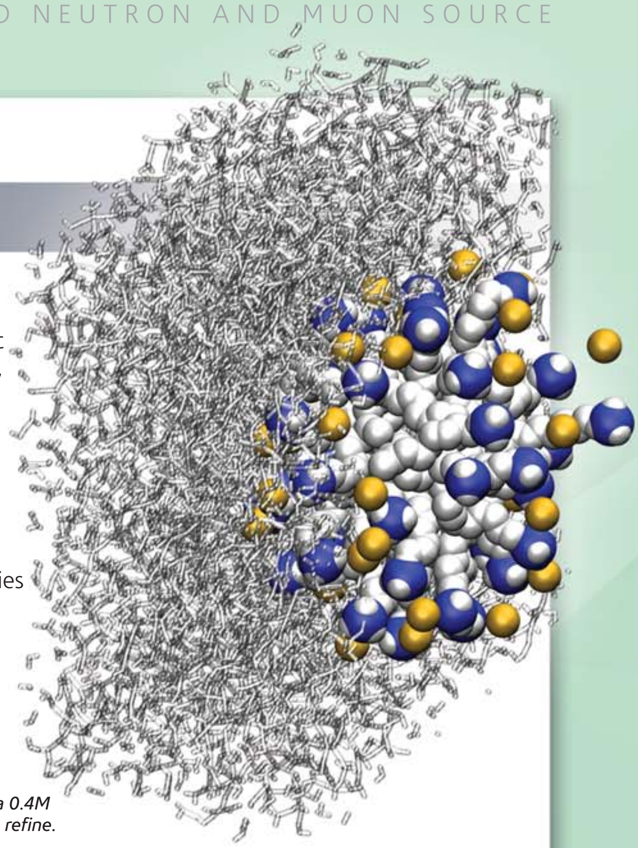
Aligned phospholipid membrane stacks give rise to multiple diffraction peaks on OFFSPEC, allowing the subtle effects of oxidative stress to be determined.

The atomistic structure of a micelle in solution

R Hargreaves, DT Bowron (ISIS), K Edler (University of Bath)
Support for research: University of Bath

In aqueous solution, surfactant molecules can aggregate into micelles that act as a tiny compartment where oily, nonpolar species (oily dirt, non-polar drugs, etc) can be hidden inside and carried through water without separating out. They play an important role in many household products from shampoo to cosmetics, medicines, paints, and foods. To optimise the properties of formulations containing micelles, a detailed understanding of their structure and interactions with the surrounding solution is needed. Previously, micelle structure has been characterised by a number of indirect or low-resolution techniques, meaning that a detailed atomic picture has been lacking. The combination of neutron scattering methods with modern computing capabilities has allowed us to address this limitation. We have used the ISIS liquids and disordered materials diffractometers Sandals and Nimrod to investigate the structure of a simple micelle as a starting point for future investigations of interactions between these aggregates and other ions and molecules.

Contact: Dr K Edler, k.edler@bath.ac.uk
Further reading: R Hargreaves et al., J. Am. Chem. Soc. 133 (2011) 16424



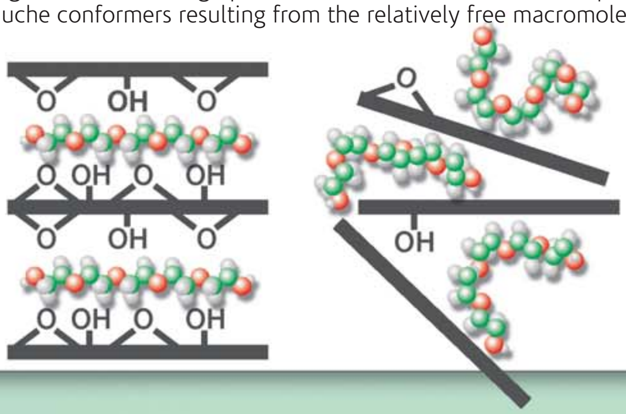
Refined structure of a decyltrimethylammonium bromide (C10TAB) surfactant micelle in a 0.4M aqueous solution. The model contains 29,592 atoms and took 1,250 CPU days to refine.

SCIENCE

Neutron spectroscopy to probe polymer structure under extreme spatial confinement

F Barroso-Bujans, S Cerveny, S Arrese-Igor, JA Pomposo, A Alegría, J Colmenero (CSIC/UPV-EHU, Spain),
F Fernandez-Alonso (ISIS)
Support for research: Spanish Ministry of Education, Basque Government, BERC-MPC

Infrared and Raman spectroscopy represent the most versatile methods to characterise bulk polymer structure and conformation. However, these techniques are of very limited utility to study macromolecular adsorption and intercalation in layered and nanostructured host media, as the substrate often dominates the overall optical response. These difficulties can be circumvented via the use of high-resolution neutron spectroscopy. Using the Tosca spectrometer, we have gained fresh insights into the conformational structure of ethylene glycol and poly(ethylene oxide) chains intercalated into graphite oxide galleries as well as adsorbed onto graphene sheets. For intercalation into graphite oxide, we observe drastic changes to polymer conformational and collective vibrational modes as a consequence of a predominantly planar zigzag chain conformation of the confined polymer phase. Surprisingly, these effects are largely insensitive to polymer chain length. In the case of graphene sheets, the neutron data unequivocally show a substantial increase in the population of gauche conformers resulting from the relatively free macromolecular conformations adopted by the polymer chains.



Contact: Dr F Barroso-Bujans, fbarroso@ehu.es
Further reading: F Barroso-Bujans et al., Macromolecules 45 (2012) 3137; ACS Macro Lett. 1 (2012) 550; Carbon 50 (2012) 5232

Schematic representation of the structure of poly(ethylene oxide) chains in graphite oxide (left) and graphene sheets (right) inferred from inelastic neutron scattering data.

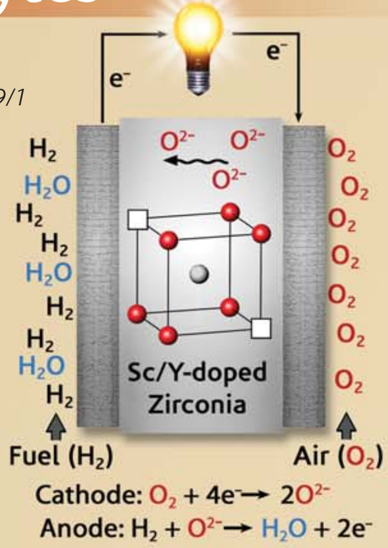
Understanding structure-property relationships in zirconia-based solid electrolytes

ST Norberg, SG Eriksson (Chalmers University), D Marrocchelli (Edinburgh University), PA Madden (Oxford University), JTS Irvine, P Li (St Andrews University), S Hull (ISIS)

Support for research: Vetenskapsrådet (Swedish Research Council), EPSRC grant EP/H003819/1 and others, STFC Centre for Materials Physics and Chemistry (CMPC), China Scholarship Council (CSC).

Solid-oxide fuel cells are an important part of the search for more environmentally friendly methods of power generation. A key component is the solid electrolyte, which transfers O^{2-} ions from the air side (cathode) to the fuel side (anode) of the cell, and is commonly zirconia, ZrO_2, doped with trivalent cations (such as Y^{3+}) to introduce anion vacancies. The latter give high oxide-ion conductivity at temperatures above 1100K. To better understand the ionic conductivity in these materials, we have performed complementary studies using neutron diffraction, Molecular Dynamics simulations and impedance spectroscopy. The size of the dopant cation species has a major influence on the oxide-ion conductivity, since the anion vacancies are preferentially bound to the smaller of the host/dopant species. This size effect explains the higher conductivity when ZrO_2 is doped with similarly sized Sc^{3+} ions. Irrespective of the type of dopant, the ionic conductivity reaches a maximum at a relatively low level of doping owing to the formation of immobile vacancy pairs.

Contact: *Dr ST Norberg, stn@chalmers.se; Dr S Hull, stephen.hull@stfc.ac.uk*
Further reading: *ST Norberg et al., Chem. Mater. 23 (2011) 1356; D Marrocchelli et al., Chem. Mater. 23 (2011) 1365*



Schematic diagram showing the operation of a solid-oxide fuel cell, together with a picture of a pair of anion vacancies within the crystal structure.

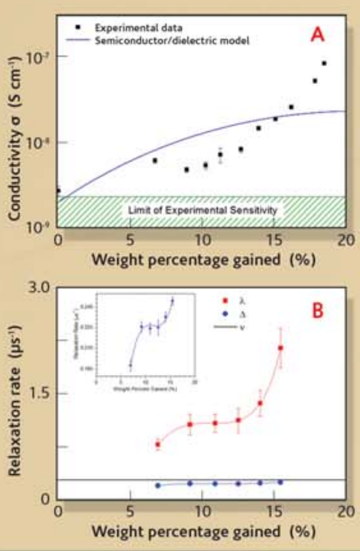
MATERIALS *AND TECHNOLOGIE*

The human skin pigment melanin is a hybrid ionic-electronic electrical conductor

AB Mostert, BJ Powell, GR Hanson, T Sarna, IR Gentle, P Meredith (University Queensland), FL Pratt (ISIS)

Support for research: Australian Research Council (ARC) Discovery Program (DP0879944), ARC QEII Fellowship (DP0877875), Queensland Smart State Senior Fellowship, Queensland Vice Chancellor's Senior Research Fellowship, Access to Major Research Facilities Programme (AMRFP) of the Australian Nuclear Science and Technology Organisation (ANSTO).

Melanin is the pigment found in human hair, skin, and eyes that protects us from the harmful effects of UV radiation. It is also found in the brain and the disappearance of melanin is linked to neuro-degenerative diseases such as Parkinson's disease. Melanin is ubiquitous in the natural world and found in organisms from bacteria to squid ink. Its bio-functionality aside, melanin has intriguing and potentially very useful electronic and optical properties. For example, in 1972 it was proposed that melanin in the solid state was a natural organic semiconductor, a rare beast indeed. We have shown that its electrical properties are even more exotic. Melanin's electrical conductivity is critically dependent upon its hydration state, the physics of which is embedded in a local chemical reaction whereby protons and electrons are released to take part in the flow of current. This 'hybrid' behaviour opens new possibilities for creating biocompatible electrical materials that can transduce between ion and electronic signals – a key requirement for the emerging field of bioelectronics, as it will allow semiconductor control circuitry to 'talk to' biological systems.



Contact: *P Meredith, Meredith@physics.uq.edu.au; BJ Powell, powell@physics.uq.edu.au*
Further reading: *AB Mostert et al., PNAS 109 (2012) 8943; Appl. Phys. Lett. 100 (2012) 093701*

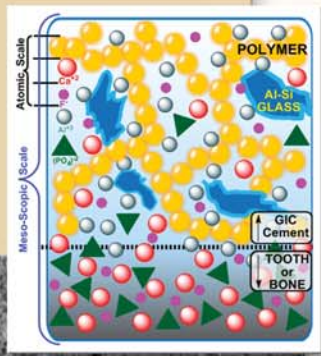
(A) The electrical conductivity of melanin increases super-exponentially with hydration – an organic semiconductor model does not describe the behaviour. (B) Muon-spin relaxation data follows the conductivity, showing that both protons and electrons contribute to current flow.

Gold teeth are passé – glassy teeth (and bones!) are now ‘in’

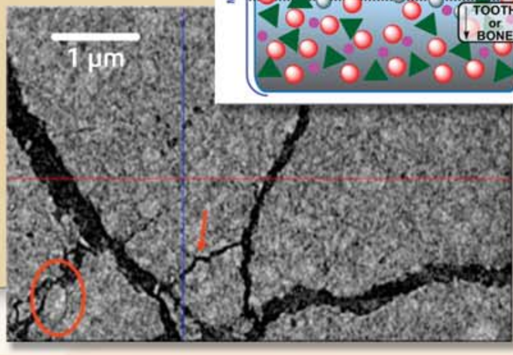
KV Tian, C Dobo-Nagy (Semmelweis University, Budapest), DT Bowron, J Mayers, F Fernandez-Alonso (ISIS), JW Nicholson (St. Mary’s University), GA Chass (Queen Mary, University of London), GN Greaves (University of Cambridge)

Support for research: EPSRC-funded project equipment (EP/H030077/1 and EP/H030077/2).

The historic implantation of foreign materials into the human body is epitomised by dentistry, which continues to be by far its most pervasive example. Successes in dental materials have generated leads in orthopaedics and beyond. However, the rational optimisation and design of tooth and bone replacements remains an unmet challenge. Problems stem from the as-yet unresolved conflict between strength and toughness. Problems of adhesion, biocompatibility, appearance and cost beleaguer materials that do satisfy mechanical thresholds. Glass Ionomer Cements (GICs) show promise of resolving this material dichotomy in filling and adhesion applications, complemented by ideal bonding to tooth and bone surfaces. Although the brittleness of these biocompatible composites has confined their use to non-load bearing applications, new evidence signals their potential to match the high toughness of teeth and bones.



Neutron diffraction on Nimrod and scattering on Vesuvio have provided valuable clues as to the factors controlling toughness and strength, through quantitative tracking of changes in structure and dynamics at the atomic and microscopic scales during cementation of GICs.



Contact: *GA Chass, g.chass@qmul.ac.uk*

Further reading: *KV Tian et al., J. Mater. Sci. Mater. Med. 23 (2012) 677; Adv. Mater. (submitted)*

Top: *Structure of ion exchange layer between GIC and tooth/bone; polymer (orange), glass (blue) and interface are shown.* ***Bottom***: *Tomographic image of fractured GIC.*

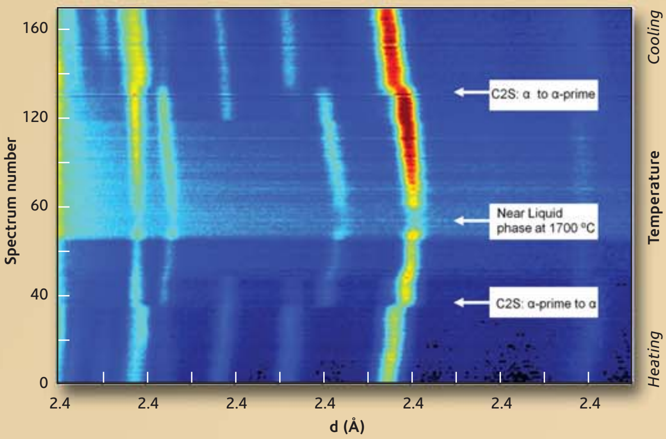
High-temperature behaviour of the multi-component oxide system in the Basic Oxygen Steelmaking process

Z Li (Tata Steel RD&T), SY Zhang, W Kockelmann (ISIS)

Support for research: Tata Steel Europe

Basic Oxygen Steelmaking (BOS) is currently the dominant process whereby hot metal is refined to liquid steel via slag flotation. The BOS slag is a liquid/solid multi-component oxide system with a complex and varied chemistry due to the operating conditions. One of the key challenges in the BOS process is to efficiently remove phosphorus impurities from the hot metal to the BOS slag. This step requires a very accurate control of the BOS-slag chemistry and an in-depth understanding of its behaviour at steelmaking temperatures. We have used neutron diffraction on Gem to probe the solid-liquid, liquid-solid, and solid-solid transitions, and to quantify the components of this multi-phase system at temperatures up to 1700 °C. The present study enables the development of new thermodynamic models accounting for the high-temperature behaviour of the multi-component oxide system, and provides new insights into the optimisation of the steelmaking process for the production of high-quality steel.

Contact: *Dr Z Li, zushu.li@tatasteel.com*

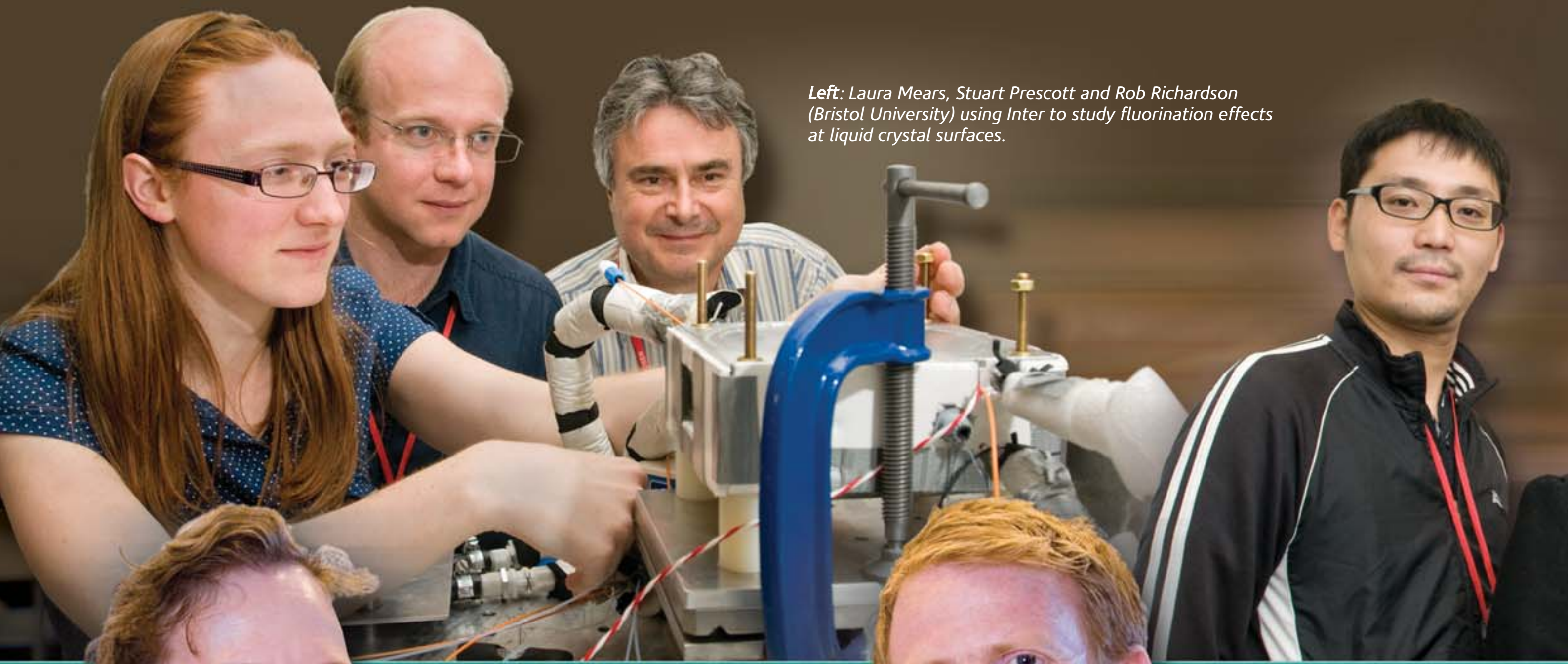


Thermo-diffractogram showing the evolution of dicalcium silicate phases in a BOS slag into and out of the liquid phase

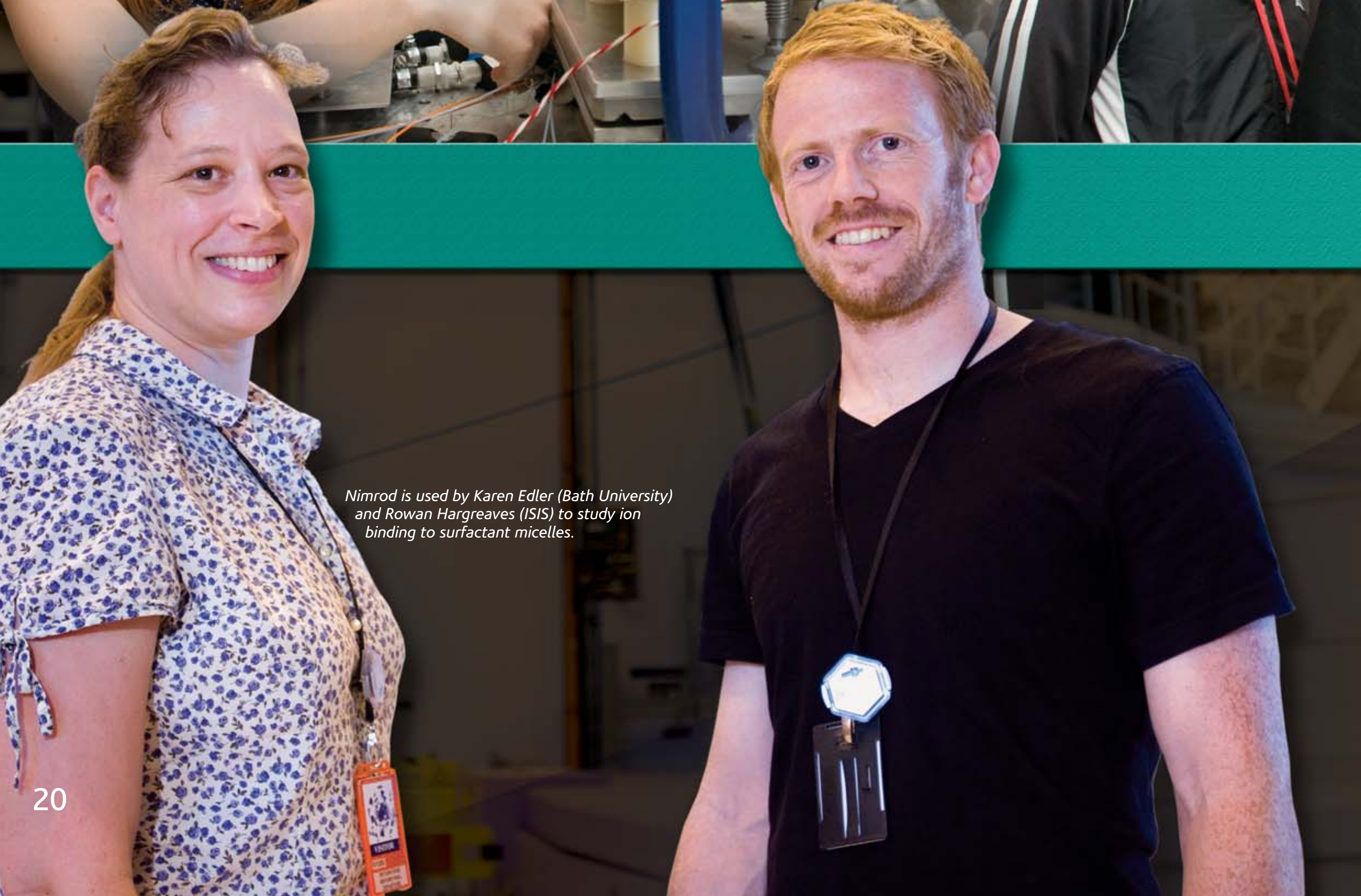
Above: Rubia Gouveia (Kings College London), Margarita Valero (Universidad de Salamanca, Spain) and Ann Terry (ISIS) use Loq to tune the functionality and bulk behaviour of micelles with cyclodextrins.

Above: Stephen Skinner (Imperial College London) uses HRPD to study structural changes in $CeNbO_4$ for energy conversion and CO_2 mitigation.

Above: David Buckley and Patrick Cullen (University College London) prepare samples of aprotic and aromatic solvents to investigate their structure using Sandals.



Left: Laura Mears, Stuart Prescott and Rob Richardson (Bristol University) using Inter to study fluorination effects at liquid crystal surfaces.



Nimrod is used by Karen Edler (Bath University) and Rowan Hargreaves (ISIS) to study ion binding to surfactant micelles.

***Right**: Pietro Carretta and Samuele Sanna (University of Pavia, Italy) investigating the evolution of the electronic structure and of the magnetic correlations in $Sr_2Cu_{1-x}(Zn,Mg)_xO_2Cl_2$ on Emu.*

***Left**: Riniaro Inove, Tian Xia, Toshi Kanaya (Kyoto University) and Hiroko Osawa (Japanese Synchrotron Institue Reserach) exploring phase separation and dewetting of dPS/PVME thin films by neutron reflectivity on Surf.*

ISIS USERS **AT WORK**

Louise Collins (Kings College London) prepares samples to investigate phosphatidylcholine and its interaction with 1,2-propandiol and water using Sandals.

Rais Singh (University of Warwick) uses MuSR to probe the superconducting state of non-centrosymmetric Heusler superconductors.

Ilaria Idiui (Bath University) prepares samples to study the influence of polymer molecular weight on polymer stabilised lipid nanodiscs using Loq.

Development at ISIS is a continuous process, driven in response to the changing needs of the user community and to maintain ISIS as a world-class neutron and muon source. Evolution of existing instruments and construction of new ones, together with advances in neutron and muon techniques, provide fresh opportunities for materials investigations. Technology developments within the ISIS accelerator complex are designed to improve ISIS reliability and performance.

The past year has seen work continuing on four new instruments – Imat, Chipir, Zoom and Larmor – for the Second Target Station, together with first neutrons on the newly-upgraded Polaris diffractometer on TS-1. Alongside technical developments comes a wide range of other activities – science workshops, training courses, user meetings, public understanding of science events, 25 years of ISIS muons – to name but a few.

DEVELOPMENTS *& EVENTS*

ADVANCES IN **INSTRUMENTS**

ISIS Target Station 2 *phase 2 instrument progress*

Zoom

The detailed design and actual construction is under way for Zoom, a flexible small angle neutron scattering (SANS) beamline capable of polarised and grazing incidence SANS. The delivery of key components, like the JJ X-ray sample stack, the 11m long detector vacuum tank and the detector motion system, is expected in the autumn of 2012.

Simulations of the high energy neutron background on Zoom have indicated that it would be better with a vertical rather than horizontal supermirror bender filter. The simulation results have also helped to improve the layout of collimation in the beam shutter and shielding around the bender, this then reducing the amount of steel shielding further along the beam line.

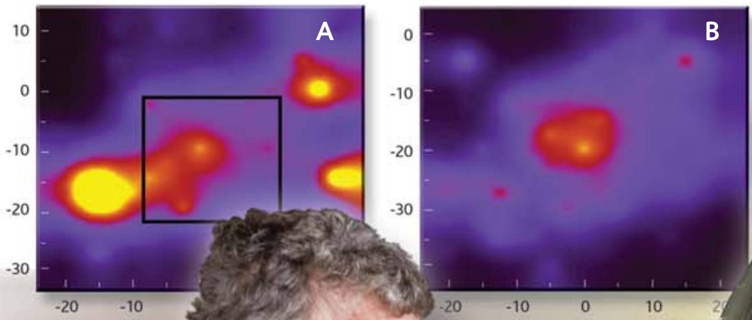
***Bottom**: Peter Galsworthy (ISIS) working on the double disc neutron chopper for Zoom.*

***Below**: Background distribution from high energy neutrons at the exit of the shutter for Zoom. (a) The original horizontal and (b) the vertically inclined shutter with improved shielding insert. The shutter is marked by the black outline. The high intensity in the bottom left hand side of (a) is due to the direct view of the target through gaps around the shutter insert. These gaps have now been reduced leading to (b) with a corresponding 1000 fold reduction in the background noise.*

Chipir

Chipir will be an instrument for rapid testing of the effects of high energy neutrons on electronic systems. Substantial progress has been made with construction this year. Large concrete blocks, an electronically shielded room, beam-stop and sample positioning table have recently appeared in the second target station hall. The concrete sections form part of the substantial block-house which has been designed to contain the MeV neutron beam that will mimic atmospheric cosmic ray neutrons once the instrument is completed next year.

***Right**: Construction of the Chipir beamline*



& TECHNIQUES

Surveying Larmor beamline components into place in June.

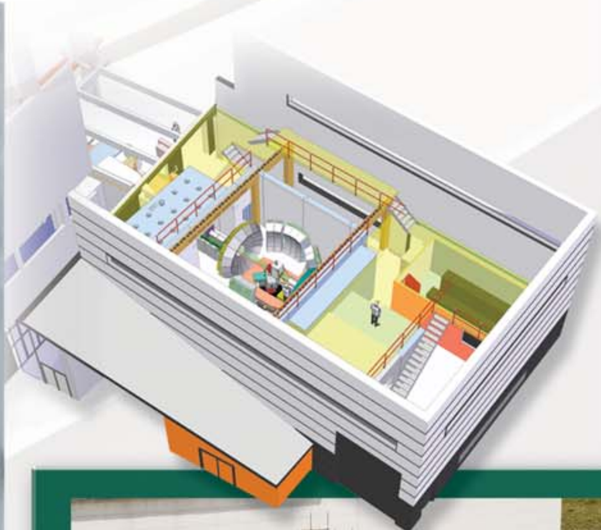
Larmor

Larmor will be a multi-purpose instrument for small angle neutron scattering (SANS), diffraction and spectroscopy utilising the Larmor precession of polarised neutrons. Larmor will provide a suite of techniques not currently possible at ISIS and will also expand the range of spatial and temporal length scales to new areas.

The Larmor guide, blockhouse and shielding will be installed before the end of the year. The bulk of the major instrument components such as the polarising system and sample stack are now being manufactured, with many due to be installed during 2013. The significant investment from the Netherlands and TU-Delft (see News section, page 39) in the development and construction of the spin-echo components of the instrument will continue in parallel, with the aim to deliver SESANS and Larmor diffraction at the earliest possible opportunity.

***Below**: Design drawing of the Imat extension building.*

***Bottom**: Construction of the steel structure outside the main experimental hall for the Imat extension building.*



Imat

Imat will be the first time that neutron radiography, tomography and diffraction techniques are available on a single instrument, making it a unique facility for testing of engineering components and materials analysis.

The construction of the instrument has started. Concrete shielding blocks are being installed in the experimental hall and the first sections of the Imat neutron guide will be put in place shortly. Construction of the Imat extension building outside the main experimental hall is well underway.

Polaris

Installation of the Polaris detector tank in November

During the past year the major upgrade to the Polaris diffractometer (funded by the STFC Facility Development scheme and with significant contributions from partners in Sweden and Spain) was completed, with first neutrons collected on the upgraded instrument shortly before Christmas 2011. Extensive commissioning and calibration tests showed that the instrument now has large increases in count rate (especially at low scattering angles) and improvements in resolution at backscattering angles. Following an opening ceremony on 10th May, Polaris resumed full user operation on 21st May.

The Mighty Flynn

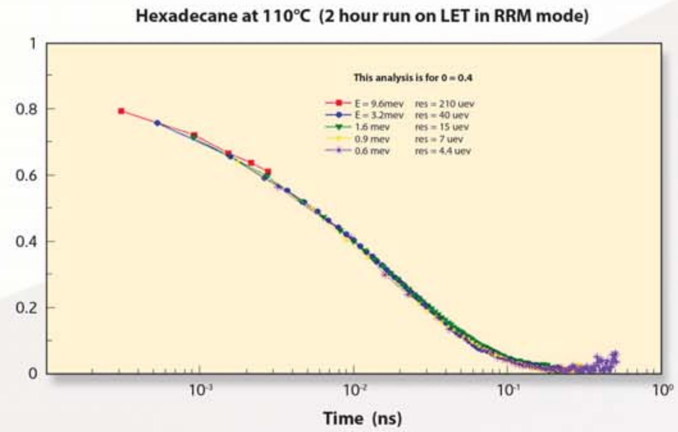
ISIS took delivery of its brand new ^{3}He spin-filter filling station 'Flynn' in March 2012. This state-of-the-art machine, built at the Institut Laue Langevin (ILL) in Grenoble, is capable of polarizing and filling a ^{3}He spin-filter in about an hour, with an in-cell ^{3}He polarization of 75% being routinely achievable. The major users of polarizing filters from Flynn will be the Wish and Let instruments. Special thanks go to the team at ILL who designed and built this remarkable machine.

__Right__: The Flynn ^{3}He spin-filter filling station with the installation team. Left to right: Ross Stewart, Jon Taylor, Joe Donaldson (ISIS), David Jullien (ILL), Stephen Boag (ISIS) and Pascal Mouveau (ILL).

One year of Let

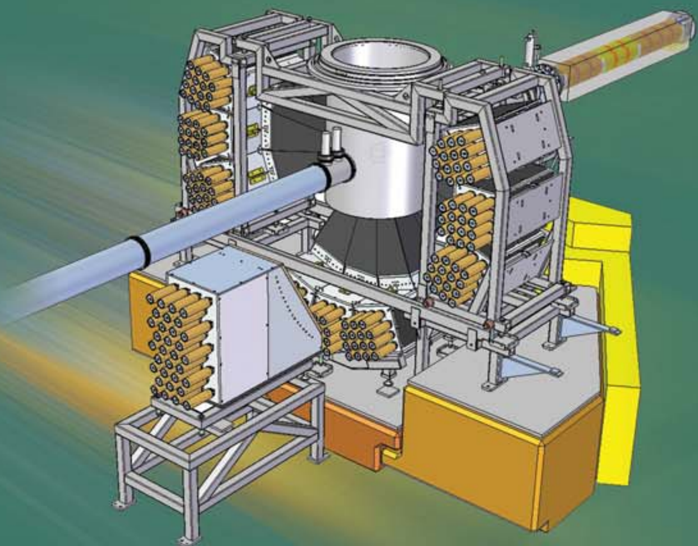
Let has been operational for one year now and has seen many exciting experiments in extreme conditions of low temperatures (30 mK) and high magnetic fields (9 T). To make use of the long 100ms time frame on the Second Target Station, Let runs regularly in multi repetition rate (MRR) mode with typically around 5 incident energies per frame covering the full dynamic range. MRR mode has proved to be particularly suitable for quasielastic experiments, allowing access to 3 decades of time in one single measurement for dynamics studies.

Dynamics of hexadecane measured using MRR mode on Let. The picture shows constant Q = 0.4 Å^{-1} cuts of the data taken at 110°C, Fourier transformed and divided by 'resolution run' taken at low T.



Pearl

Following the partial completion of the upgrade project the Pearl user program was resumed in July 2011. Over 20 user experiments have now been completed since then and the new instrument is performing very well. In April 2012 a new low angle detector was installed to complete the instrument upgrade. This new low angle detector has a higher resolution than its predecessor and will enable more detailed studies of magnetic or large unit cell materials.



Above: *Design drawing of the upgraded Pearl instrument.*

Muon data rate increases

The ISIS muon group and STFC Technology Department have been working to increase the count rate on the muon suite of instruments. The rate has been limited by the detector electronics, but a new time to digital convertor (TDC) electronics card has resulted in at least a doubling of the count rate on Emu, from 50 million events per hour to over 120 for a large sample. The new electronics will be put on to all the muon instruments over the coming year.

Right: *Matt Roberts (ISIS) testing the new TDC card for the muon suite of instruments.*

Iris and Osiris Express

In July 2011, we started running a quasi-elastic neutron scattering (QENS) Xpress programme on our backscattering spectrometers Iris and Osiris. This has proved very successful with a total of 16 requests to date, half of which are from users new to the technique. Measurements have been helped by the standard closed cycle refrigerator now being equipped to allow a large temperature range (4-600K) to be measured without manual intervention.

Simon Cassidy, Alex Corkeit and David Free (Oxford University) using Osiris for studies of magnetism, structure and superconductivity in $Sr_{1-x}Na_xFe_2As_2$.

ISIS support laboratories

This year we have refurbished two of the sample preparation laboratories in Target Station 1. Both labs were completely rebuilt with new fume cupboards, benching, and storage and lab gas systems, as well as upgraded facilities for managing active samples and a walk-in fume cupboard.

The Materials Characterisation Lab has benefited from considerable investment too, with replacement of the X-ray diffraction set by a brand new state-of-the-art one.

Marek Jura (ISIS) working on the new Rigaku x-ray diffractometer in the ISIS Materials Characterisation La

Synchrotron steering and trim quadrupole magnet power supplies

New power supplies have been installed for the synchrotron vertical and horizontal steering magnets. The 10 defocusing trim quad magnets will also have their new power supplies installed in the August 2012 shutdown and the upgrade will be completed in the January 2013 shutdown when the remaining 10 focusing trim quad power supplies are replaced. The new power supplies are capable of a higher current output and greater current slew rate than the existing units.

Team involved in the installation of the 180kW Bipolar pulsed power supplies for the synchrotron trim quadrupole and steering dipole magnets.

***Back, left to right**: Jonny Ranner, Steve West, Martin Hughes, Steve Ruddle.*

***Front left to right**: Tim Carter, Mike Van De Mortel, Kenny Rodgers, Adrian McFarland, Chris Tyrrell, Noel McNammee and Steve Gray.*

ACCELERATOR AND TARGET

Main magnet power supply upgrade

In August the Electrical Engineering Group completed the tendering process for a 1.44MW DC power supply to replace the existing obsolete synchrotron main magnets DC Bias power supply. When installed in 2014 this power supply will improve the stability of the sine wave current used to drive the synchrotron magnets, as well as allowing these magnets to operate in a mode suitable with higher injection energies possible in future ISIS upgrades. The new power supply and associated systems will be housed in a new extension building due for completion later this year.

Architects impression of the building extension for the synchrotron main magnet power supply upgrade program.

New pumps for ISIS cooling water

The cooling tower water circuit is the backbone ISIS, but the pumps and tower gearbox drive fans were installed around 1962. They have therefore recently been replaced with more efficient pumps, motors and inverter drives, reducing electricity costs, water usage and chemical treatment costs.

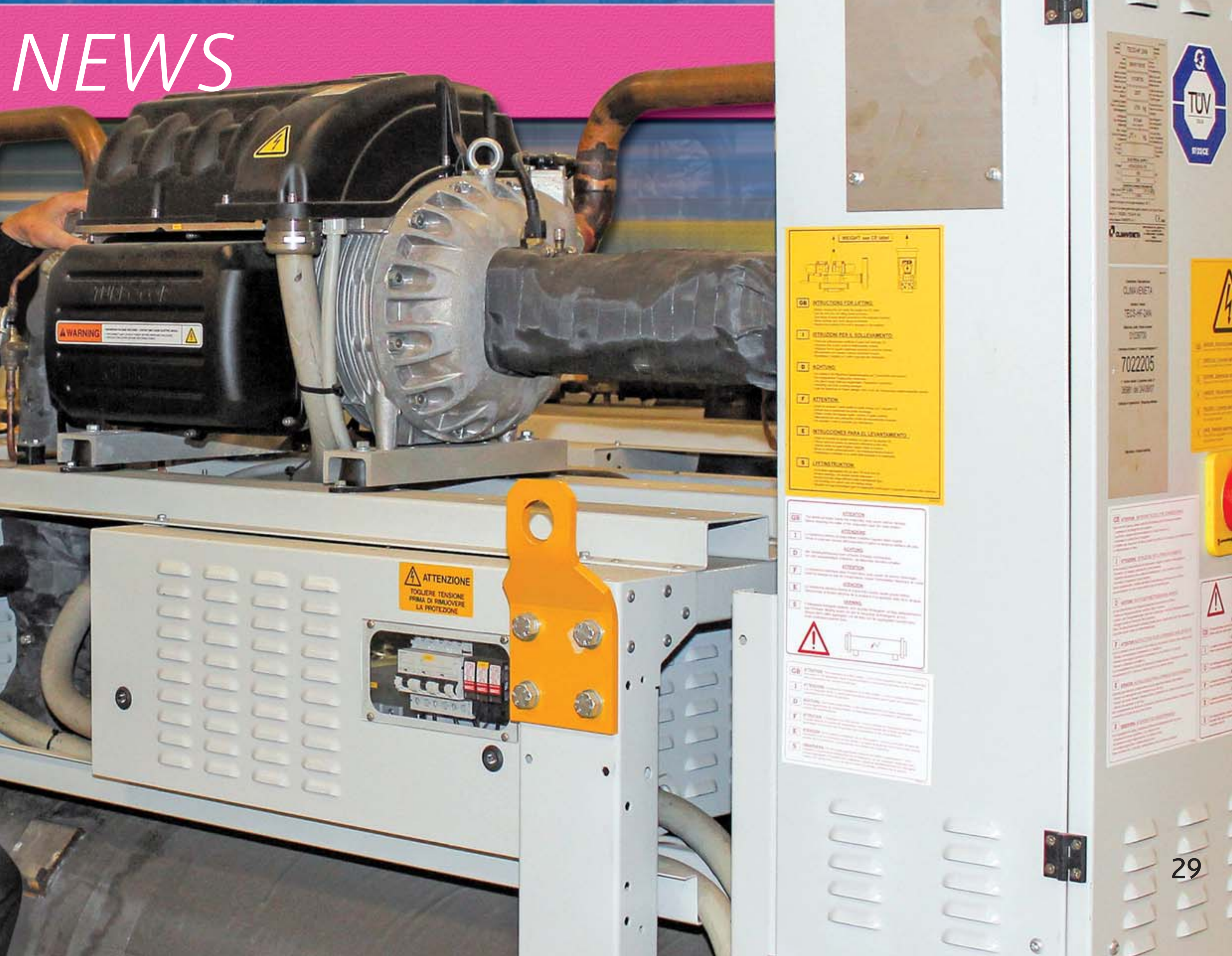
***Right**: Brian Hipwell working on one of the cooling water pump units.*

The most efficient chillers on Earth

ISIS synchrotron hall air conditioning is a vital for ISIS operations. The old unreliable chillers, which were continually under repair, have been replaced by state of the art Turbo-Corr units. These have magnetic levitation bearings with only one moving part, and are oil free, low noise, light-weight and low maintenance unit, with an energy usage of 30% - 50% of the old units.

***Below**: John Govans - alongside one of the chillers*

NEWS



Making stripping foils for ISIS

Stripping foils are used to remove the electrons from the negative hydrogen ions that are accelerated in the ISIS linac. This process creates bare protons, which are then accelerated in the synchrotron.

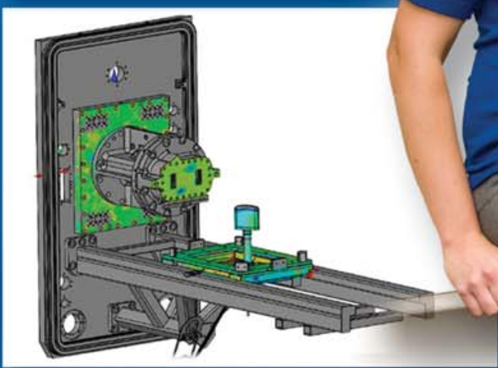
The ISIS Vacuum Section is responsible for making these stripping foils. This is a time consuming and delicate operation. The process starts with annealing a 0.1mm thick sheet of aluminium which is then anodized before being etched in a solution containing bromine until it is 0.3mm thick. The foil is then coated with approximately 10nm of aluminium before being stored in specially designed containers. Last year a new coating machine was purchased which has greatly improved the foil manufacturing process, with fewer breakages now occurring during the coating process.

***Below**: Geoff Matthews (ISIS) loading foils into the new coater.*

Replacing tank 4 of the ISIS linear accelerator (linac)

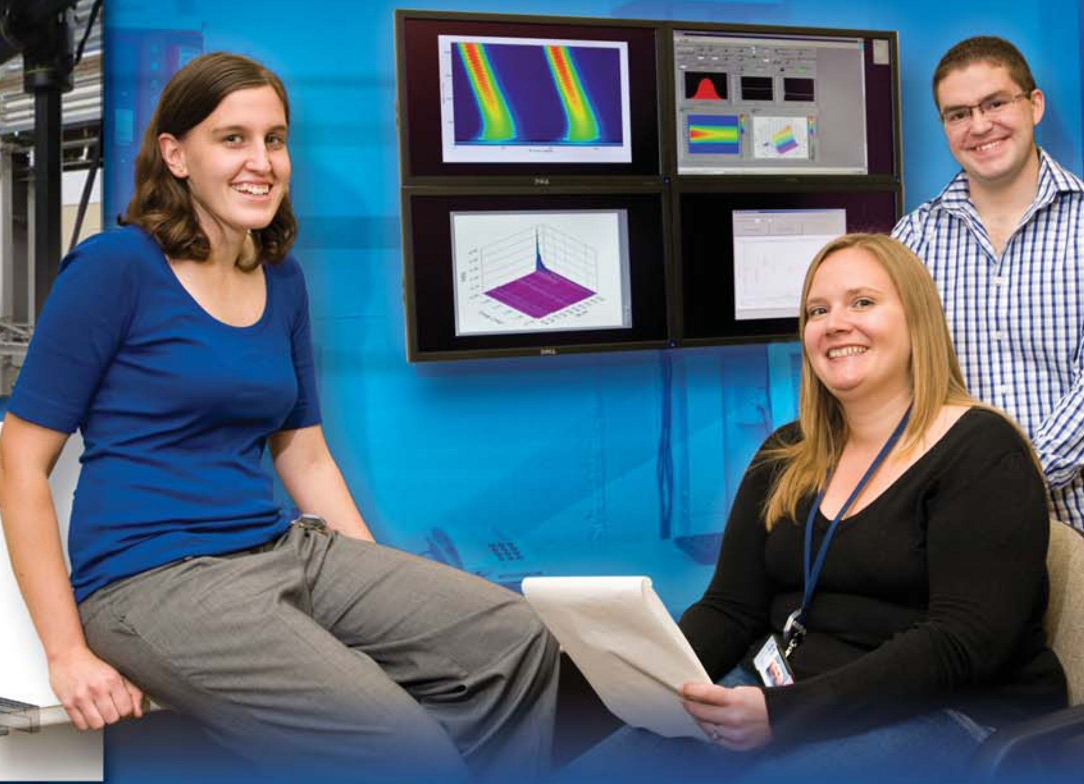
Design drawing of the linac test tank.

The largest components of the ISIS linac are four drift tube tanks. Tank 4 was designed back in 1973 and is now showing signs of wear after many years of service. Its replacement is due to happen in 2018, which means already starting the design, build and testing process of the new 12m long tank. A test tank (1/6 the length of the current tank) is being designed first to provide proof of concept.



Left: Scanning the mock-up of the TS-1 target, with CAD comparison of the scanned data below.

Below: ISIS accelerator diagnostics team members Hayley Smith, Sarah Fisher and Bryan Jones.



3D digitising and scanning

The ISIS accelerator design group have purchased a 3D digitising and scanning system from GOM UK. The system allows areas to be scanned to provide detailed position information of components. Once data has been captured and processed it can be exported into CAD software, or CAD models can be imported into the GOM software for comparison and or Inspection.

The RF section of the ISIS Synchrotron Group. Left to right: Andrew Seville, Rob Mathieson, Ian Gardner, Derek Bayley and Julian Brower.

Spent target disposal

The ISIS Target Transportation flask loaded with a spent target ready for transportation to Sellafield.

The ISIS neutron target is replaced periodically. Used targets, which are very radioactive, need to be disposed of at Sellafield, but the project to transport them is complex and requires very careful planning. Disposal of two targets was a major project for Target Operations Group this year, working with ISIS and RAL radiation protection staff.

Cara Morgan (Oxford University) and Jordan Petkov (Unilever) using Inter for adsorption of surfactant mixtures.

ISIS AND INDUSTRY

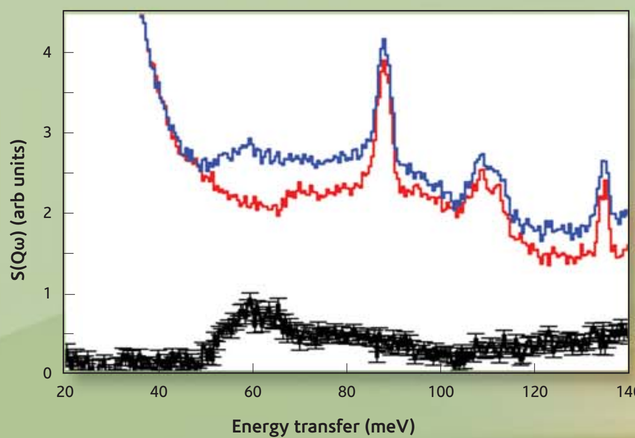
As one of the key scientific tools in the investigation of matter, neutrons have a major role to play in the solution of near-market and applied scientific problems that are tackled in both industry and academia.

Traditionally, industry has made effective use of ISIS through its collaborations with the university sector. These projects, some of which are co-funded by UK research councils, access the ISIS instrument suite through the standard beam time proposal system.

In the two proposal rounds of 2012, ISIS received 120 proposals with industrial partners. These involved between them around 50 separate companies, and requested 420 days of beamtime on 20 different ISIS instruments. Typical science areas include soft matter and polymer studies, engineering strain measurements and catalysis.

A recent ISIS study has enabled catalyst researchers at Evonik Industries to understand exactly how the widely-used Lindlar catalyst, which the company makes and supplies to a range of industrial customers, works at the atomic scale in unprecedented detail. Dr Peter Albers of Evonik Industries' central analytical service provider AQura GmbH explains; "The results generated by ISIS provided us with the missing piece of the jigsaw. We now know precisely how the Lindlar catalyst behaves and why it is so effective at preventing alkane production."

Inelastic neutron scattering spectra of the Lindlar catalyst recorded on Maps. The clean catalyst is shown in red and after absorption of hydrogen in blue. The difference spectrum in black demonstrates the generation of PdH.

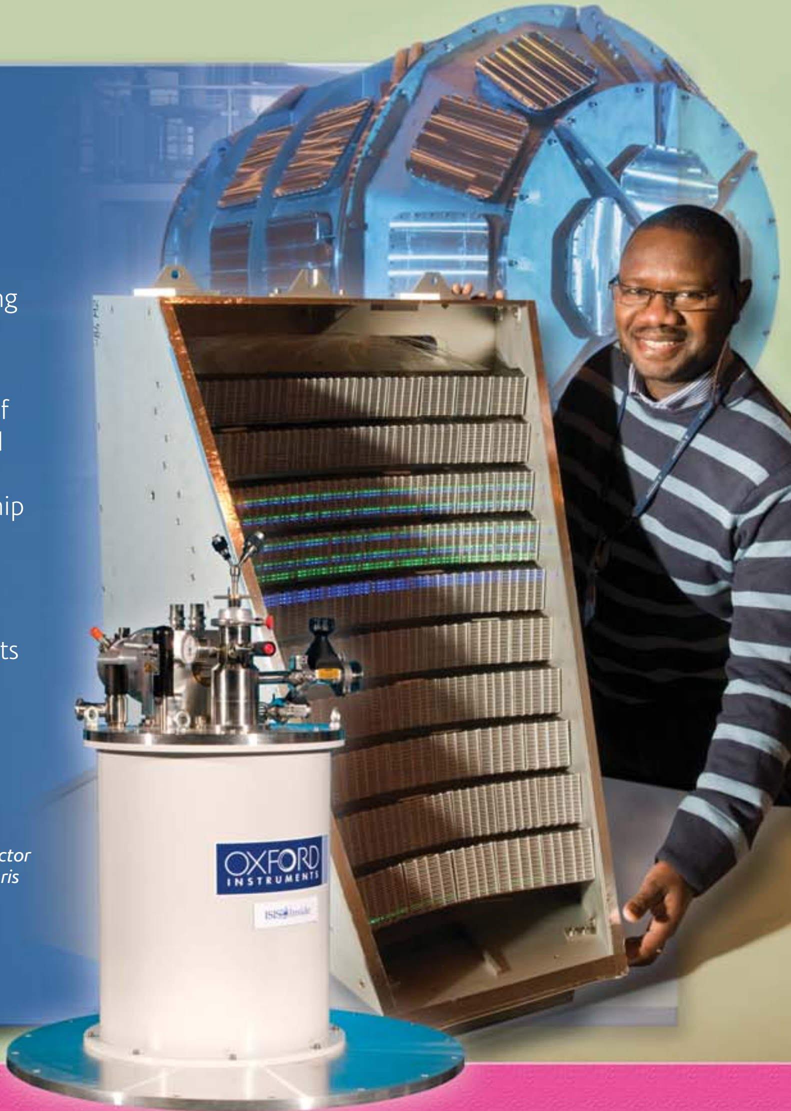


Technology development in partnership with industry

In addition to industry using neutron and muon beams to investigate commercially-relevant materials, ISIS also works with industrial partners to develop new capabilities – resulting in benefits both to ISIS and to the company involved.

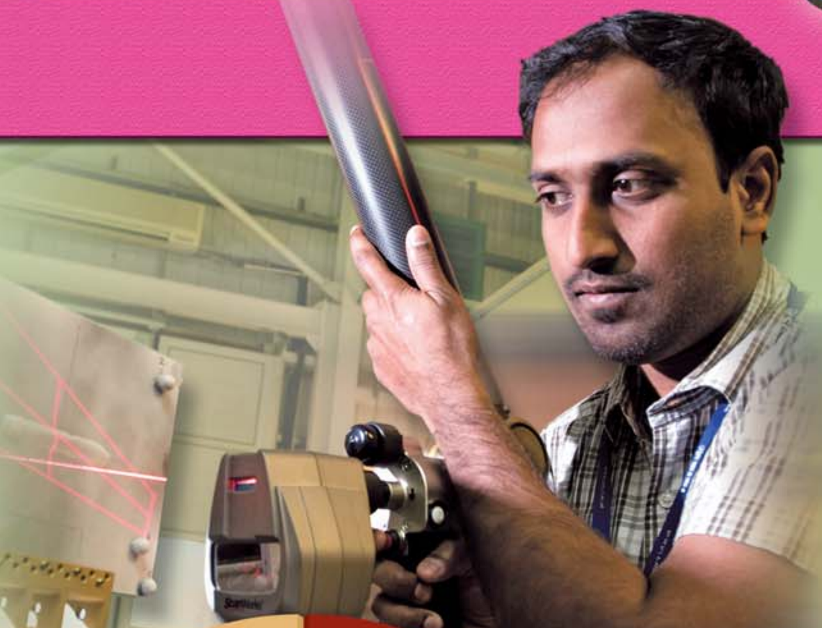
For example, ISIS has worked with Applied Scintillation Technologies Ltd, based in Harlow, UK, a specialist supplier of scintillator materials for neutron detectors. AST has supplied over 180 square metres of specialist scintillator for neutron detectors to ISIS since 1988. "Our long and valued relationship with the detector scientists at ISIS has helped keep us at the forefront of neutron detection technologies", says Stuart Quinn, Sales and Commercial Director at AST.

ISIS has a long-standing collaboration with Oxford Instruments (OI) which has included working together with OI on designs for cryogen-free magnet systems and cryostats suitable for very low temperature applications.



***Far right**: Quintino Mutamba of the ISIS detector group with a fibre coded neutron scintillator detector module for the Polaris diffractometer. Thirty-eight of these detector modules, encompassing more than 400,000 m of fibre optic, are installed in the Polaris vacuum tank visible in the background.*

***Near right**: The Oxford 'Isistat', a cryogen-free system designed by a collaboration between ISIS and Oxford Instruments.*

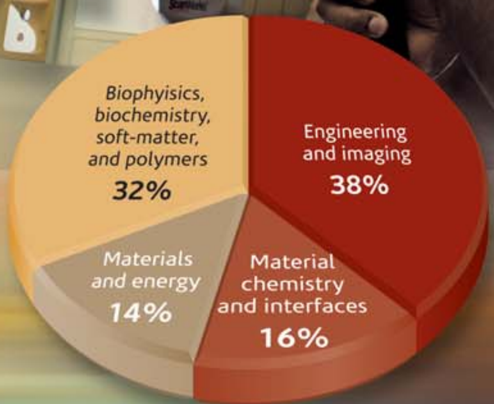


The ISIS collaborative R&D programme

A new venture between ISIS and STFC's Innovations Department has further reinforced the neutron's position as a fundamental industrial research tool: the ISIS Collaborative R&D (ICRD) programme.

This scheme was started in 2011 to widen the use of ISIS by industry. The programme offers a new way for industry to work in partnership with ISIS, aiming to provide the right conditions for industry to tackle its research problems.

The 2011/12 year saw an enthusiastic take-up by the industrial sector with 53 days being allocated to 9 proposals involving 7 different companies. In the first six months of the 2012/13 year, 6 proposals involving 16 companies have been allocated a further 41 days of time under the scheme with several more proposals in the preparation stage.



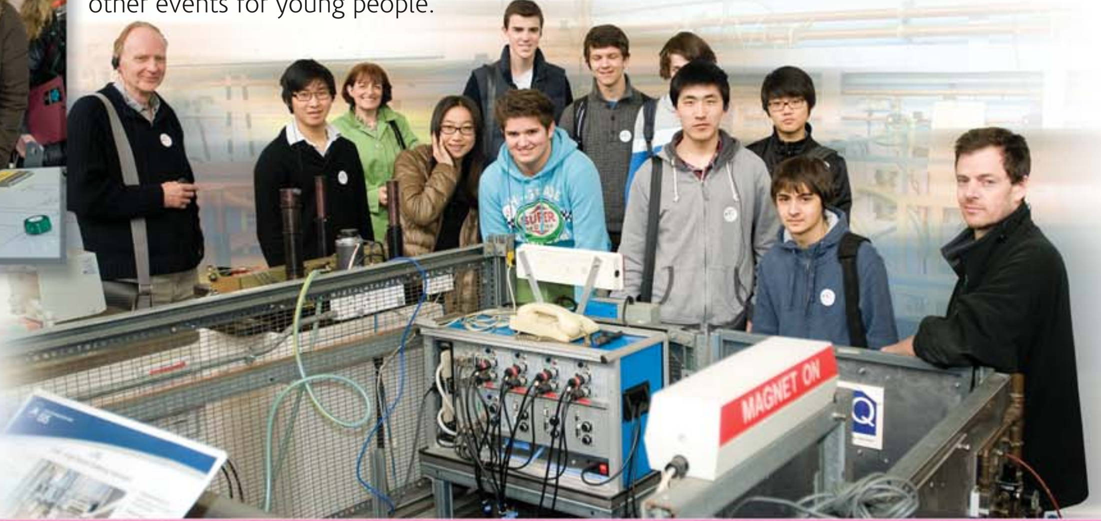
***Above**: Shanmukha Moturu (Open University) preparing to measure residual stresses in stainless steel plates with a three-pass groove weld. This measurement was part of an ICRD proposal from EdF Energy in collaboration with the Open University.*

***Left**: ICRD programme beam days by scientific theme.*

Training the next generation of scientists and engineers is a key feature of the work that goes on at ISIS. From visits by school students, work experience student placements, apprentices, sandwich students and graduates, to training courses for PhD students, ISIS provides many opportunities young people to learn about science and engineering.

Schools visits

ISIS regularly hosts visits from school students. In the 2011/2012 year, around 700 students aged between 11 and 18 visited. In addition, ISIS staff members are science and engineering ambassadors who will visit schools and help with other events for young people.



***Above**: Rob Williamson (ISIS) touring ISIS with students from Marling School, Stroud, plus some French exchange students from Lycée Maine de Biran High School, Bergerac.*

***Right**: Students from Royal Grammar School, Guildford, visiting ISIS as part of the Particle Physics Masterclass held at RAL in March.*

TRAINING *THE NEXT GENERATIO*

Third year apprentice Daniel Smith working on the 7 kbar pressure system in the ISIS pressure lab.

Johnny Boxall (former graduate trainee, now an ISIS staff member) and current graduate trainee Hayley Smith, talking about their work during a visit from Marling School, Stroud.

Tim Hellyer from Magdalen College School, Oxford, gaining work experience at ISIS.

Apprentices

ISIS takes apprentices from age 16 as part of the STFC apprentice scheme. They train in electrical, electronic or mechanical engineering, and spend time working on ISIS projects as well as learning at college. Their four-year apprenticeship equips them with valuable skills for their future work.

STFC Graduate Scheme

ISIS regularly takes graduates as part of the STFC Graduate Training Scheme. Graduates work alongside ISIS staff on real instrument, sample environment or accelerator projects, and benefit from an in-house training programme in personal and professional skills.

Work experience students

ISIS regularly takes work experience students for a one or two week period over the summer, as part of STFC's work experience scheme.

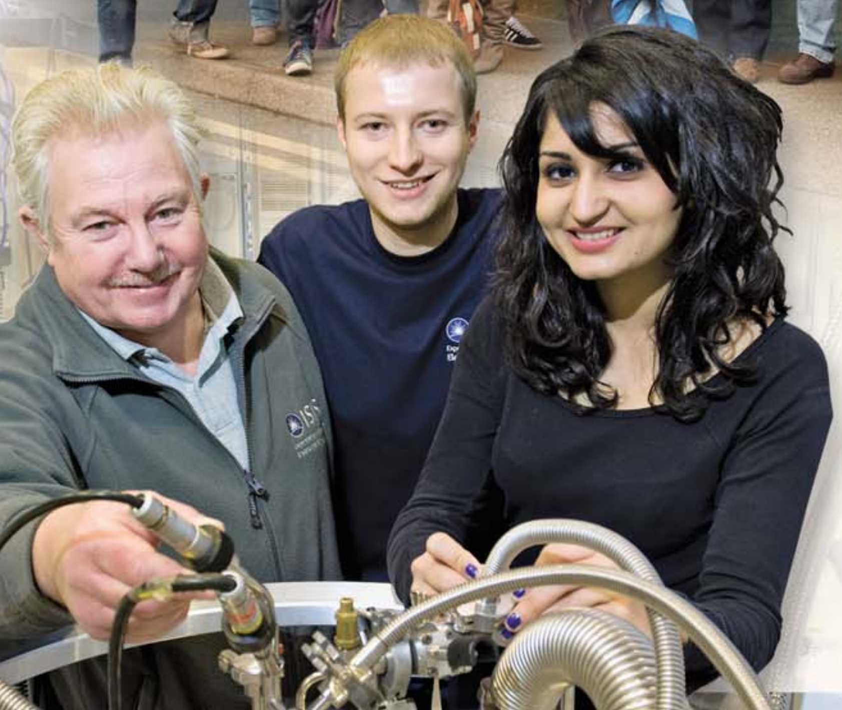
Training for PhD students

Around 60%-70% of UK proposals to ISIS involve students. In year 2011/12, over 330 individual UK PhD students came to ISIS to be involved with experiments. Their experiences whilst at the facility provide valuable training – not just in neutron scattering or muon spectroscopy, but also in use of low temperature systems, computing and data analysis.

In addition, ISIS provides more formal training courses – for example, the regular Neutron Training Course, the Muon Training School and the Oxford Neutron Summer School. Through such events PhD students get a good grounding in the theory and applications of neutrons and muons, as well as practical experience running experiments on ISIS instruments.

__Above right__: Lucy Clark (St. Andrew's University) and Christina Schaeffler (Nottingham Trent University) using the Argus muon spectrometer during the ISIS muon training school.

__Below right__: Students at the Oxford Neutron Summer School visiting ISIS.



Sandwich students

ISIS hosts several sandwich students each year. They normally come for one year, part-way through their university course, to gain experience of using their learning in a real-world environment.

__Left__: Amandeep Hundal (right) during her sandwich year at ISIS as part of the ISIS communications team. She is seen here with Stephen Cox and Peter Phillips (ISIS) with a dilution refrigerator in the ISIS hall.

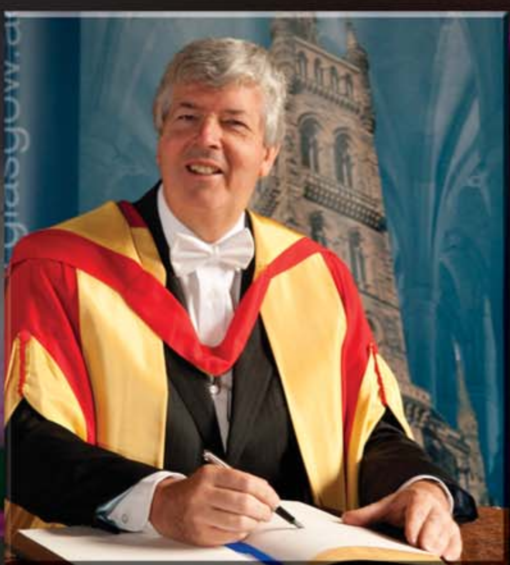
ISIS bids a fond farewell to Andrew Taylor…

…but he's not going very far! Andrew was Director of ISIS for almost 20 years. Early this year he was appointed STFC Executive Director for National Laboratories, which includes ISIS but also the wide variety of other facilities and departments at Rutherford Appleton and Daresbury Laboratories. As Uschi Steigenberger notes in her Foreword to this review, Andrew leaves behind him a huge legacy of investment, development and success at ISIS.

Prof Robert McGreevy has been appointed to succeed Andrew as ISIS Director starting in September 2012. Robert returns to ISIS from his current position as Deputy Associate Laboratory Director at Oak Ridge National Laboratory. Before moving to the Spallation Neutron Source in Oak Ridge, Robert was Head of the Diffraction Division at ISIS. Prior to this he was Director of the Studsvik Neutron Research Laboratory at Uppsala University, Sweden.

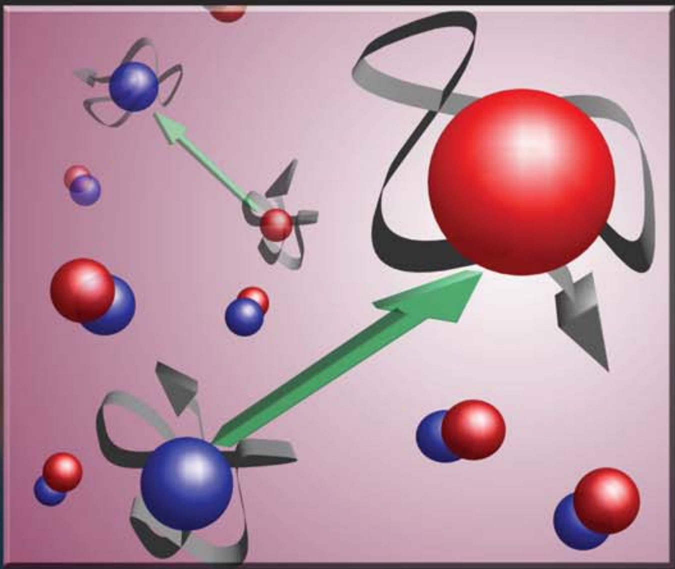
Uschi Steigenberger presents Andrew Taylor with framed photos of the ISIS target stations.

A YEAR *AROUND ISIS*



***Left**: Andrew Taylor receiving an honorary Doctor of Science degree from Glasgow University in 2010.*

***Right**: Andrew Taylor became ISIS Director in 1993.*



Above: Magnetic charge moving apart under the influence of an applied magnetic field.

ISIS researchers win prestigious Europhysics prize

The 2012 Europhysics Prize for condensed matter physics was awarded to ISIS user Professor Steve Bramwell (London Centre for Nanotechnology and University College London), Claudio Castelnovo (Royal Holloway University of London and ISIS Theoretical Physics Group) and their colleagues, for the prediction and measurement of magnetic monopoles in a magnetic material known as a spin ice.

Claudio Castelnovo and colleagues predicted that individual tetrahedral of atoms in spin ice could develop a slight imbalance in their spins and act as tiny, localised north or south poles. The prediction of free magnetic monopoles was verified in a series of neutron scattering and muon spectroscopy experiments by Bramwell and others at ISIS and elsewhere.

Above: Students at the ISIS Muon Training School in May.

Muon training school

ISIS ran a muon training school in May with lectures to give postdoctoral and postgraduate students an introduction to the muon technique, together with practical experience of running muon experiments on ISIS muon spectrometers.

Twenty-five years of muons at ISIS!

Friday 23 March 2012 saw the 25th anniversary of muon science at ISIS. First muons at ISIS were produced on a single beamline and instrument on 23 March 1987. Since then the ISIS muon facilities have grown from one to seven experimental areas, including the Japanese-funded RIKEN-RAL muon facility. During the past 25 years, over 1000 science publications have come from the ISIS muon instruments, and many hundreds of researchers have visited ISIS to use muons.

A gathering of ISIS muon group members, muon users and ISIS staff to celebrate 25 years of muons at ISIS. Other cakes were also provided in addition to just the one shown!

Over 500 visitors discover the joy of science at ISIS open day

More than 500 people visited ISIS on Saturday 28 January 2012. The ISIS Family and Friends Open Day allowed staff to proudly showcase their work to those closest to them who listen every day to their tales from the workplace. Visitors explored the vast buildings learning about atoms and molecules, particle accelerators and modern science.

"There was a great atmosphere in the place – and it was extremely rewarding to see staff from ISIS showing off their facility to their family and friends. There was a fantastic feeling of pride in their achievement of running their facility."
A visitor to the facility.

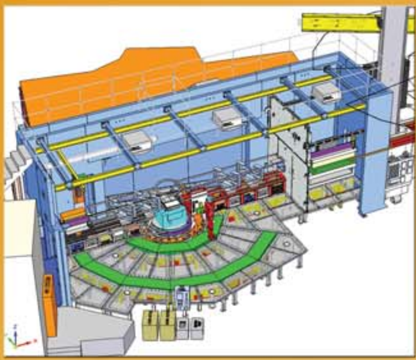
***Below**: Science demonstrations at the ISIS family and friends day.*

The ISIS Neutron Training course

Richard Heenan (ISIS) helping students on the neutron training course to analyse data.

The ISIS Practical Neutron Training Course is aimed at PhD and post-doctoral researchers who have little or no experience of neutron scattering, but whose future research program aims to make use of neutron scattering techniques. The 10-day course was run again in May this year, and saw students learning about the theory, applications and practicalities of neutron scattering through hands-on time on the ISIS neutron instruments.

Netherlands funding for Larmor



Design drawing of the Larmor instrument.

Larmor is a new ISIS instrument presently under construction on the Second Target Station. It will use the spin of the neutron to open up new techniques for studies of the atomic and molecular properties of materials. In addition to UK contributions for the instrument construction, the Netherlands Organisation for Scientific Research (NWO) and a consortium of Netherlands Universities (led by TU Delft) are adding to the fund. The Dutch team have been awarded around €4M for the development of spin manipulation devices for Larmor.

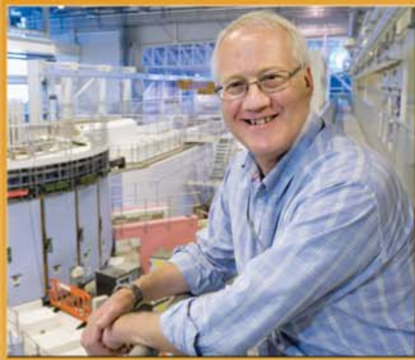
Oxford researcher scoops top neutron prize for ISIS research

Dr Sylvia McLain of the University of Oxford was awarded the prestigious B.T.M. Willis Prize for neutron scattering at the UK Neutron and Muon User Meeting held at RAL in April.

Sylvia McLain, winner of the Willis Prize for neutron scattering, being presented with her award by Ali Zarbakhsh, Chair of the Neutron Scattering Group of the Institute of Physics and Royal Society of Chemistry.

The award was in recognition of her studies of a broad range of biological molecules and their interactions at the atomic and molecular level in the presence of water.

Congratulations to Jeff Penfold!



Prof Jeff Penfold, winner of the 2013 Rideal Award from the Society of the Chemical Industry.

Professor Jeff Penfold, STFC Senior Fellow and ISIS Senior scientist, has won a prestigious award from the Society of the Chemical Industry, The Rideal Lectureship. Jeff's work has been highlighted because of his major scientific contributions to surfactant, colloid and interface science. Next year there will be a special symposium in honour of Jeff's work: 'The Impact and Future of Scattering Techniques in Soft Matter', 18-19 March 2013, Keble College Oxford.

ISIS saw two retirements from the Molecular Spectroscopy science group this year: John Tomkinson (left) and Jerry Mayers, both left ISIS after many years of neutron scattering.

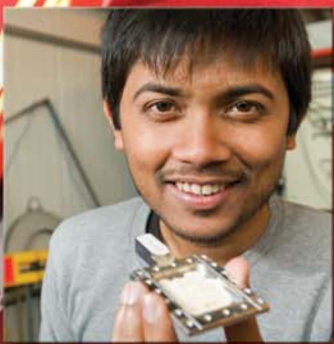
Delegates at the ISIS-run European Spallation Source symposium 'Materials engineering at a long pulse source' held at RAL in December.

The Molecular Spectroscopy User Group met at Cosener's House in November. User Groups provide a valuable way for ISIS users to hear about latest science and development news from ISIS, and discuss future facility requirements.

ISIS USERS **AT WORK**

Andrea Perrin (University of Durham) uses Sandals to study the mechanism of action of clathrate hydrate inhibitor relevant to the petrochemical industry.

***Below**: ISIS users Rap Smith and Michael Smidman (University of Warwick) with instrument scientist Adrian Hillier investigate the role of the electron-phonon interaction in non-centrosymmetric superconductors using MuSR.*



Debsundhu Bhowmik (Donostia Inter-national Physics Centre, Spain) investigating the dynamics of polymer/ polymer nanocomposites on IRIS.

Samples are prepared by Francesca Baldelli Bombelli and Paul McNaughter (University of East Anglia) to understand the structure of constrained polymer thin-films using Offspec.

***Below**: Ines Collings (Oxford University) using Gem to explore the local structure of the order/disorder ferroelectric transition in $[ND_4][Zn(DCOO)_3]$.*

There are seven ISIS Facility Access Panels (FAPs) covering the variety of science areas studied by neutrons and muons. Each FAP consists of experts in their subject field from the international research community. The FAPs meet twice per year, roughly six weeks after each ISIS proposal deadline. They judge all proposals received based on their scientific merit and timeliness.

Above: *The Molecular Spectroscopy FAP in action.*

Bella Lake (Berlin) discussing Excitations proposals.

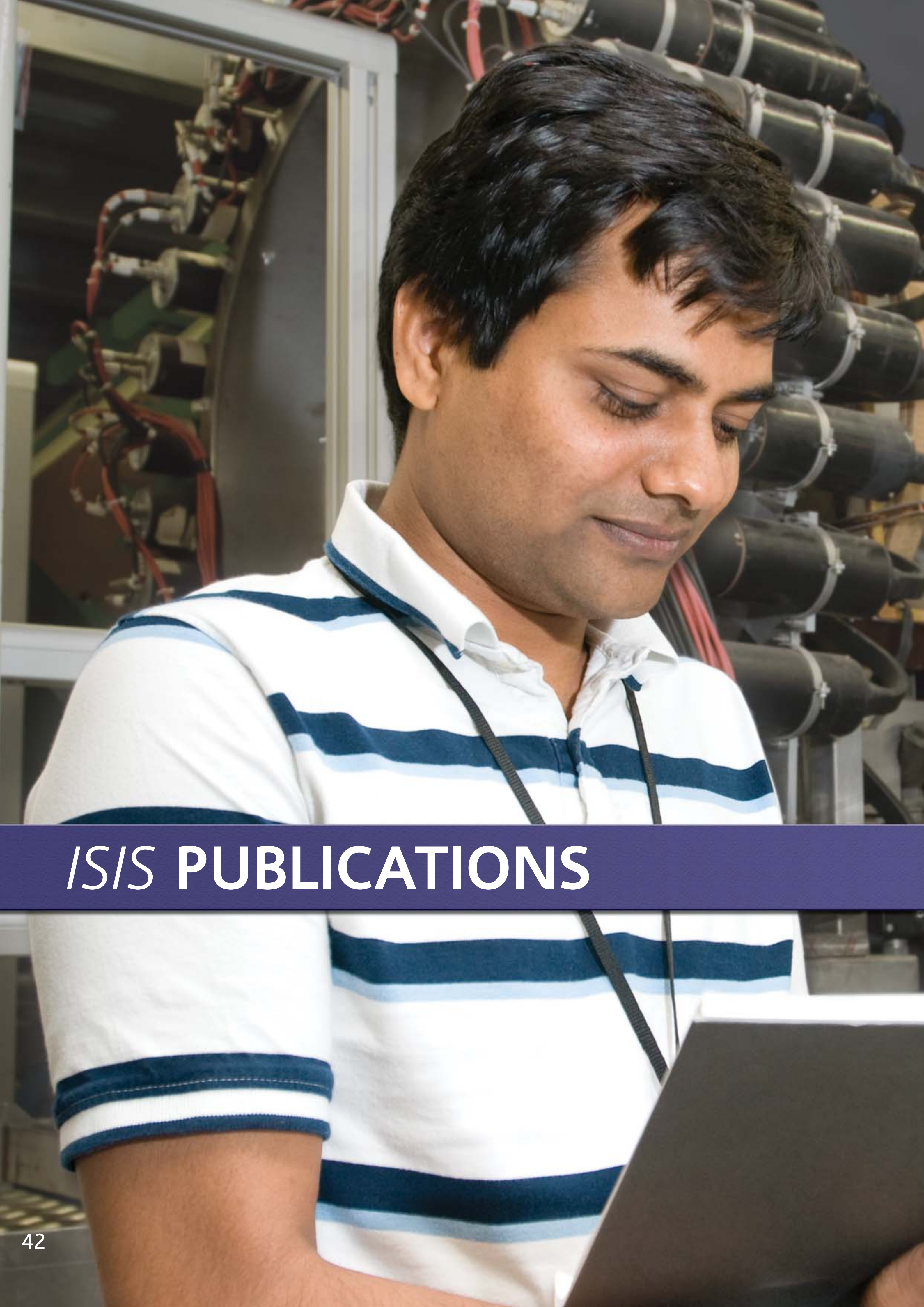
Members of the Engineering FAP.

Chris Hardacre (Queen's University Belfast) and Daniel Bowron (ISIS) considering disordered materials science.

Meigan Aronson (Stony Brook, USA) during the muon FAP.

ISIS FACILITY ACCESS PANELS

Below: *Ali Zarbakhsh (Queen Mary University of London), right, considering proposals in the Large Scale Structures FAP with Max Skoda (ISIS).*



ISIS PUBLICATIONS

Publications relate to all work carried out at ISIS.

Listed here are 402 publications resulting from work at the facility that were published in calendar year 2011.

B. Abbey, S. Y. Zhang, W. Vorster, and A. M. Korsunsky: **'Reconstruction of axisymmetric strain distributions via neutron strain tomography'**, *Nuclear Instruments & Methods in Physics Research Section B-Beam Interactions with Materials and Atoms, 2011, 270, 28-35.*

B. Abbey, S. Y. Zhang, M. Xie, X. Song, and A. M. Korsunsky: **'Neutron strain tomography using Bragg-edge transmission'**, *International Journal of Materials Research, 2011, 103(2), 234-241.*

T. Adachi, Y. Tanabe, K. Suzuki, Y. Koike, T. Suzuki, T. Kawamata, and I. Watanabe: **'Development of Cu-spin correlation in $Bi_{1.74}Pb_{0.38}Sr_{1.88}Cu_{1-y}Zn_yO_{6+d}$ high-temperature superconductors observed by muon spin relaxation'**, *Physical Review B, 2011, 83(18).*

P. C. Aeberhard, K. Refson, P. P. Edwards, and W. I. F. David: **'High-pressure crystal structure prediction of calcium borohydride using density functional theory'**, *Physical Review B, 2011, 83(17).*

H. Afifi, M. A. da Silva, C. Nouvel, J.-L. Six, C. Ligoure, and C. A. Dreiss: **'Associative networks of cholesterol-modified dextran with short and long micelles'**, *Soft Matter, 2011, 7(10), 4888-4899.*

H. Afifi, G. Karlsson, R. K. Heenan, and C. A. Dreiss: **'Solubilization of oils or addition of monoglycerides drives the formation of wormlike micelles with an elliptical cross-section in cholesterol-based surfactants: a study by rheology, SANS, and cryo-TEM'**, *Langmuir, 2011, 27(12), 7480-7492.*

S. Agrestini, C. L. Fleck, L. C. Chapon, C. Mazzoli, A. Bombardi, M. R. Lees, and O. A. Petrenko: **'Slow magnetic order-order transition in the spin chain antiferromagnet $Ca_3Co_2O_6$'**, *Physical Review Letters, 2011, 106(19).*

R. Ahmed, N. H. Faisal, A. M. Paradowska, M. E. Fitzpatrick, and K. A. Khor: **'Neutron diffraction residual strain measurements in nanostructured hydroxyapatite coatings for orthopaedic implants'**, *Journal of the Mechanical Behavior of Biomedical Materials, 2011, 4(8), 2043-2054.*

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ISIS SEMINARS 2011-2012

ISIS hosts seminars on topics covering the range of science undertaken at the facility by researchers from the UK, Europe and further afield.

5 April 2011
Leonid Sandratskii
Max Planck Institute, Germany
Non-adiabatic spin-dynamics of complex magnetic systems

12 April 2011
Ken Andersen
European Spallation Source, Lund, Sweden
Progress on neutron instruments for the European Spallation Source

19 April 2011
Amit Keren
Technion Institute of Technology, Israel
A magnetic analog of the isotope effect in cuprates

10 May 2011
Hardy Gross
Max Planck Institute, Germany
Ab-initio theory of superconductivity: how to predict the critical temperature

17 May 2011
Mike J Gillan
University College London
High-accuracy energetics of condensed matter with quantum chemistry and quantum Monte Carlo

26 May 2011
Achim Rosch
University of Cologne, Germany
2nd SEPnet Summer Programme: Condensed Matter Physics in the City Spintorques and skyrmions in chiral magnets

26 May 2011
Joe Bhaseen
University of Cambridge
2nd SEPnet Summer Programme: Condensed Matter Physics in the City Quantum Phase Transitions in Pairing Systems

26 May 2011
Joseph Betouras
University of Loughborough
2nd SEPnet Summer Programme: Condensed Matter Physics in the City. On the Lifshitz transition in a model of 2D dipolar fermions and in $NaxCoO_2$

2 June 2011
Andrew Briggs University of Oxford
2nd SEPnet Summer Programme: Condensed Matter Physics in the City Quantum Mesoscopics

2 June 2011
Andrew Boothroyd
University of Oxford
2nd SEPnet Summer Programme: Condensed Matter Physics in the City Magnetic fluctuations in Fe-based superconductors

2 June 2011
Suchitra Sebastian
University of Cambridge
2nd SEPnet Summer Programme: Condensed Matter Physics in the City. Nodal pockets revealed by quantum oscillations in underdoped YBCO

2 June 2011
Adrian Hillier
ISIS
2nd SEPnet Summer Programme: Condensed Matter Physics in the City Evidence for non-unitary superconductivity

2 June 2011
Elizabeth Blackburn
University of Birmingham
2nd SEPnet Summer Programme: Condensed Matter Physics in the City. The superconducting states of $CeCoIn_5$

7 June 2011
Nic Shannon
University of Bristol
Quantum ice

14 June 2011
Helen E Hermes
Heinrich-Heine-University Düsseldorf, Germany
Neutron radiography of soft and complex matter systems: an experimenter's viewpoint

28 June 2011
Amy Briffa
University of Birmingham
The magnetic structure of gadolinium titanate

2 August 2011
Stefan Kowarik Humboldt
Universität Berlin, Germany
Growth and structure of molecular semiconductors:real-time XRR, energy dispersive and anomalous reflectivity, and X-ray miscroscopy studies

16 August 2011
Brent Fultz
California Institute of Technology
Non-harmonic phonon thermodynamics

27 September 2011
Matthias Ballauff
HZB, Germany
Neutron scattering and supramolecular chemistry

25 October 2011
Rex Godby
University of York
The GW approach to spectral, ground-state and transport properties

1 November 2011
Kimitoshi Kono
RIKEN, Japan
Free surface of superfluid 3He and rotating supersolid: recent activity of RIKEN low temperature physics laboratory

22 November 2011
Leonardo Bernasconi CSED, STFC
Electronic excitations and dynamics in the condensed phase

25 November 2011
Heribert Wilhelm
Diamond Light Source
Precursor phenomena at the magnetic ordering of the cubic helimagnet FeGe

29 November 2011
Ulrich K. Rössler
Leibniz Institute, Dresden, Germany
Skyrmion matters in chiral magnets

12 December 2011
Michele Benzi
Emory University, USA
Decay properties of spectral projectors with applications to electronic structure computations

12 December 2011
Boualem Hammouda
National Institute of Standards and Technology, USA
Nanoscale structures using small-angle neutron scattering

17 January 2012
Brent Heuser
University of Illinois at Urbana-Champaign, USA
Hydrogen trapping at dislocations in deformed Pd at low temperature: Results from SANS, IINS, and DFT

31 January 2012
Serena Corr
University of Kent
Local structure studies of functional metal oxides

28 February 2012
Joachim Dzubiella
Humholdt University of Berlin, Germany
Theoretical and computational approaches to the modelling of (bio) molecular fluids

13 March 2012
Arno Schindlmayr
University Paderborn, Germany
Electronic excitations in itinerant ferromagnets from first principles

27 March 2012
Pietro Ballone
Queen's University, Belfast
Coarse graining dynamical properties: the excess entropy route

19 April 2012
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)

15 May 2012
Ferruccio Renzoni
University College London
Control of atomic motion with ac fields: from the ratchet effect to vibrational mechanics

29 May 2012
Ludovic Jaubert
Okinawa Institute of Science and Technology (OIST), Japan
Spin ice dynamics and spin liquid Curie law

Vesuvio is used by Andrew Seel (Oxford University) to examine the state of the proton in lithium-ammonia solutions and solids via deep inelastic neutron spectroscopy.

ISIS FACTS & FIGURES

ISIS Facility Access Panel

FAP 1	FAP 2	FAP 3	FAP 4	FAP 5	FAP 6	FAP 7
Diffraction	**Liquids**	**Large Scale Structures**	**Excitations**	**Molecular Spectroscopy**	**Muons**	**Engineering**
D Gregory Chair	C Hardacre Chair	A Zarbakhsh Chair	A Boothroyd Chair	N Skipper Chair	D Paul Chair	J Bouchard Chair
D Allan	M Arai	D Barlow	P Dai	C Andreani	M Aronson	C Davies
L Chapon	C Cabrillo	W Bouman	B Lake	D Book	H Dilger	T Holden
J Claridge	R McGreevy	S Clarke	S Raymond	F Bresme	A Drew	A Lodini
E Cussen	G Monaco	K Edler	D Reznik	S Golunski	A Suter	J Quinta da Fonseca
A Goodwin	J Tse	T Hase	H Ronnow	M Jones	I Terry	R Reed
M Hofmann	R Winter	S Lee	N Shannon	M Krzystyniak	J Titman	H Stone
B Kennedy		T Nylander	C Stock	MP Marques	T Veal	M Yescas
C Knee		E Sivaniah		A Nogales Ruiz	I Watanabe	
S Skinner		I Tucker		R Senesi		
A Thompson						
R Walton						
I Wood						
M Tucker	D Bowron	M Skoda	R Ewings	F Demmel	S Cottrell	J Kelleher
S Hull	A Hannon	J Webster	J Taylor	J Mayers	A Hillier	SY Zhang

ISIS Facility Access Panel membership for the June 2012 meetings. The FAPs meet twice per year to review all proposals submitted to the facility based on scientific merit and timeliness.

ISIS User Committee

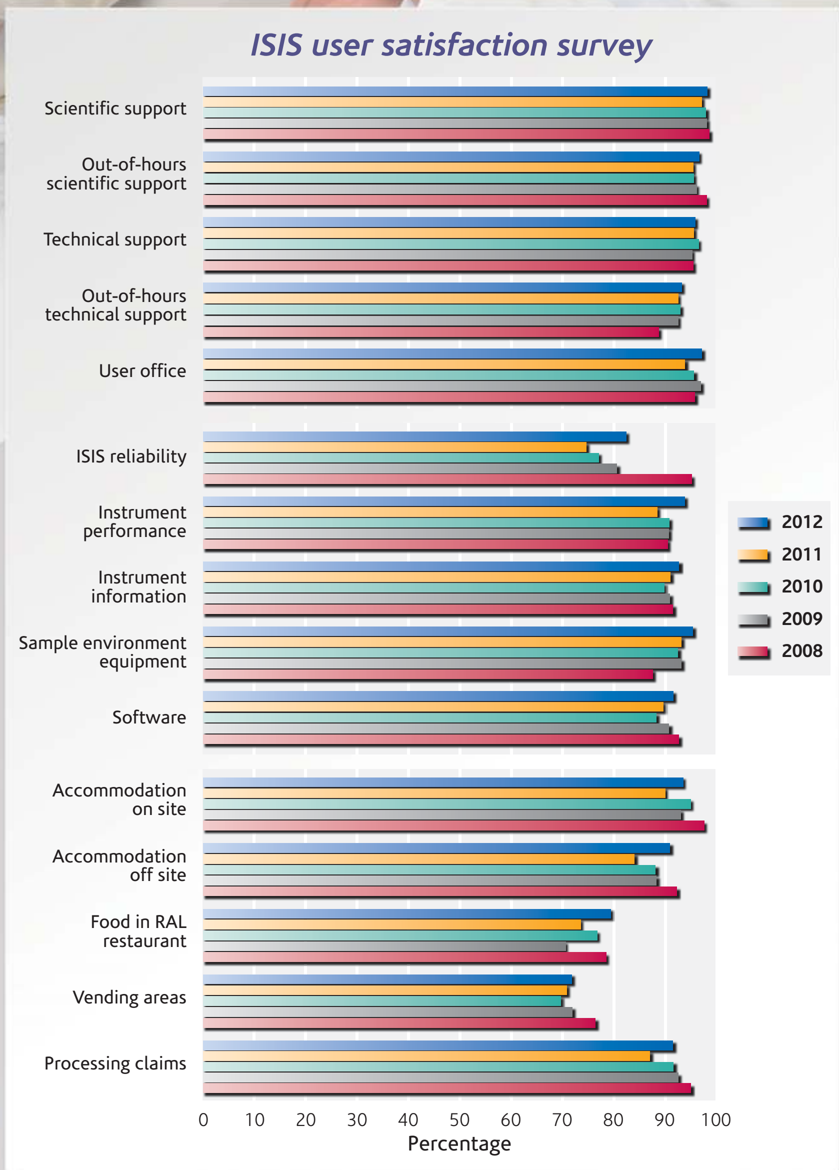
	Chair	D Lennon	University of Glasgow
IUG1	**Crystallography**	A Powell Vacancy	Heriot-Watt University
IUG2	**Liquids and Amorphous**	J Holbrey B Webber	Queen's University Belfast University of Kent
IUG3	**Large Scale Structures**	J Lakey A Zarbaksh	University of Newcastle Queen Mary College, London
IUG4	**Excitations**	J Goff P Salmon	Royal Holloway University London Bath University
IUG5	**Molecular Spectroscopy**	D Lennon S McLain	University of Glasgow University of Oxford
IUG6	**Muons**	A Drew D Paul	Queen Mary University of London University of Warwick
IUG7	**Engineering**	D Dye M Preuss	Imperial College London Manchester

	ISIS Director	U Steigenberger
	ISS Division Head	P J C King
	IDM Division Head	S Langridge
	IEO Division Head	Z A Bowden
	II Division Head	D Greenfield
	ISIS User Programme Manager	A D Kaye

ISIS User Committee Membership for June 2012. The IUC exists to represent the user community on all aspects of facility operation.

User **Satisfaction**

All users visiting the facility are invited to complete a satisfaction survey which addresses the quality of the scientific, technical and User Office support, the ISIS, instrument and support equipment performance and reliability, and the quality of the accommodation and restaurant facilities. The feedback obtained in this way helps to ensure a high quality service is maintained and improved where necessary.



ISIS user survey results from 2008 to 2012.

ISIS FACTS & FIGURES

Beam Statistics 2011-2012

For the period of this report and during scheduled operating cycles, ISIS delivered a total of 583 mA.hrs of user proton beam to the muon and neutron targets.

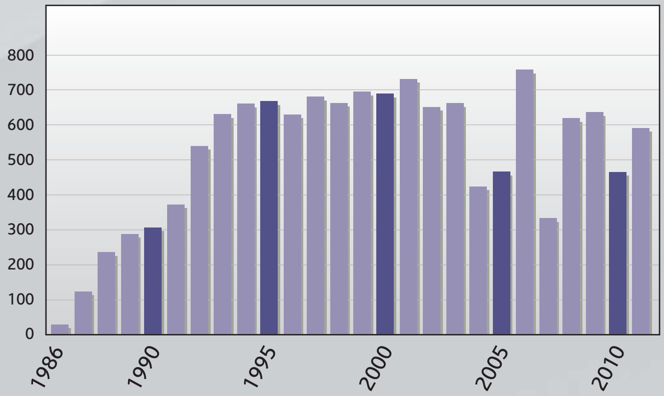
The tables below give beam statistics for the individual cycles in the year 2011-2012, together with year-on-year statistics for ISIS performance.

Cycle	11/1	11/2	11/3	11/4	11/5
	17 May - 9 Jun 2011	5 Jul - 4 Aug 2011	4 Oct - 4 Nev 2011	22 Nov - 23 Dec 2011	21 Feb - 29 Mar 2012
Beam on target 1 (hr)	476	645	622	596	650
Total beam current delivery to both targets (mA-hr)	90	122	119	120	133
Average beam current for beam on target (targets 1 & 2 combined)	188.0	188.0	190.9	201.2	205.0

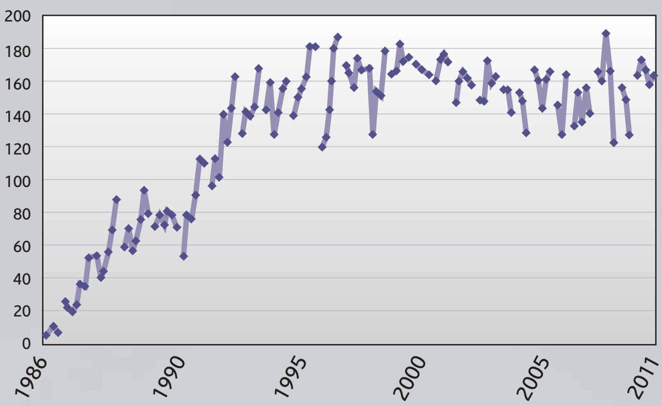
ISIS operational statistics for year 2010-2011.

Year	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011
Total Scheduled Days	168	156	165	106	134	196	92	163	156	116	138
Total Time on Target (days)	158	144	152	96	107	174	74	144	126	97	125
Total Integrated Current (mA-hrs)	725	612	647	409	459	749	326	612	630	460	583
Average Beam Current (for beam on target) (μA)	192	178	177	177	178	179	183	177	179	197	194

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



The ISIS integrated beam current year-on-year.



Average ISIS beam current per cycle

The ISIS Pulsed Neutron and Muon Source

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