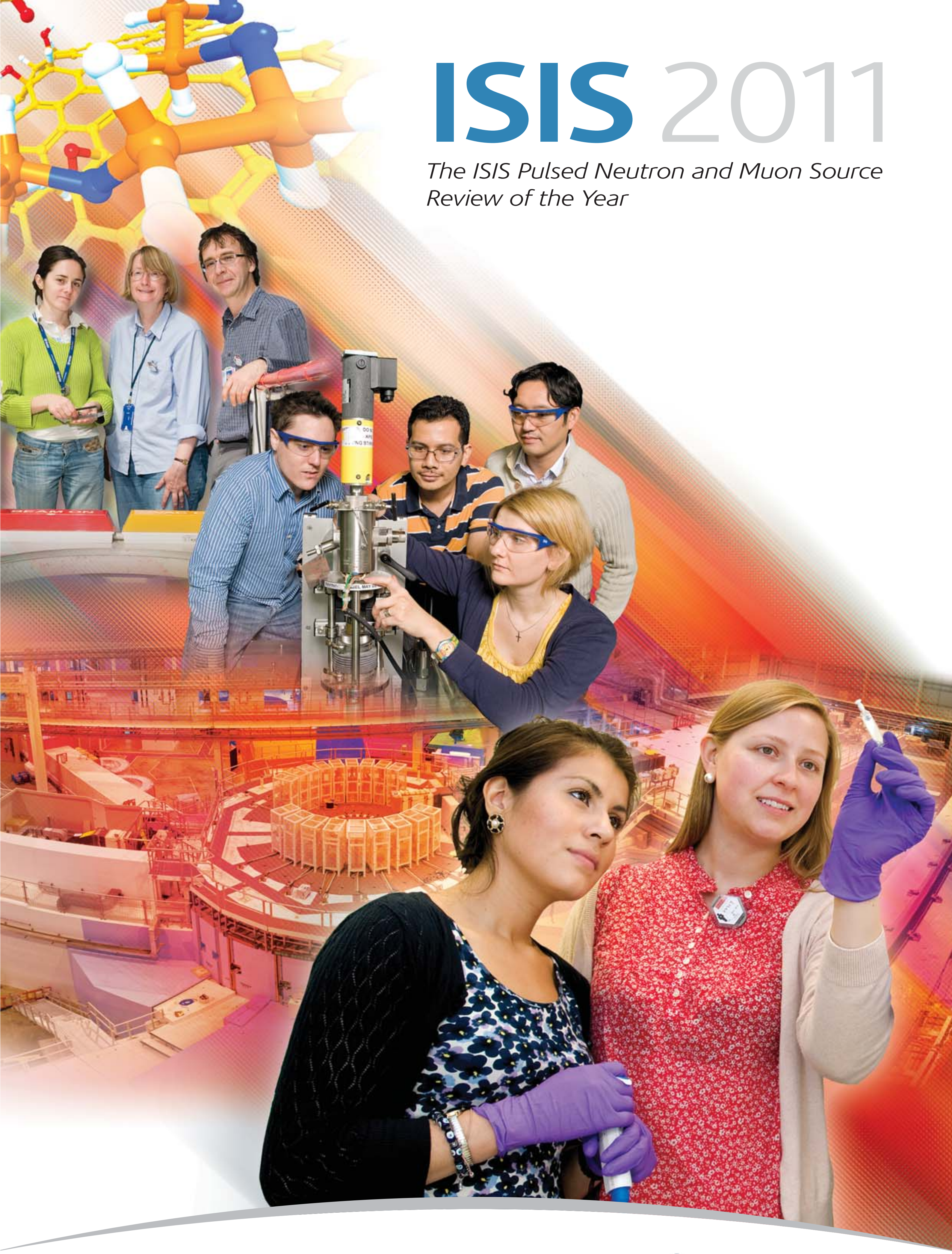
ISIS 2011

The ISIS Pulsed Neutron and Muon Source Review of the Year



Science & Technology Facilities Council

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September 2011

ISIS 2011

ISIS provides world-class facilities for neutron and muon investigations of materials across a diverse range of science disciplines. ISIS 2011 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 year.

Contents

Lord Alec Broers, Chairman of Diamond Light Source Ltd., with the Offspec instrument in the ISIS Second Target Station.

Right: Andrew Smith MP learning about neutron reflectometry from Rob Dalgliesh (ISIS) during his visit in July.

Right: Patxi Lopez, Lehendakari Basque Government President visited ISIS in March. He is seen here discussing ISIS science with ISIS Director Andrew Taylor.

Above: Nicola Blackwood MP touring the ISIS Second Target Station with Sarah Rogers (ISIS) in February.

Below: John Howell MP (left) visited ISIS in June with Andrew Taylor (Director, ISIS).

David Willetts MP, Minister for Universities and Science, visited ISIS in March. During his visit he announced £11M funding for the Chipir instrument, to be built on the ISIS Second Target Station, and near right: considering soft matter science at ISIS with Julian Eastoe (Bristol University).

Foreword

During a visit to ISIS on 14 March 2011, Universities and Science Minister David Willetts announced an £11 million investment to start the second phase of instruments at the ISIS second target station. This was closely followed by a further £10 million announced by Chancellor George Osborne in the budget on 23 March.

This is fantastic news for ISIS and a superb reflection on the outstanding work of the ISIS user community and staff in delivering world-leading science and technology. The success of ISIS continues to be recognised at the highest levels within the UK government, and the impact of ISIS science is clearly appreciated.

The combined funding of £21 million, together with additional contributions from ISIS partner countries, will finance the construction of four new instruments within the ISIS second target station: Chipir, Imat, Zoom and Larmor. These instruments will add world-class capabilities in microchip screening, neutron imaging and small angle scattering, together with extending the time- and length-scales of neutron experiments. Exciting days ahead.

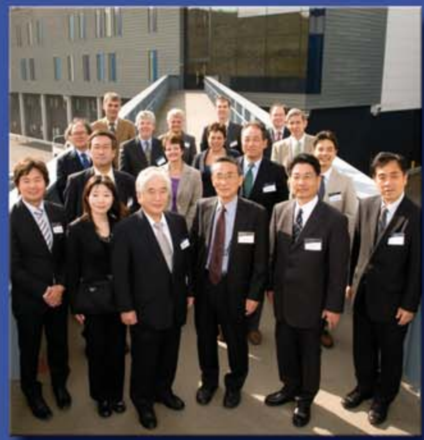
Creating new instruments enables us to deliver world-class science. From novel magnetism to new types of solar cell; practical hydrogen storage materials to antibiotics for life-threatening illnesses; human tissue protein studies to silicates for catalysis – research at ISIS spans a huge range pure and applied science areas, a range that will continue to grow as new instrument capabilities are added.

But also part of enabling ISIS science is the work of keeping the ISIS accelerator complex up and running. This year saw a six month maintenance shut-down which was several years in the planning. A huge amount of work – some 700 small projects, together with several large projects – took place to keep the ISIS machine and instruments going well into the future. I would like to thank ISIS staff for all their work not just in the shut-down itself, but for the years of preparatory work beforehand.

We deliver world-class science with impact in many areas, and we maintain, operate and develop our accelerators and instruments – these things are central to ISIS. But also key are the many other activities that form part of the life of the facility – ISIS engineers working with AS level school students on detector projects; ISIS scientists and engineers winning prizes for their work in national competitions; staff enthusing school children at UK science fairs; receiving students and members of the public as visitors to explain what we do and to encourage the next generation of scientists. These are all signs of the health and maturity of the ISIS community.

ISIS is not immune to the current financial pressures, and we find ourselves facing a reduced level of operations. Despite this, we are seeking to maintain ISIS at the forefront of neutron and muon science. Together with our user community we will strive to deliver another exciting year of excellent science.

Andrew Taylor
Director



Above right: In October ISIS welcomed the Mayor of Tokai-Mura, Japan, Mr Tasuya Murakami, together with other members of the Tokai-Mura village and senior staff from J-PARC (Japan Proton Accelerator Complex) and the Japan Atomic Energy Agency (JAEA). J-PARC is located on the Tokai site of JAEA.

Above centre: The Rt Revd John Pritchard, Bishop of Oxford, visited ISIS in March with other members of the Wallingford Deanery. He is seen here in the ISIS Second Target Station with Andrew Kaye and Philip King (ISIS).

Above left: RAL held an open day for the general public on 9th June 2011. Here we see Sean Langridge (ISIS) with visitors in the ISIS Second Target Station.

Left: The Schools Science Prizes were presented at RAL in October. Pupils were nominated by their teacher and received a certificate and book tokens to encourage their future development as scientists. Here Christopher Stewart (Lord Williams's School, Thame) is helping Stephen Boag and Max Skoda (ISIS) during their demonstrations of the science of the very (very) cold and how it is used in superconducting magnets in ISIS and the Large Hadron Collider.

The STFC Science Board visited ISIS in October. Science Board members provide advice on all aspects of STFC's science and technology programme. Left to right: Prof Anthony Watts (Oxford University), Prof Steven Rose (Imperial College London), Prof Guenter Rosner (Glasgow University), Prof Shiela Rowan (Glasgow University), Prof Bob Newport (University of Kent), Prof Tony Ryan (Sheffield University), Prof Matt Griffin (Cardiff University), Prof Neville Greaves (Aberystwyth University), Prof Jon Butterworth (University College London).

ISIS has had ongoing collaborations with KEK in Japan for many years. Osamu Shimomura, Director, Institute of Materials Structure Science, KEK, and other KEK members, visited ISIS in June. Here, Prof Shimomura is presenting Andrew Taylor, ISIS Director, with a gift to mark the ISIS-KEK collaboration.

Prof Andrew Hamilton (Vice-Chancellor, Oxford University) and colleagues visited ISIS in September. Left to right: Prof Ian Walmsley (Pro-Vice Chancellor, Research, Oxford University), Prof Richard Wade (STFC Chief Operating Officer) Prof Andrew Hamilton, Dr Andrew Taylor (Director, ISIS) and Prof Angus Kirkland (Department of Materials, Oxford University).

Right: In December ISIS had an exhibition at the Cornerstone gallery in near-by Didcot. The exhibition enabled members of the public to experience ISIS science and technology through photos, pictures and hands-on displays. Bill Heine, BBC Radio Oxford presenter, was one of the visitors to attend the opening evening.

Below: In January ISIS hosted visitors from the King Abdulaziz City for Science and Technology (KACST), Saudi Arabia. Here David Barlow (left) and Jayne Lawrence (right), Kings College London, are discussing biomolecular science applications of neutrons with Muhanna Al Muhanna (KACST) and Hamid Al-Shejni (STFC).

A year around ISIS

Johnson Matthey scientists Barry Murrer, Peter Bishop, Jonathan Sharman and Sue Ellis visited ISIS in November.

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

How does the antibiotic amphotericin work?

F Foglia, A Dabkowska, MJ Lawrence, DJ Barlow (King's College London), R Barker (University of Bath), AE Terry, SE Rogers, AV Hughes, JRP Webster (ISIS)

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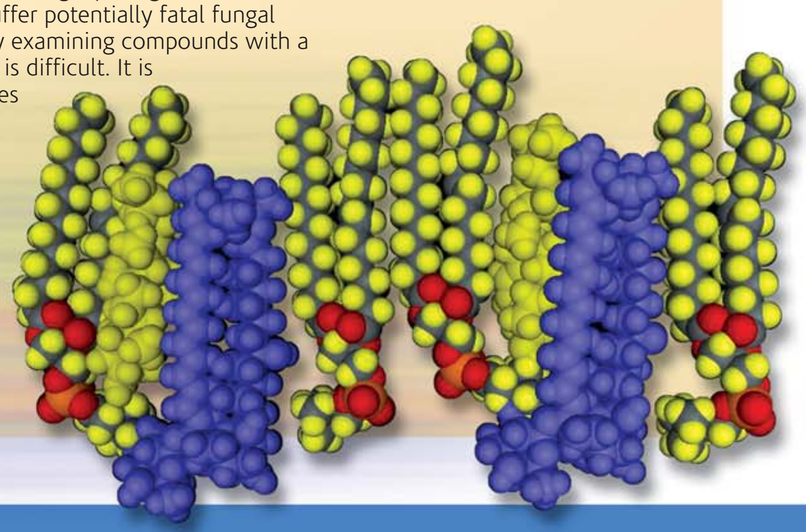
Further reading: F Foglia et al., Biochim. Biophys. Acta 1808 (2011) 1574

Amphotericin has been the first line of defence against fungal infections since the mid-1950s. Unfortunately, resistance to this drug is beginning to emerge, posing serious problems for AIDS and chemotherapy patients who often suffer potentially fatal fungal infections. Normally, replacement drugs would be sought by examining compounds with a similar mechanism of action. For amphotericin, though, this is difficult. It is established that the drug punches holes in cells, which makes them leaky and so causes them to die, but how it does this, and why it causes more damage to fungal cells than human cells remains unclear. Neutron reflectivity and small-angle scattering studies have been performed to study the effects of amphotericin on model human and fungal cell membranes, to find out why the drug is so selective. Rather surprisingly, the drug is found to insert into both fungal and human cell membranes but the neutron studies also clearly show that it perturbs these two types of membranes in markedly different ways.



Molecular model of a lipid monolayer showing the fungal sterol ergosterol (yellow) interacting with the inserted antibiotic amphotericin (blue).

Dynamics in lipid vesicles

Y Gerelli (Università di Parma, Italy and ILL, France), A Deriu, (Università di Parma, Italy), V Garcia Sakai (ISIS)

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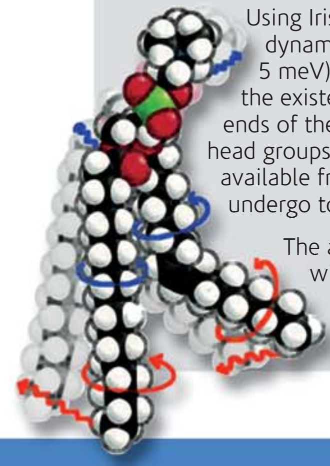
Further reading: Y Gerelli et al., Soft Matter 7 (2011) 3929

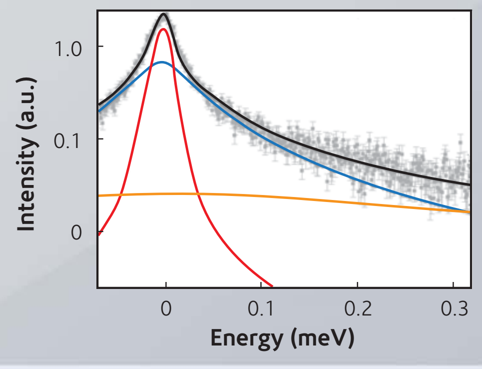
Interest in the fundamental properties of systems based on lipids (fat-like molecules that are insoluble in water) has increased owing to a growing number of applications in pharmacy, medicine and food science. Investigation of the internal dynamics of lipid aggregates raises some important and yet-to-be-answered questions, including the effects of temperature on these motions.



Using Iris at ISIS and IN6 at ILL, we have explored a wide range of dynamics of lipid-based systems (energy-transfer range 10 μeV – 5 meV). The quasielastic neutron scattering (QENS) data confirm the existence of dynamical heterogeneities, whereby the terminal ends of the acyl chains experience faster motions than those of the head groups and neighbouring chain segments. Owing to the larger available free volume, the terminal CH_2 and methyl groups can also undergo torsional structural changes.

The addition of chitosan, a charged polysaccharide used along with lipids in drug-delivery applications, affects the localised hydrogen motions on the upper part of the molecule yet they do not seem to influence the structural changes.

The structure of a lipid molecule is shown on the left, where coloured arrows indicate the motions investigated in this work. Using the same colours, the corresponding contributions to the QENS spectrum are shown on the below.



Life sciences

'We must not forget that when Radium was discovered, no one knew that it would prove useful in hospitals' – M Curie

The unusual behaviour of a plant seed defence protein

LA Clifton, MR Sanders, SE Rogers, RK Heenan, C Neylon (ISIS), V Castelletto, RA Frazier, RJ Green (University of Reading)

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Further reading: LA Clifton et al., Phys. Chem. Chem. Phys. 13 (2011) 8881

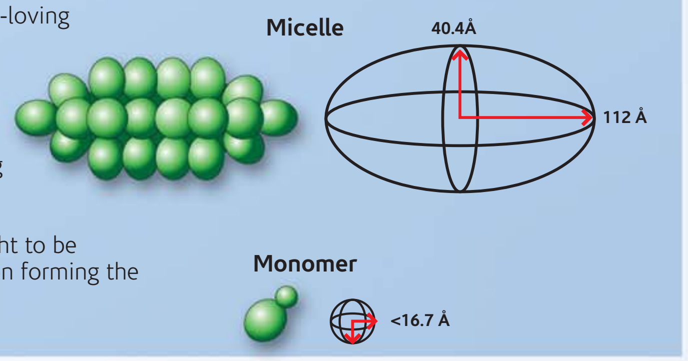
A combination of small angle neutron scattering, dynamic light scattering and size-exclusion chromatography has been used to uncover a protein's unique structuring behaviour in solution.

Puroindoline-a is a plant seed defence protein found in wheat. It has a broad spectrum of antifungal and antibacterial activity, and has potential applications such as novel antibiotics or targeted drug-delivery systems.

Puroindoline-a forms micelles in aqueous solution. One part of a puroindoline-a molecule is water-loving; the other end is water-insoluble. Micelles are groups of the protein molecules in which the water-loving parts all point outwards, into the surrounding solution. Proteins which form micelles are rare, with only one other protein known to spontaneously form these assemblies in solution.

We have been able to discover that the structure formed by puroindoline-a is unique amongst known protein micelles, being highly elongated rather than spherical. Puroindolines contain a tryptophan-rich part which is responsible for the protein's antimicrobial membrane-binding activity. This part is also thought to be responsible for its solution-structuring behaviour, with this region forming the water-insoluble interior of the micelle.

Structures of puroindoline-a micelle (top) and monomer (bottom) obtained from small angle neutron scattering, dynamic light scattering, and size-exclusion chromatography.



Protein motion in red blood cells

AM Stadler (Jülich, Germany), L van Eijck (ILL, France), F Demmel (ISIS), G Artmann (Aachen University, Germany)

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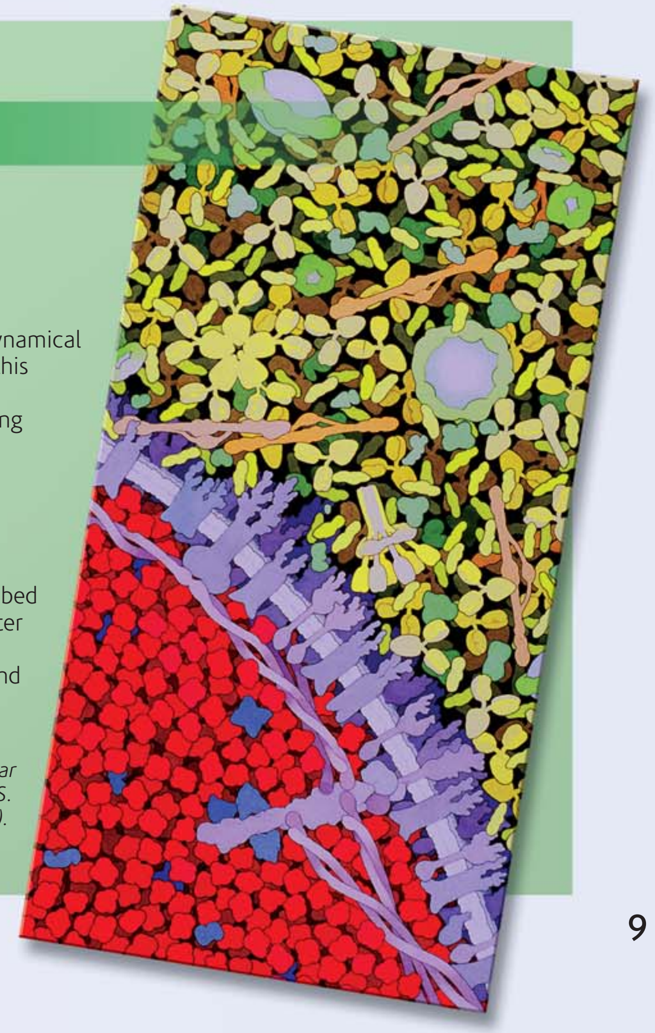
Further reading: AM Stadler et al., J R Soc Interface 8 (2011) 590

Ongoing cell research aims at a coherent picture of the interactions and dynamical properties of proteins inside living cells under physiological conditions. In this context, red blood cells are exceptional, as they are highly specialized and relatively simple in composition, the main macromolecular component being haemoglobin.

We have used high-resolution quasielastic neutron scattering to study the motions of haemoglobin in whole red blood cells. Neutron scattering is exceptionally useful as measurements on living cells are possible without damaging these highly sensitive specimens. We find that the diffusion of haemoglobin in the crowded environment of a red blood cell can be described using concepts from colloid physics. Furthermore, interfacial hydration water has a large influence on protein diffusion. This work demonstrates how neutron scattering allows the measurement of internal protein dynamics and global macromolecular diffusion in whole cells, thereby contributing to a better understanding of cellular phenomena at the molecular level.



Schematic diagram of a red blood cell (lower left) and surrounding extracellular medium. The cell is densely filled with haemoglobin, shown in red (© David S. Goodsell 2000).

Energy and catalysis

'Chemistry without catalysis would be a sword without a handle, a light without brilliance, a bell without sound' – A Mittasch

Spreadable polymer solar cells

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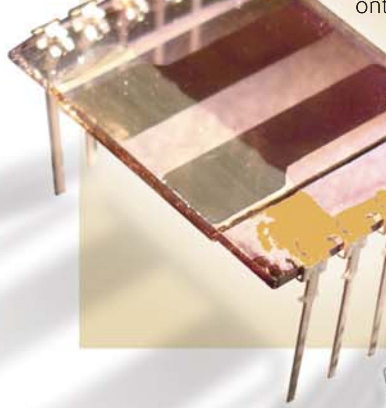
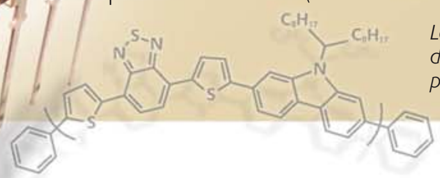
Further reading: PA Staniec et al., Adv. Energy Mat. 1 (2011) 499

Over the next fifty years society is going to need to supply the growing energy demands of the world's population without using fossil fuels, and the only renewable energy source that can do this is the Sun. Plastic (polymer) solar cells are much cheaper to manufacture than conventional silicon solar cells and have the potential to be produced in large quantities. Using neutron reflectivity, we have shown that when complex mixtures of molecules in solution are spread onto a surface, like varnishing a table-top, the different molecules separate to the top and bottom of the layer in a way that maximises the efficiency of the resulting solar cell. These results have given important insights into how ultra-cheap solar energy panels for domestic and industrial use can be manufactured on a large scale. Rather than using complex and expensive fabrication methods to create a specific semiconductor nanostructure, high-volume printing could be used to produce nanoscale (60 nanometer) solar cell films.





Left: A polymer-based, test solar cell with the structure of the donor polymer, PCDTBT. Right: Dr Rob Dalgliesh (ISIS) holding a polymer solar-cell sample.

Understanding a catalyst from formula to mechanism

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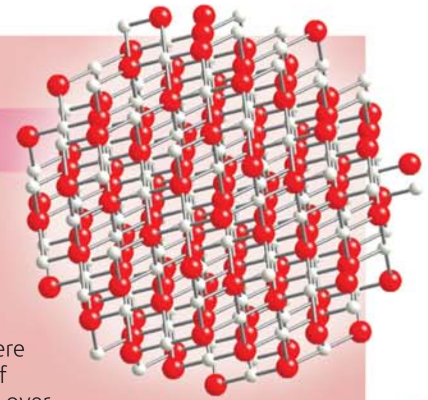
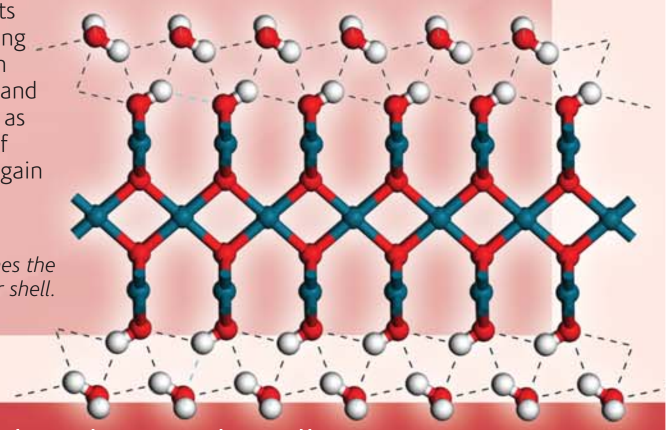
Further reading: SF Parker et al., J Phys Chem C 114 (2010) 14164



Palladium catalysts are a key component of the three-way catalytic converter used in cars, where they effect complete oxidation of hydrocarbons and carbon monoxide. To discover the effect of palladium, we have investigated the low-temperature catalytic conversion of carbon monoxide over hydrous palladium oxide powders. This oxidation reaction is remarkable in that it readily occurs at room temperature and pressure.

However, almost all that has been known about hydrous palladium oxide is its empirical formula, namely, $PdO{\bullet}H_2O$. We have characterised the material using a combination of neutron and x-ray powder diffraction, transmission electron microscopy, inelastic neutron scattering spectroscopy, infrared spectroscopy and computational methods. The results show that the material is best described as PdO nanocrystallites around 2 nm in size, terminated by a monolayer or so of hydroxyl groups, and capped by 4-7 layers of water. This model allows us to gain insight into the mechanism of catalytic oxidation of CO over a supported palladium catalyst.



Right: The structure of hydrous palladium oxide. Neutron diffraction (Gem, upper) defines the PdO core while vibrational spectroscopy (Tosca, Mari, Maps, lower) defines the water shell.

Getting the hole picture: porosity in activated carbons for hydrogen storage

Z Mileeva, DK Ross, D Wilkinson (University of Salford), S King (ISIS), T Ryan, H Sharrock (Chemviron Carbon Ltd)

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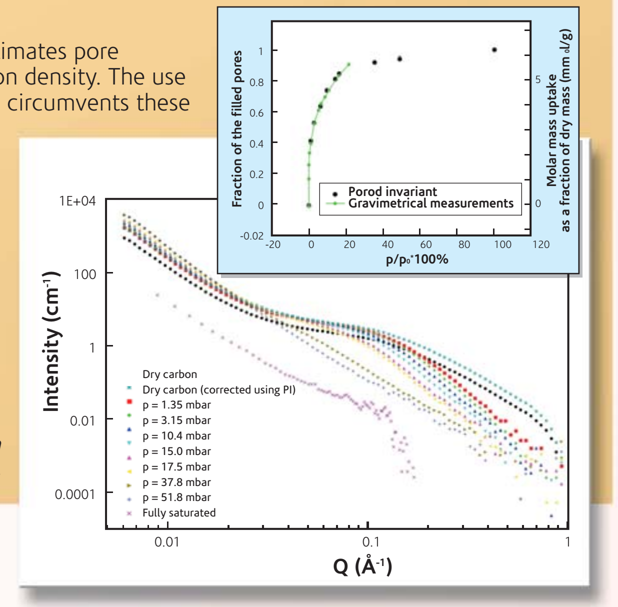
Further reading: Z Mileeva et al., in preparation

Activated carbons are of interest for hydrogen storage because hydrogen molecules can be trapped on the carbon surface. Such trapping works best in nanoscale 'slit pores' where adsorbate molecules interact with both walls.

The standard method to measure porosity, helium pycnometry, overestimates pore volumes because condensation of the gas increases the apparent carbon density. The use of small angle neutron scattering (SANS) and contrast-matching liquids circumvents these difficulties. Using mixtures of H/D-toluene to match the scattering from carbon, we can obtain the carbon density at different length scales. On the scale of atomic distances, this density is close to that of graphite. At larger, nanometer length scales, the density drops owing to the presence of porous structure.

SANS data for carbon show fractal behaviour at the larger length scales, and a well-defined hump at atomic scales caused by the activation (oxidation) process. From these data, the minimum pore radius as a function of toluene partial pressure can be found. The SANS data also allow us to compare the accessible pore volumes at each partial pressure with those obtained gravimetrically.



SANS data as a function of toluene partial pressure. The inset shows a comparison between SANS and gravimetric data.

You want it where?

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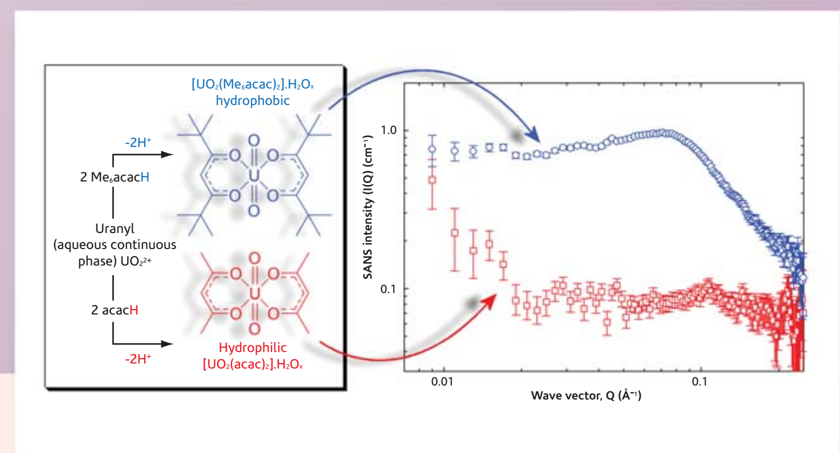
Nuclear power has played an important role in Britain's history, and with plans to build 10 new facilities, it is set to play an equally important role in its future. There is a need to develop rapid, selective methods for the detection and speciation of transuranic radioisotopes (e.g. Np, Pu, Am, Cm) in solution, as these elements represent hazardous by-products of the nuclear power industry. In collaboration with Magnox Ltd we are developing microemulsion systems to speciate these radionuclides in liquid wastes, to determine not only the element type and concentration, but also its oxidation state.

In essence, a range of water soluble complexing agents have been synthesised that display selectivity towards the radionuclides of interest. The binding of these agents to a radionuclide cation causes them to separate out within the microemulsion. The properties of the cations can then be studied. Small angle neutron scattering (SANS) is being used to probe the separation within the microemulsion system and to discover unique complexing agent – metal cation combinations.



Hydrophobic ligands selectively sequester ions and transport them to specific places within microemulsion systems for detection.

Good chemistry between magnetism and superconductivity

E Coronado, C Martí-Gastaldo, E Navarro-Moratalla, A Ribera (University of Valencia), SJ Blundell (University of Oxford) and PJ Baker (ISIS)

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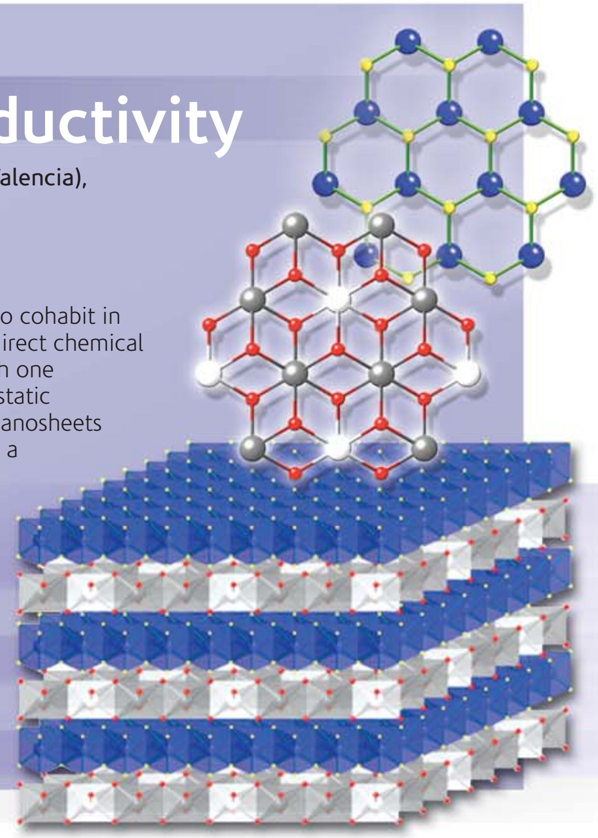
Further reading: E Coronado et al., Nature Chemistry 2 (2010) 1031

Superconductivity and magnetism are usually sworn enemies and often refuse to cohabit in the same compound. In a new method to make a multifunctional material by direct chemical design, layers of superconducting material and layers of magnetic material, each one molecule thick, have been pre-assembled and then brought together by electrostatic attraction. Thus, rather than building up the material one molecule at a time, nanosheets with different functionalities have been self-assembled. This is like constructing a building by adding entire pre-fabricated floors rather than brick by brick, and is the secret behind combining these two inimical properties. Putting magnetic and superconducting layers together in close proximity offers the possibility of using one property to alter the effect of this coupling in this new class of materials, we have used ISIS muons to determine the volume of the sample that becomes magnetically ordered as well as the strength of the superconducting state.



Alternating superconducting and magnetic layers combine to form a hybrid material.

Antiferromagnetic tendencies in superconducting LiFeAs

AE Taylor, MJ Pitcher (University of Oxford), RA Ewings, TG Perring (ISIS), SJ Clarke, AT Boothroyd (University of Oxford)

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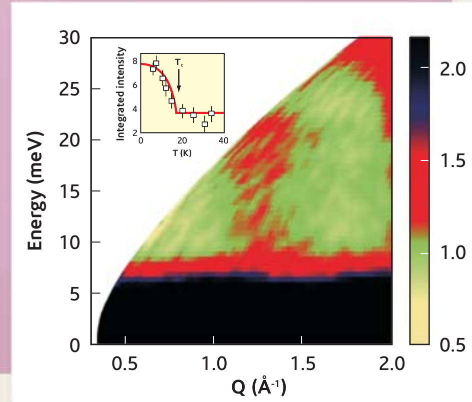
Further reading: AE Taylor et al., Phys. Rev. B 83 (2011) 220514(R)

Superconductors are metals whose electrical resistance vanishes below a certain 'critical temperature' T_C. This remarkable phenomenon was first observed in 1911, so 2011 was the 100th anniversary. Before 1986 the highest known T_C of any superconductor was only 18 degrees above absolute zero, or a chilly minus 255 Celsius. Despite such low operating temperatures, superconductors are widely used to provide high magnetic fields for magnetic resonance imaging and other applications.

The material we have studied, LiFeAs, is a member of a new family of iron-based superconductors discovered in 2008. Compounds in this family tend to develop antiferromagnetic order, and this property is believed to offer a possible route to higher T_C. In the case of LiFeAs, however, theoreticians had predicted an anomalous tendency for ferromagnetism. In our experiment we probed the atomic-scale magnetic dynamics in LiFeAs directly by neutron spectroscopy and found an antiferromagnetic tendency after all. We also found that the magnetic signal increased on cooling below T_C, providing clear evidence that antiferromagnetic fluctuations in LiFeAs are intimately linked to superconductivity.



Neutron scattering spectrum of superconducting LiFeAs taken on Merlin at 6K, showing a plume of intensity at Q = 1.2 Å^{-1} due to antiferromagnetic fluctuations and evidence for a superconductivity-induced spin resonance (inset).

Quantum Matter 1

'What we observe is not nature in itself but nature exposed to our method of questioning' – W Heisenberg

Understanding the role of oxygen vacancies in a spintronics semiconductor

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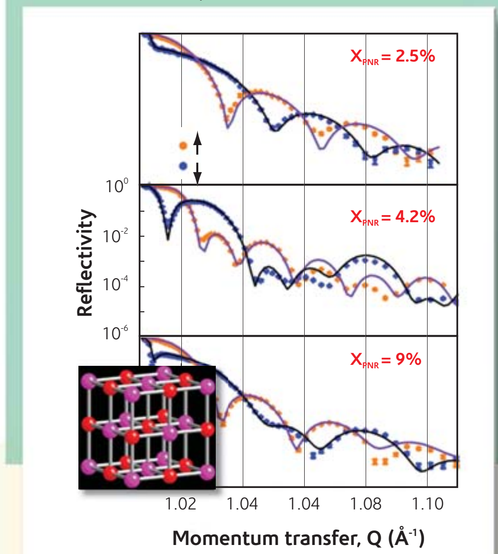
Further reading: M. Barbagallo et al., Phys. Rev. B. 84 (2011) 075219

Electron-doped europium oxide (EuO) is a semiconductor which undergoes a simultaneous ferromagnetic and metal-to-insulator phase transition, across which the resistivity drops by 8 to 13 orders of magnitude. The conduction electrons are nearly 100% spin polarized, making EuO an excellent material for next generation spintronic devices – devices in which the spins of the electrons are exploited instead of, or as well as, their charge.



An unanswered question is what effect electron doping has on the interactions and, crucially, on the degree of spin polarisation. By combining polarised neutron reflectometry with magnetometry and crystallography, we have been able to obtain precise values of oxygen-vacancy concentrations and relate this quantity to the enhanced magnetic moment in thin films and the increase in conduction-band polarisation. The results indicate that electron doping mediates an additional ferromagnetic interaction leading to an increase in ordering temperature, a result confirmed using theoretical models. These insights help to provide a fundamental understanding of the interactions in this fascinating material, as well as suggesting ways of increasing the ordering temperature in similar materials.

Polarised neutron reflectivity data and model calculations as a function of oxygen deficiency. The inset shows the crystal structure of stoichiometric EuO.

Slow magnetic crossover in the frustrated magnet $Ca_3Co_2O_6$

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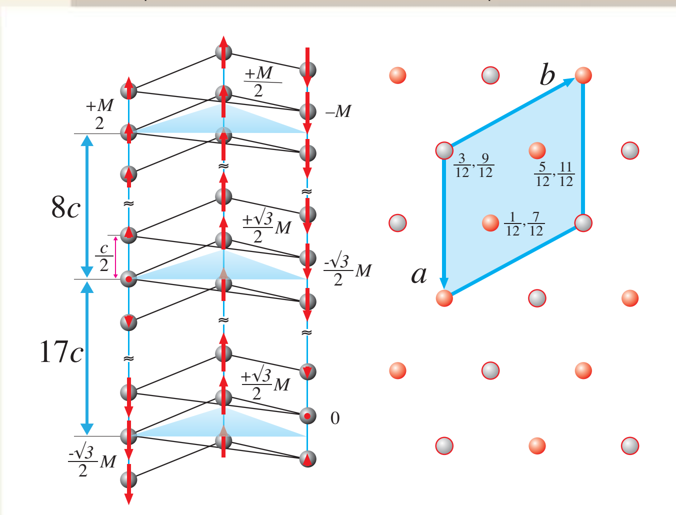
Further reading: S. Agrestini, et al., Phys. Rev. Lett. 106 (2011) 197204

Temperature-induced phase transitions between two magnetically ordered states usually correspond to lock-in transitions, transitions from collinear to non-collinear order, or magnetic ordering of symmetry-independent ionic sites. Very rarely, transitions between two magnetically ordered phases involve a change of translational symmetry, especially at low temperatures. A recent time-resolved powder diffraction study of the frustrated $Ca_3Co_2O_6$ compound has shown that below 12 K, the known magnetic structure (a nearly 600 Å longitudinal spin-density wave) transforms slowly into a commensurate magnetic phase (in which the magnetic structure follows the atomic structure). The broadening of diffraction features suggests that this new phase forms as an inter-growth within the matrix of the initial magnetic phase, i.e., the sample does not undergo macroscopic phase separation. This phenomenon appears below the freezing point of 12 K, where bulk dynamical behaviour is also known to change dramatically and steps appear in the magnetization. Both effects, however, still defy explanation at the atomic level.



Schematic representation of the spin-density-wave and commensurate phases. In the former case, the figure shows three sets of spin chains. In the latter case, the moments are aligned ferromagnetically perpendicular to the page.

Nanostructured ionic liquids

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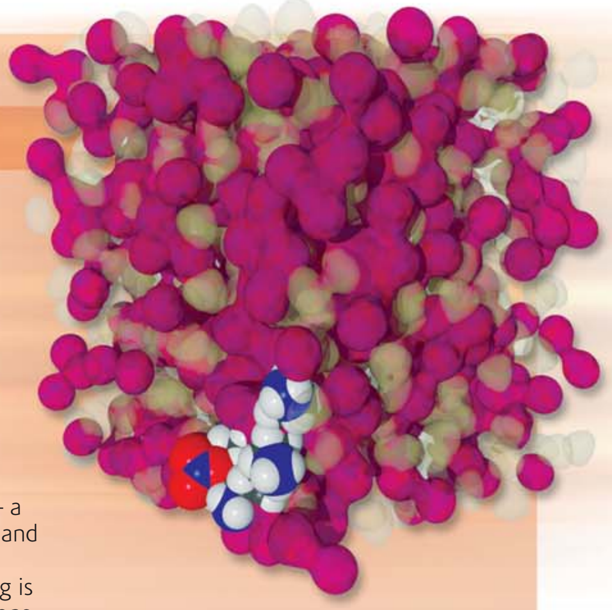
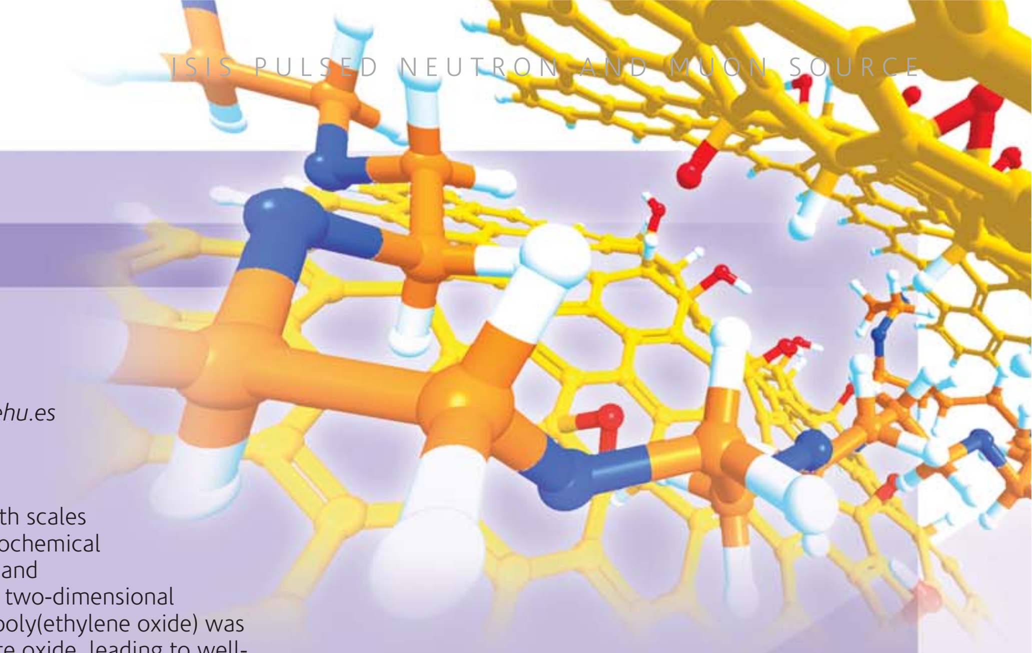
Further reading: Hayes et al, Phys. Chem. Chem. Phys, 13 (2011) 13544

The Greek philosopher Aristotle once suggested 'No reactions in the absence of solvent.' Whilst chemists have long since demonstrated solid- and gas-phase transformations, the vast majority of reactions are still conducted in the liquid phase. The choice of solvent can have a profound influence on reaction outcomes (yields, kinetics, etc.) and yet there are relatively few studies which characterize the structural origin of solvent properties. In this work, we have examined the bulk structure of ionic liquids – a special class of solvents composed entirely of ions – using neutron diffraction and computer simulation. The results show that ionic liquids self-assemble into bicontinuous nanostructures of polar and apolar domains. This solvent ordering is structurally analogous to thermodynamically stable bicontinuous microemulsions (microemulsions of two immiscible liquids stablised by a third component, such as oil and water stabilised by a surfactant), but with characteristic length scales at least an order of magnitude smaller. Interestingly, the nature of the bicontinuous arrangement could be modified via simple variations in ion structure, meaning that, in principle, the solvation properties of ionic liquids can be designed for particular chemical reactions.



Snapshot of the bulk structure of ethylammonium nitrate from neutron diffraction and computer simulation. Two interpenetrating networks of polar (red) and apolar groups (grey) can be identified.

Polymers in prison



F Barroso-Bujans, S Cerveny, A Alegría,
J Colmenero (CSIC/UPV-EHU, Spain),
F Fernandez-Alonso, SF Parker (ISIS)

Contact: Dr F Barroso-Bujans, fbarroso@ehu.es

Further reading: F Barroso-Bujans et al., Soft Matter 7 (2011) 7173

Polymer confinement at nanometer length scales can lead to significant changes in physicochemical properties including chain conformation and macromolecular relaxation. In this work, two-dimensional confinement of the ubiquitous polymer poly(ethylene oxide) was achieved via its intercalation into graphite oxide, leading to well-defined (subnanometer) polymer layers of thickness ~3.4 Å. The extreme spatial confinement of the polymer phase is responsible for the suppression of crystallization and cooperative relaxation processes. For the first time, high-resolution inelastic neutron scattering experiments on Tosca show that poly(ethylene oxide) under these extreme confinement conditions adopts a planar zig-zag conformation which in no way resembles the characteristic helical structure of the bulk crystal. Moreover, the neutron data also account for a drastic reduction in long-range order and chain mobility.

Poly(ethylene oxide) confined between two graphite-oxide sheets, leading to a single polymer layer of thickness ~3.4 Å. Neutron spectroscopy shows that the polymer is forced to adopt an unfolded planar conformation.

Supramolecular science and nanotechnology

*'There is plenty of room at the bottom'
– RP Feynman*

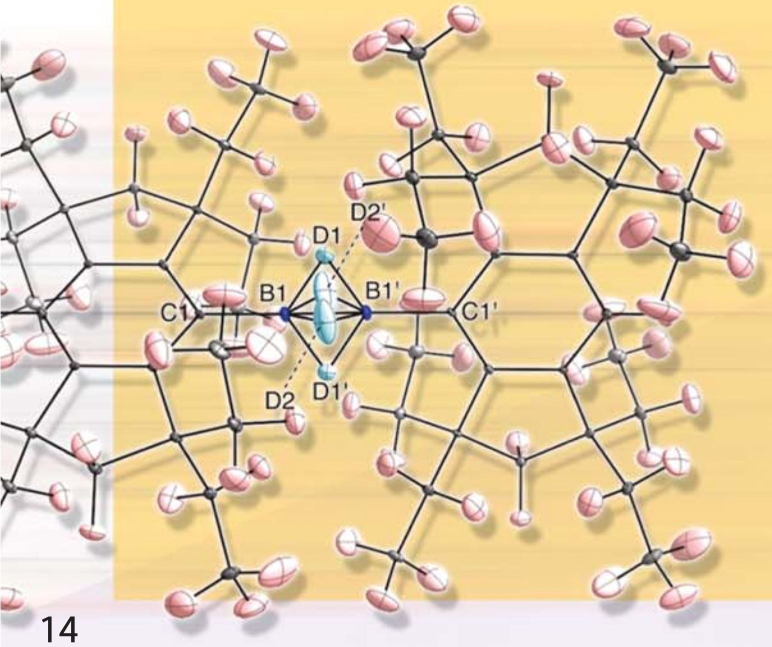
Butterflies and bridges

Y Shoji, T Matsuo, D Hashizume, K Tamao (RIKEN), H Fueno, K Tanaka (Kyoto University), MJ Gutmann (ISIS)

Contact: Dr T Matsuo, matsuo@riken.jp

Further reading: Y Shoji et al., J. Am. Chem. Soc. 133 (2011) 11058

While covalent bonds are usually formed by sharing two electrons between two atoms, some compounds contain B–H–B bonds in which an electron pair is distributed over three sites. The electron-deficient nature of these '3-center, 2-electron' bonds can give rise to various distinct chemical structures, some of which have only been predicted theoretically. We have isolated the stable diborane(4), $[B_2H_4]^{2-}$, with butterfly-shaped B–H–B bonds and a boron-boron link with triple-bond character. Neutron data were collected on a large-size single crystal of ^{11}B-labeled and deuterated diborane(4) using the SXD neutron diffractometer. The two bridging deuterium (μ-D) atoms are found to be located over two positions, which have been refined with occupancy factors of 0.5. An extraordinarily short B-B distance of 1.483(3) Å is comparable to computational predictions of B-B triple bonds. These structural features indicate that the chemical bonding at the B atoms can be described in terms of sp-hybridization.



Molecular structure of $(\mu\text{-D})_2(\text{Eind})^{11}B^{11}B(\text{Eind})$ determined using single-crystal neutron diffraction (50% probability ellipsoids). Eind is a large hydrocarbon molecule used to stabilise the compound.

Influence of lone-pair cations on the germanate anomaly in glass

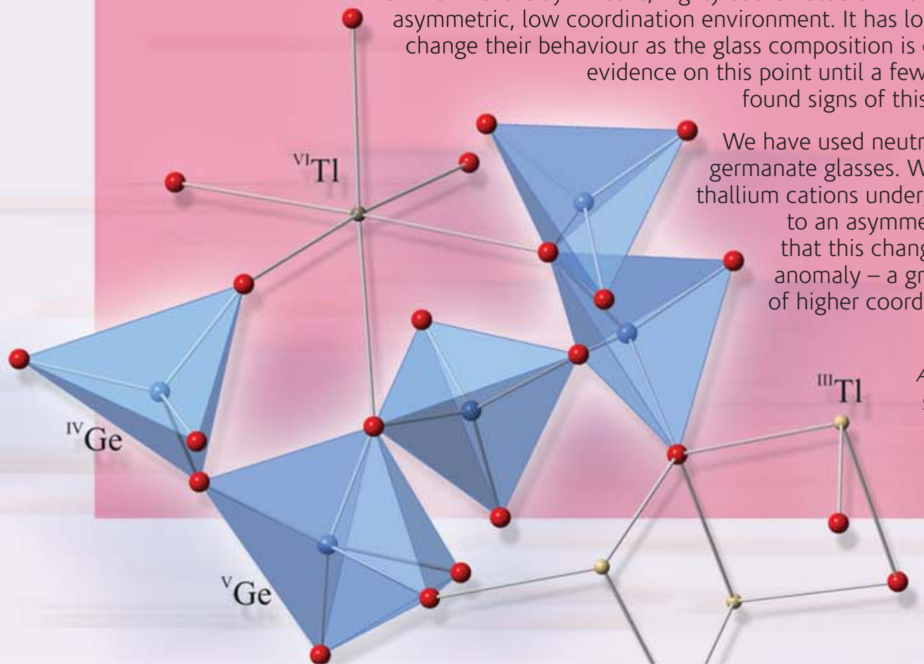
ER Barney, AC Hannon (ISIS), N Laorodphan, D Holland (University of Warwick)

Contact: Dr ER Barney, emmacruddace@gmail.com

Further reading: ER Barney et al., J. Phys. Chem. C in press (DOI: 10.1021/jp202279b)

Lone-pair cations in glasses are important due to the strong non-linear optical properties which they impart to the glass. Cations with a non-bonding (lone-pair) of electrons, such as lead or thallium, can adopt two different types of environment: a symmetric, highly coordinated environment, or a much more optically active, asymmetric, low coordination environment. It has long been believed that lone-pair cations change their behaviour as the glass composition is changed. However, there has been little evidence on this point until a few recent studies which have mostly not found signs of this.

We have used neutron diffraction to study a series of thallium germanate glasses. We have shown firstly that the lone-pair thallium cations undergo a change in behaviour from a symmetric to an asymmetric environment. Secondly, we have shown that this change is associated with the germanate anomaly – a growth and subsequent decline in the number of higher coordinated germanium ^{V}Ge sites in the glass.



A fragment of the network in a thallium germanate glass

Low energy spin-gap studies of $LiErF_4$

N Nikseresht (EPFL, Switzerland), B Dalla Piazza, HM Rønnow (Ecole Polytechnique Federale de Lausanne), R Bewley, J Taylor (ISIS), C Kraemer (ETH-Zurich)

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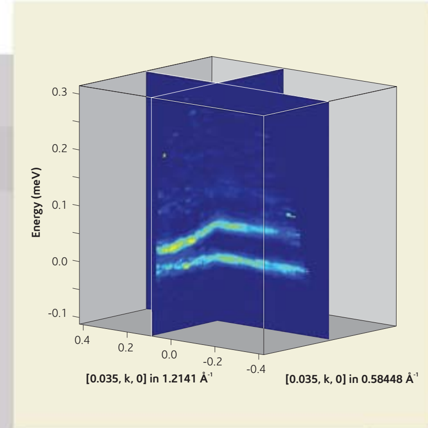
Further reading: C. Kraemer Phd Thesis ETH-Zurich 2009 (http://infoscience.epfl.ch/record/144121)

Arguably the most fundamental collective physics problem in magnetism is that of interacting dipoles. Yet investigations of antiferromagnetic dipolar-coupled magnets have been scarce due to lack of materials exhibiting this property and due to the low energy scale involved.

We have established the material $LiErF_4$ as a dipolar antiferromagnet exhibiting both classical and quantum phase transitions. The excellent resolution of the new Let instrument on the ISIS Second Target Station has allowed direct observation of the full pattern of magnetic interactions in the material, including accurate measurement of a tiny 25 μeV energy gap. The excellent signal and low background allowed full 4-dimensional datasets (3 momentum directions and one energy axis) to be recorded. While detailed analysis and a follow-up experiment are still ongoing, the results so far are providing detailed information on the nature of the phase transitions and how the behavior of $LiErF_4$ is linked to that of other materials. The excellent instrument resolution and high flux of Let open a new range of low energy scales that can be exploited by neutron spectroscopy to address fundamental questions in quantum physics.



3D image of part of the 4D data set at low temperature. The spin gap has a minimum at the high symmetry point (0 0 1). The spectra is essentially dispersionless along the (0 K 0) within the covered space (40% of a unit cell).

Mapping out a quantum spin liquid

FL Pratt, PJ Baker (ISIS), SJ Blundell, T Lancaster (Oxford), S Ohira-Kawamura (J-PARC), C Baines (PSI), Y Shimizu (Nagoya), K Kanoda (Tokyo), I Watanabe (RIKEN), G Saito (Kyoto)

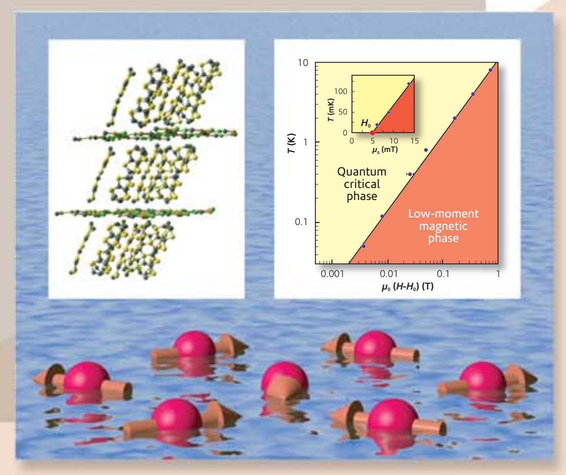
Contact: Dr FL Pratt, francis.pratt@stfc.ac.uk

Further reading: FL Pratt et al., Nature 471 (2011) 612

In magnetism, the idea of a quantum spin liquid phase has fascinated theoretical and experimental physicists for many decades. In such a phase, the ordered magnetic state, as usually found in systems of interacting magnetic spins, is completely absent due to the destabilising effect of strong quantum fluctuations.

Although the idea of the spin liquid is quite old, it is only recently that experimental systems have become available that show all the hallmarks of such a state. This is particularly the case in materials containing triangular lattices of spin-1/2 molecular radical dimers. One such system, κ-$(ET)_2Cu(CN)_3$, has been the focus of intense study since its discovery a few years ago. Muons provide an exquisitely sensitive local probe of magnetic properties. Recent muon experiments at ISIS show that a weak magnetic phase can be recovered from the spin-liquid phase using a very small magnetic field.

The ordering expected for a triangular lattice S=1/2 Heisenberg antiferromagnet (background). Left: the κ-$(ET)_2Cu_2(CN)_3$ spin liquid. Right: field-induced recovery of its suppressed magnetism.



Quantum Matter 2

'More is Different' – PW Anderson

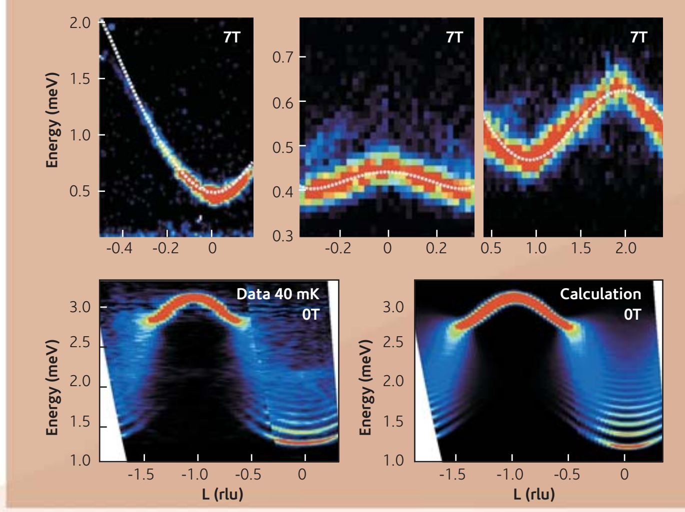
Let probes excitations in a quantum Ising chain

IM Cabrera, R Coldea (Oxford University), R Bewley, J Taylor (ISIS), D Prabhakaran (Oxford Univesity)

Contact: Dr R Coldea, r.coldea@physics.ox.ac.uk

Further reading: R Coldea et al., Science 327 (2010) 177

The newly commissioned Let spectrometer on the ISIS Second Target Station, combined with the vertical-opening 9 T magnet and dilution refrigerator insert, offers unparalleled opportunities for probing atomic dynamics with high resolution and wide coverage in all three momentum directions.



We have used Let to explore the magnetic behaviour in $CoNb_2O_6$. We recently showed this material to be the first experimental realization of the much theoretically-studied Ising chain in transverse field. Here 'quantum melting' of order occurs above magnetic fields of 5.5 T, in which spontaneous long-range order is replaced by a gapped 'quantum paramagnet.' We have probed the magnetic behaviour in this high-field phase at 7 T along both interchain crystal directions and confirmed a model of frustrated interchain couplings. Knowing the strengths of these couplings is important as they are responsible for the formation of a 'Zeeman' ladder of confined bound states in zero field.

Top: Magnetic behaviour at 7 T along the chain and two inter-chain directions measured on Let. Dashed lines show behaviour expected for a model of frustrated interchaing couplings. Bottom: 'Zeeman' ladder of bound states in zero field measured on Iris.

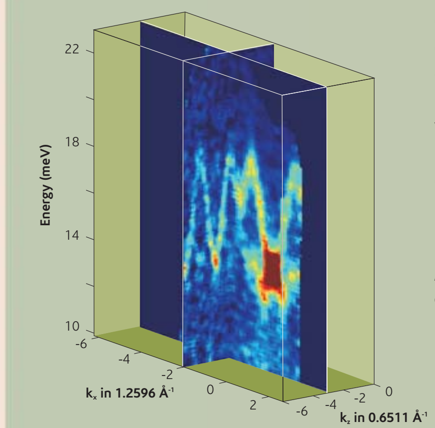
Using neutrons to probe electron clouds in crystals

MD Le (Helmholtz Center Berlin), KA McEwen (University College London), J Jensen (University of Copenhagen), M Rotter (Max-Planck Institute Dresden), RI Bewley, T Guidi (ISIS)

Contact: MD Le, e-mail: duc.le@helmholtz-berlin.de

Further reading: MD Le et al., submitted to J. Phys.: Condens. Matt. (2011).

Contrary to the popular view that an electron is a ball-like particle orbiting the nucleus, quantum mechanics dictates that it ought to be described in terms of a spatial probability distribution – a charge cloud, rather than a rigid ball. The shape of such a charge cloud is uniquely defined by its orbital angular momentum, and can be conveniently decomposed into different multipoles (e.g., monopole, dipole, quadrupole, …). In general, electron clouds around different atoms are not correlated, but in certain ordered compounds they are. As neutron scattering relies on the constructive interference of rays scattered from an ensemble of many atoms, only such compounds are amenable to study. Further, the shape of a given electron cloud can also change with time, and its temporal evolution can be probed via inelastic neutron scattering. The accompanying figure shows data from a quadrupole-ordered UPd_3 crystal measured on the Merlin spectrometer. From an analysis of the energy- and momentum-transfer dependence of the scattered intensity, it is possible to deduce how electron clouds around particular atoms evolve in time.



Left: measured UPd_3 dispersion relations at T=3.5 K. Below: time-resolved snapshots of the electronic charge distribution associated with the intense inelastic mode around 14 meV.

ISIS helps UK magnesium producer with a cracking problem

M Turski (Magnesium Elektron, Manchester, and Open University), AM Paradowska, S-Y Zhang (ISIS), D Mortensen, H Fjaer (Institute for Energy Technology, Norway), J Grandfield (Grandfield Technology Pty Ltd, Australia), B Davis, R DeLorme (Magnesium Elektron North America, Madison, USA)

Contact: Dr. M Turski, Mark.Turski@magnesium-elektron.com

Further reading: M Turski et al., submitted to Metallurgical and Materials Transactions A (2011)

Direct chill (DC) cast slab being positioned on Engin-x.

Scientists from ISIS have worked in partnership with UK company Magnesium Elektron to solve manufacturing challenges.

Magnesium Elektron is a world leader in magnesium technology and alloy development. The company, who first produced magnesium in Manchester in 1936, specialises in the development, manufacture and supply of magnesium products to technology industries worldwide. Their alloys are extensively used for applications in the aerospace and automotive industries.

"Magnesium is 30% lighter than aluminium, and therefore it could be used for components in the transport industry to help reduce emissions. For magnesium to be a financially viable alternative to aluminium, we need to be able to mass produce it. However, we were unable to mass produce it as large slabs because they cracked during casting," explained Dr Mark Turski, a senior metallurgist at Magnesium Elektron.

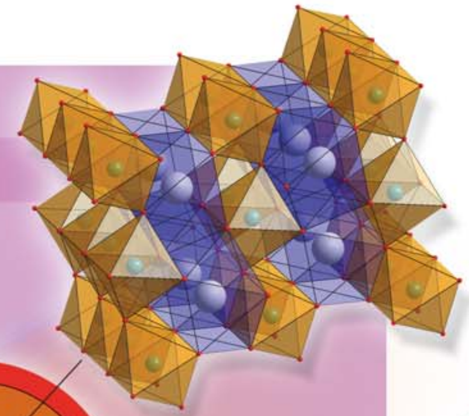
The company used Engin-X, the engineering beamline at ISIS, to examine the residual stress in large magnesium alloy slabs that caused the cracking. Using neutrons, scientists from Magnesium Elektron were able to build up an accurate picture of where the strain and stress were within the casted slabs.

Understanding the deep Earth

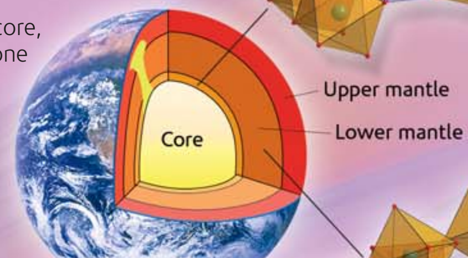
A Lindsay-Scott, IG Wood, DP Dobson, L Vočadlo, JP Brodholt (University College London), T Taniguchi (National Institute for Materials Science, Japan), KS Knight, MG Tucker (ISIS)

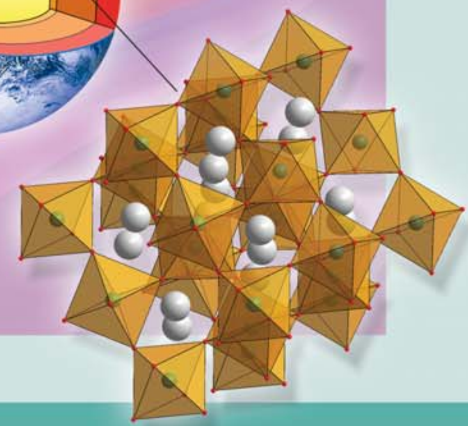
Contact: Dr I Wood, ian.wood@ucl.ac.uk

Further reading: Lindsay-Scott et al., Phys. Earth. Plan. Int. 182 (2010) 113



At the bottom of the Earth's lower mantle and just above the liquid outer core, there is a ~300 km thick region termed the D''-zone. Although thin, this zone plays a crucial role in Earth's evolution as it regulates heat exchange from the metallic core to the silicate mantle and is the source of plume-style mantle convection. D'' is associated with a change in crystal structure of $MgSiO_3$ perovskite – the major mineral in the lower mantle – to a denser 'post-perovskite' form. Post-perovskite $MgSiO_3$ is stable only at million-atmosphere pressures and so it is impossible to measure directly many of its physical properties. Instead, measurements must be made on other materials with the same structure and combined with computer simulations to estimate values for the D'' $MgSiO_3$ structure. Our experiments at ISIS on $CaPtO_3$, one of very few post-perovskites stable at atmospheric pressure, show that its structure responds to temperature differently from $MgSiO_3$ and so it may not be a suitable substitute. The search for good post-perovskite analogues must, therefore, continue.





The structure of the deep Earth and the D'' region between lower mantle and core. Post-perovskite $MgSiO_3$ in D'' consists of layers of octahedra and hendecahedra. In the lower mantle, $MgSiO_3$ is made up of corner-linked octahedra.

Materials and technologies

'Nothing tends so much to the advancement of knowledge as the application of a new instrument' – H Davy

Magnetic imaging using a time of flight neutron beam

Dr A S Tremsin (University of California at Berkeley), Dr M Strobl (Hahn-Meitner-Institut), Dr C J Kinane, (STFC), Dr S Boag (STFC), Dr R M Dalgliesh (STFC), Dr J Kelleher (STFC)

Contact: Dr A S Tremsin (ast@ssl.berkeley.edu), Dr C J Kinane (christy.kinane@stfc.ac.uk)

Further reading: A. S. Tremsin et. al., in print, Nucl. Instr. and Meth. A. 652 (2011) 400.

The recent development of fast, highly pixelated neutron detectors capable of performing transmission radiography at a pulsed source, along with ^{3}He spin filters, has opened up a number of interesting new possibilities in polarised neutron imaging from magnetic materials. For instance, by combining the inherently good energy resolution of a time of flight (TOF) instrument at a pulsed source with high spatial resolution it is possible to perform detailed structural and compositional analysis of complex materials. By the addition of neutron polarisation (provided by polarised ^{3}He spin filters) it also becomes possible to directly image magnetic flux both in vacuum and within materials, akin to using the neutrons as iron filings to show magnetic field patterns. The additional image contrast observed in polarized neutron imaging results from the precession of the neutron spin in a magnetic field, e.g. within the sample. The amount of rotation depends on the wavelength of the neutron. The good wavelength resolution of a pulsed neutron source (<0.1% $\Delta\lambda/\lambda$) should produce better resolution than that of a reactor (>1% $\Delta\lambda/\lambda$). The Crisp reflectometer was used to demonstrate that polarised neutron imaging can be performed at ISIS with these advantages of the TOF technique.

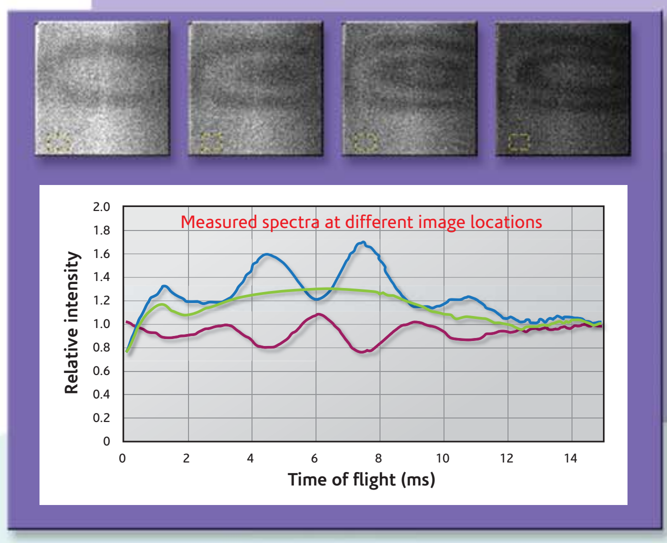


Image of measured intensity variation caused by neutron precession in the magnetic field of a simple DC coil. The coil is oriented horizontally along the fringes. The variation of image intensity is shown as a function of TOF (wavelength) for three regions of interest. This can be used to reconstruct the magnetic field of the coil.

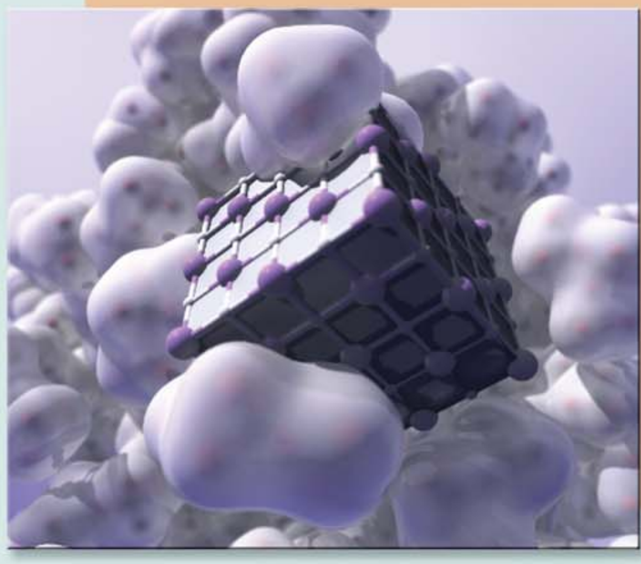
Neutron Compton scattering in moderate-mass systems

AG Seel, A Sartbaeva, PP Edwards (University of Oxford), J Mayers, AJ Ramirez-Cuesta (ISIS)

Contact: Prof. PP Edwards, peter.edwards@chem.ox.ac.uk

Further reading: AG Seel et al., J. Chem. Phys. 134 (2011) 114511

This study suggests for the first time that the technique of neutron Compton scattering (NCS) may be extended beyond the study of the lightest elements (such as H or He isotopes) to provide additional information about the profile widths of heavier nuclei in complex systems. If the relative stoichiometry of heavier elements in a material is known, fixing it in the standard Vesuvio data-analysis procedures enables a determination of neutron Compton widths.

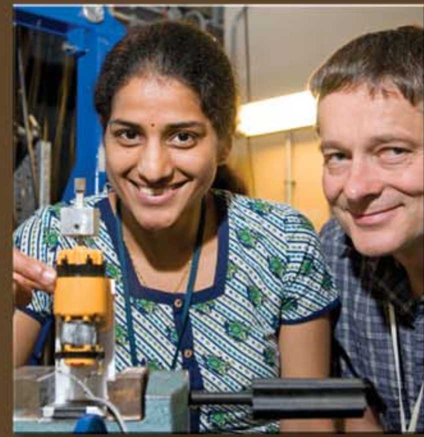


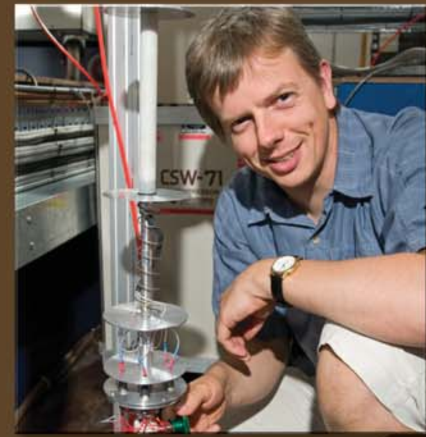
Measurements were conducted on three systems: bulk NaH, amorphous Na within a silica gel framework (SiGNa), and a system with both amorphous Na and NaH nanocrystallites encapsulated in the framework (SiGNaH). In addition to subtle differences in the proton momentum distribution in NaH and SiGNaH, a systematic increase in Na Compton widths is demonstrated in SiGNa, SiGNaH and bulk NaH. This sensitivity to chemical environment is further supported by examination of O and Si widths in the gel samples.

NaH nanocrystallites (or amorphous Na) can be encapsulated in a silica gel framework, and studied by neutron Compton scattering.

Right: Anton Tremsin (University of California) developing high resolution Bragg edge time of flight transmission detectors on Engin-x.

Below: Edward Bilbe, Elena Marelli, Ann Chippindale and Simon Hibble (Reading University) studying structure-property relationships in photoluminescent platinum and palladium cyanides on Gem.





Above: Yasuhtro Takabayashi and Ruth Zadik (University of Durham) using muons to study magnetism and superconductivity in hyper expanded fullerides.

Above centre: Anusha Kankanale and Jon James (Open University) using Engin-x to explore the effects of post-weld heat treatment on a dissimilar metal butt weld.

Above right: Jon Duffy (University of Warwick) investigating the dynamics of confined CO_2 on Mari.

Left: Stephen Gaw (university of Oxford) using Merlin to investigate the origin of high-temperature magnetoelectricity in CuO.

Left: Robbie Warringham (University of Glasgow) using Maps to improve understanding of the active phase of iron-based Fischer-Tropsch catalysts.

Below: Fabio Bruni (University of Rome), Katrin Winkel (University of Innsbruck), Alessia Giuliani (University of Rome) and Mark Adams (ISIS) using Vesuvio to study the environment of water protons in amorphous ices.

ISIS users at work

Tristan Youngs and John Holbrey (Queens University, Belfast) using Sandals to conduct studies on the hydration of the nootropic drug piracetam.

Nancy Ross (Virginia Tech, USA) determining the thermodynamic properties of the hydration layers on porous alumina nanoparticles using Tosca.

Technology development at ISIS is a continuous process, driven in response to the changing scientific 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.

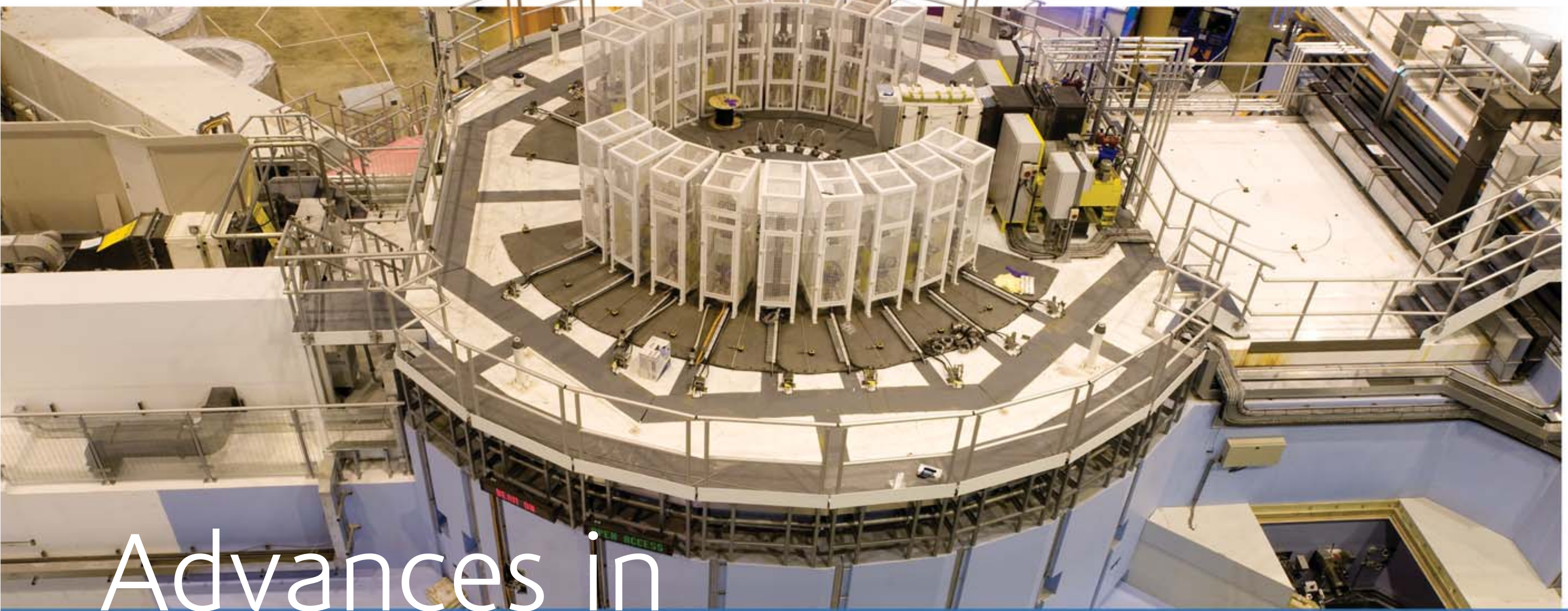
The past year has seen work starting on four new instruments for the Second Target Station. In addition, a huge amount of work was carried out across ISIS during the planned maintenance shut-down at the end of 2010. Alongside technical developments comes a wide range of other activities – science workshops, training courses, user meetings, public understanding of science events, schools visits – to name but a few.

Technology and training

Rachel Evans (Trinity College, Dublin) preparing samples to study the controlled assembly of cationic polythiophene-surfactant complexes on Loq.

From Phase One to Phase Two!

Alongside the seven instruments that are up and running on the ISIS Second Target Station, construction has started on four new ‘Phase 2’ instruments following the announcement of funding by David Willetts MP, Minister for Universities and Science, in March. Chipir, Larmor, Zoom and Imat will all be built over the next few years.

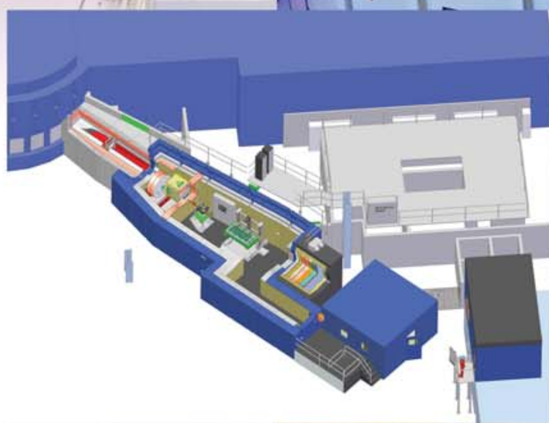


Advances in instruments and techniques

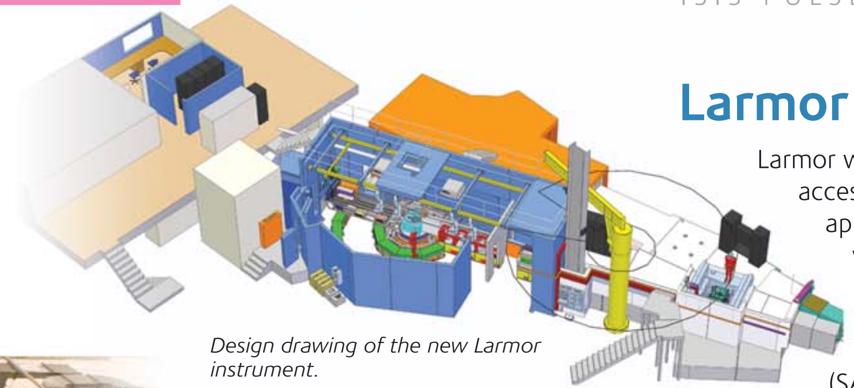
Chipir

Concrete shielding for Chipir, an instrument designed to look at the effect of cosmic radiation on microchips, has been manufactured and installed this year. This shielding stops stray neutrons from the instrument entering the experimental hall, and creates a platform on which Chipir will be placed.

Chipir will be one of only a handful of facilities outside of the US capable of looking at the response of silicon microchips to cosmic radiation. Cosmic radiation has the power to cause the failure of critical electronic systems such as those found in aircraft and road vehicles. The new neutron beam line will replicate the cosmic radiation that can affect microchips. The findings will help manufacturers build more reliable electronic systems for use in cars, planes and other devices.



Right: Beginning of the construction of the Chipir beamline.
Above: Design drawing of Chipir.



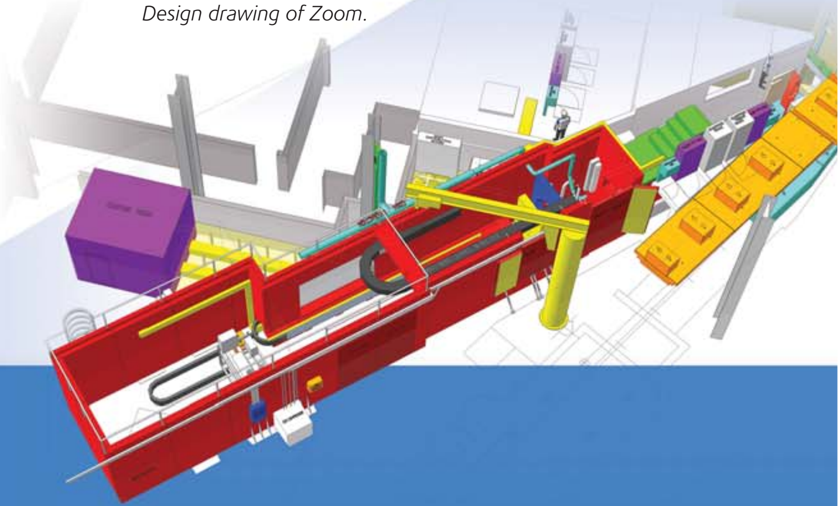
Design drawing of the new Larmor instrument.

Larmor

Larmor will extend both the spatial and temporal ranges accessible to the neutron technique and is particularly applicable to soft matter and biomolecular science. It will exploit the Larmor precession of the neutron spin to deliver a suite of techniques extending those presently available at ISIS. Larmor will initially be used for small angle neutron scattering (SANS) with polarisation analysis, spin-echo SANS and Larmor diffraction, but additional operational modes will be made available as the instrument develops. Detailed instrument design is now underway, and component procurement has started.

Zoom

Zoom will be a flexible, high count rate small-angle scattering instrument ideally suited for kinetic and dynamic experiments. Additionally, it will allow for grazing incidence techniques to study surface structures and will be able to polarise neutrons for studies of magnetic materials. It will be the first ISIS instrument to use focusing, which, when coupled with a high resolution, two dimensional detector, will enable us to reach very small Q, ~ 0.0003 $Å^{-1}$ (~ 2 μm) with a wide simultaneous Q range out to at least ~ 0.15 $Å^{-1}$. Stage 1 of the design, a highly flexible small angle instrument, is presently underway.



Design drawing of Zoom.

Imat

Imat is a neutron imaging and diffraction instrument for materials science. The instrument will offer a combination of possibilities such as neutron radiography, neutron tomography, energy-selective imaging, neutron strain scanning and texture analysis. The combination of these analytical techniques on the same instrument is unique and will allow new types of experiments to be carried out. For example, residual stresses inside engineering-sized samples can be more effectively analysed if the diffraction scans are guided by radiographic data. Conversely, diffraction analysis may be indispensable for a quantitative analysis and physical interpretation of the attenuation features observed in radiography data. Imat will have a straight neutron guide to transport the neutrons to an aperture selector giving a maximum field-of-view of 20 x 20 cm^2 at a sample position at 56 meters from the moderator.

The new Imat instrument.

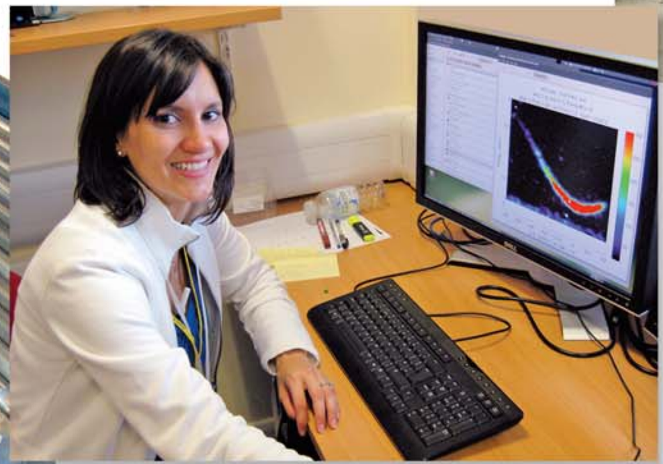
Advances in instruments and techniques

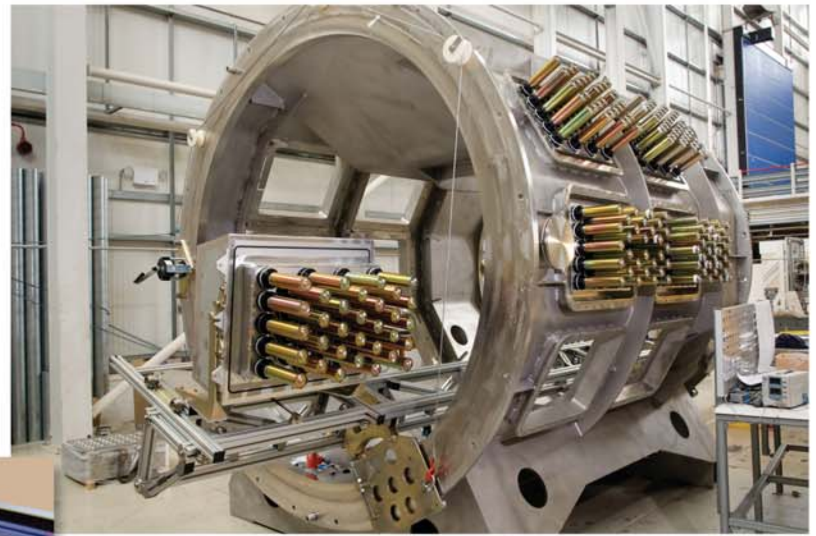
First user experiment on Let

Radu Coldea and Ivelisse Cabrera (Oxford University) were the first scheduled users on the new Let spectrometer on the Second Target Station. A single crystal of $CoNb_2O_6$, a quasi-one-dimensional Ising ferromagnet, was mounted on a rotation stage in a dilution fridge at 50 mK in the new 9T magnet which was designed specially for Let. This was therefore a complex experiment, but it was very successful nevertheless – see highlight on page 16.

Left: Construction of the 4m long position-sensitive detectors for Let.

Below: Ivelisse Cabrera (Oxford University) during the first scheduled experiment on Let.





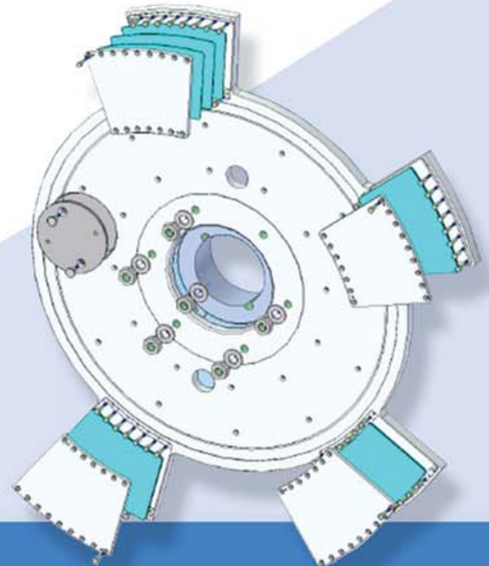
Polaris

The upgrade of the Polaris instrument is nearly completed, and commissioning experiments are planned to begin towards the end of 2011. When finished, 38 modules of fibre-coupled scintillation detectors will contain some 400,000 m of fibre optic light guides and will give Polaris a count rate up to 20 times higher than the old instrument. New opportunities in the study of disordered and nanostructured materials, in-situ investigations of chemical and electrochemical reactions and texture measurements of historical artefacts will become routinely available.

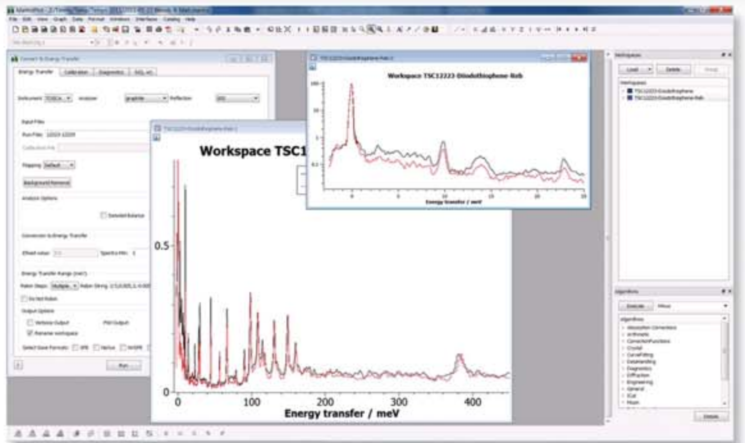
The new Polaris tank being fitted with detectors.

TOSCA Chopper Upgrade

With a new disc chopper running at 10 Hz, the energy-transfer range on Tosca has been extended below 3 meV. This development provides new scientific opportunities, particularly in the study of the interplay between low-energy excitations and molecular mobility in a wide range of applied systems (hydrogen storage, catalysis, proton conductors, soft nanocomposites, etc). It also provides a direct link to quasielastic studies on Osiris and Iris.



The new, four-bladed Tosca chopper.



The new Mantid interface showing data analysis and visualisation on Tosca.

Mantid goes International

Mantid is a data analysis framework and application to support the neutron and muon communities. The project started as a joint collaboration between ISIS and Tessella, and has now grown to include the SNS and HFIR facilities at the Oak Ridge National Laboratory (ORNL). In the last 12 months the data reduction for direct and indirect-geometry spectrometers has been moved to operate within the Mantid framework, so that, for example, Iris, Osiris and Tosca data can be fully reduced using Mantid.

Polarisation

This year saw a significant milestone in the ISIS polarized neutron project – the first wide-angle polarised neutron measurement ever performed at ISIS. A full polarisation analysis measurement of silicon powder was performed on the Wish diffractometer on the Second Target Station, using the new uniaxial field-coil polarized neutron insert. The flipping ratios of the silicon Bragg peaks (the ratio between spin-up and spin-down scattered neutrons) gives a measurement of the polarisation of the beam.

With the delivery of the ISIS ^3He ‘filling station’ at the end of 2011, polarised neutrons will be available on both Wish and Let in the coming year.

Stephen Boag (ISIS) craning the polarisation field-coil insert into the Wish diffractometer.

Pearl

Over the past year the high-pressure diffraction facility at ISIS (Pearl) has undergone a major upgrade to improve the diffraction data resolution and detector stability while maintaining as large as possible incident flux and d-spacing range. All of the detectors have been replaced, with the new modules incorporating the latest design of ZnS scintillator detector element. The commissioning trials conducted so far have demonstrated the anticipated resolution gains very well. The Pearl upgrade work has been part-funded by the Spanish government via the CSIC research council in partnership with Spanish companies AVS and Scientifica.

Geoff Eacott (ISIS) working on the Pearl detector banks.

The past year saw an extended maintenance shutdown for ISIS, from August 2010 to February 2011. The shutdown was necessary to replace a wide range of ageing ISIS equipment and components, many of which were installed over 25 years ago. Two major projects were carried out: refurbishment of part of the proton beamline for ISIS Target Station 1, and replacement of heavy-duty electrical cable for the accelerator magnets. In addition, some 700 smaller tasks were also completed: around 200 tasks on the accelerators, 200 on the neutron target systems and 300 on the neutron beam lines and instruments, including major rebuilds of Pearl and Polaris.

Accelerator and target news

Refurbishment of the proton beamline to Target Station 1

After 25 years of being bombarded by high energy protons, the proton beam exit window in front of the neutron target in target station 1 had become weak. During the six month shutdown, nearly 60 people worked on the project to replace the window.

The refit was planned in great detail over several years since special long-reach tools, machines and shielding flasks had to be designed and constructed, movable thick steel shields had to be deployed, and rehearsals of the whole refurbishment were made using a full-scale mock-up of the work area. The project involved removing the layers of concrete and steel shielding above the proton beam, a 4-week task in its own right.

In addition to replacing the proton beam window, three new quadrupole magnets were also installed, replacing older magnets and providing additional control for the proton beam.

Inset: The team who worked on the Target Station 1 proton beamline refurbishment. The three new quadrupole magnets can be seen in the foreground.

Right: Adrian Hooper and Steve Cook working on remote tooling for the proton beamline refurbishment.

Second Target Station target

The long shut-down also saw replacement of the target in TS-2. A revised design with improved cooling based on experience of operating the target since TS-2 began running was installed. The new target was designed and manufactured within 8 months – a big achievement.

Finite element modelling of heat flow in the new TS-2 target, near right, together with an initial target mock-up, far right.

Rewiring the ISIS synchrotron

Also during the long shutdown, over 2km of heavy-duty power cables were replaced in the ISIS synchrotron accelerator. The cables deliver rapidly-varying currents up to 1000 amps to the bending magnets controlling the proton beam path.

A ring of 10 bending magnets in the ISIS synchrotron keeps the proton beam within the evacuated beam tube as it is accelerated. As the beam gets faster during acceleration, the current in the magnets is increased to give the larger and larger magnetic fields needed to keep the beam following the correct path.

The power cables for the magnets were originally installed in the 1980s. The cables were jointed, and over the past two years joints have begun to fail more and more frequently. To improve performance, the entire cable installation was replaced with single continuous cable runs – a job involving many weeks of specialised work removing heavy cables, each 4 cm in diameter.

Adrian McFarland (ISIS) in the inner synchrotron during the recabling work.

Accelerator and target news

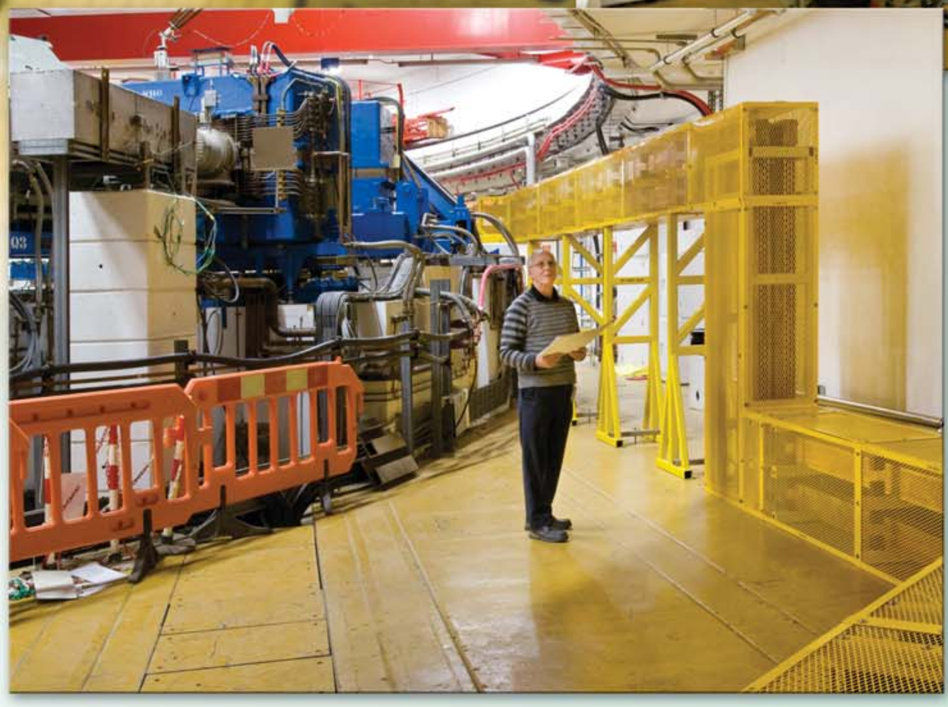
The ISIS synchrotron accelerator is a complex machine requiring people with different areas of expertise to maintain, operate and develop it. Seen here are members of the synchrotron group.

Left: Hayley Smith, from the Synchrotron Physics group, was awarded second place at this years 'Present Around the World (PATW)' competition, for her outstanding presentation on foil studies. PATW are technical competitions in which students and young professionals give a ten minute presentation on an engineering or technology subject of their choice. Having won the local and regional heats, Hayley presented her stripping foil studies at the national final in Birmingham in July and won second place. Stripping foils are used in the ISIS synchrotron to convert H^- ions to protons.

Synchrotron magnet replacement

From time to time the main bending (dipole) magnets in the ISIS synchrotron accelerator are replaced. This involves splitting a magnet in half and refitting new upper and lower coils as well as cleaning up the yoke and laminations.

Above: Jamie Searis, Steven Cook, Adrian Hooper and Oliver Newell (ISIS) working on the lower coil during replacement of a synchrotron dipole magnet.



Right: New extract and injection septum magnet busbar system for the ISIS synchrotron.

Right: Installation of new synchrotron steering magnet and trim quadrupole power supplies in the ISIS inner synchrotron. The new power supplies are capable of delivering a higher current output and a programmed current waveform with a slew rate of 300,000 Amps per second, twice that of the existing units.

A year around ISIS

Condensed Matter in the City meeting held at ISIS

Above: Attendees at the meeting on Magnetism and Strongly Correlated and Interacting Electron Systems, RAL, June 16-17.

The Centre for Materials Physics and Chemistry at STFC, together with the Hartree Centre and Hubbard Theory Consortium, held a two-day workshop at RAL in June. There was a wide range of talks from researchers from the UK, Europe and further afield. The meeting was part of the South East Physics Network (SEPNet) summer programme 'Condensed Matter Physics in the City', focused on stimulating discussions between theorists and experimentalists in the field of magnetism and strongly correlated and interacting electron systems.

Attendees at the Large Scale Structures User Group Meeting held at Cosener's House 24-25th January. The meeting included talks, posters and a discussion session.

Above: Prof Stephen Bennington from ISIS, Chief Scientific Officer for Cella Energy, showing a Cella Energy storage device.

Cella Energy Ltd

Cella Energy is a spin-out from ISIS. The company has already gained major investments from specialist chemical company Thomas Swan & Co Ltd., who signed an agreement on 24 January 2011, and Space Florida who have led further investments of $2.5m. Cella Energy has developed a novel technology that allows hydrogen to be stored in a cheap and practical way, making it more suitable for widespread use as a carbon-free alternative to petrol.

ISIS scientist wins neutron prize for novel nanoscience technique

Rob Dalgliesh from ISIS has been awarded the prestigious BTM Willis Prize for neutron scattering. This is in recognition of his development of novel neutron techniques that are opening up new areas of fundamental and applied research in nanoscience. The prize is awarded bi-annually by the Neutron Scattering Group of the Institute of Physics (IOP) and the Royal Society of Chemistry (RSC). Rob has pioneered a new instrument called Offspec, one of the instruments on the ISIS Second Target Station. It is designed to look at microscopic structures such as those found in polymer blends (plastics) and surfactants (soaps and detergents). *Right: Robert Dalgliesh receives the Willis Prize from Dr Ali Zarbakhsh.*

Faraday Discussion 151: hydrogen storage materials

Organised by the Faraday Division of the Royal Society of Chemistry and supported by ISIS, this Discussion was held at RAL in April and attracted 115 participants from 10 countries. It focused on hydrogen storage for fuel applications, and included discussion of adsorption and reaction of hydrogen by materials, from synthesis to characterisation.

Above: Faraday Discussion 151 on hydrogen storage materials was held at RAL in April.
Image courtesy of Pacific Northwest National Laboratory, USA.

Neutron Training Course

The ISIS neutron training course was held in May. The course is aimed at researchers new to neutron scattering (mainly 1st year PhD students) and provides practical experience of the set-up and running of the full suite of neutron instruments at ISIS. In addition the students receive lectures in the technique of time-of-flight neutron scattering, and learn about the production of neutrons at a spallation source. This year 25 participants attended the 8-day course.

Right: Students at the 2011 ISIS Neutron Training Course.

Students from Reading Blue Coat School have been working with ISIS scientist Johnny Boxall on neutron detector technology. This pairing is part of the nationwide Engineering Education Scheme, which matches scientists and engineers with students from local schools. The AS level students were asked to examine alternatives to photomultiplier tubes, part of the detection system in some instruments at ISIS. The students wrote a report about their findings and had to present their research at the Engineering Education Scheme Celebration Day at RAL. All four pupils are now determined to apply to engineering courses at university.

A year around ISIS

ISIS represented at The Big Bang 2011

The Big Bang 2011 is one of the UK's biggest science events for young people celebrating science and engineering, with over 20,000 people attending. The theme of the ISIS stand at the 2011 event, held in London, was low carbon energy. The stand featured mini hydrogen-powered cars and an array of novel hydrogen storage material samples, with experts from ISIS and Cella Energy on hand to answer visitors' questions.

Left: Visitors to ISIS' Big Bang exhibition learning about hydrogen-powered cars.

Right: Chinese steel company, Baoshan Iron and Steel Co., Ltd (Baosteel Co,.Ltd), visited ISIS in June. Vice President Jianfeng Zhou, together with Pijun Zhang, Xiuzhen Lin, Laizhu Jiang, Hongzhi Shi and Yang Zhao were joined by Prof Yulong Ding (University of Leeds) and Dr Hongbiao Dong (University of Leicester). The visit was hosted by Robert McGreevy (ISIS) and Shu Yan Zhang, instrument scientist on the ISIS Engin-x engineering beamline.

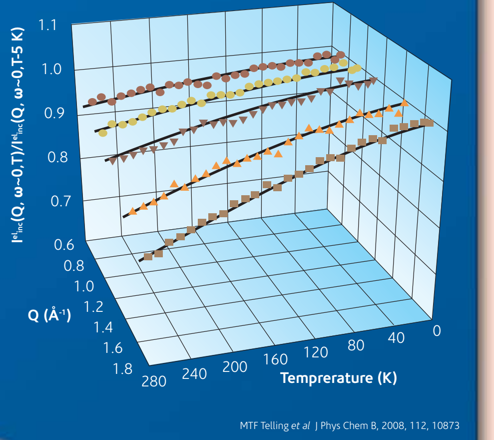
Above: ISIS presented the operating and phase 2 Second Target Station instruments at the European Conference on Neutron Scattering held in Prague in May. Here we see the ISIS team demonstrating complex scattering experiments to delegates.

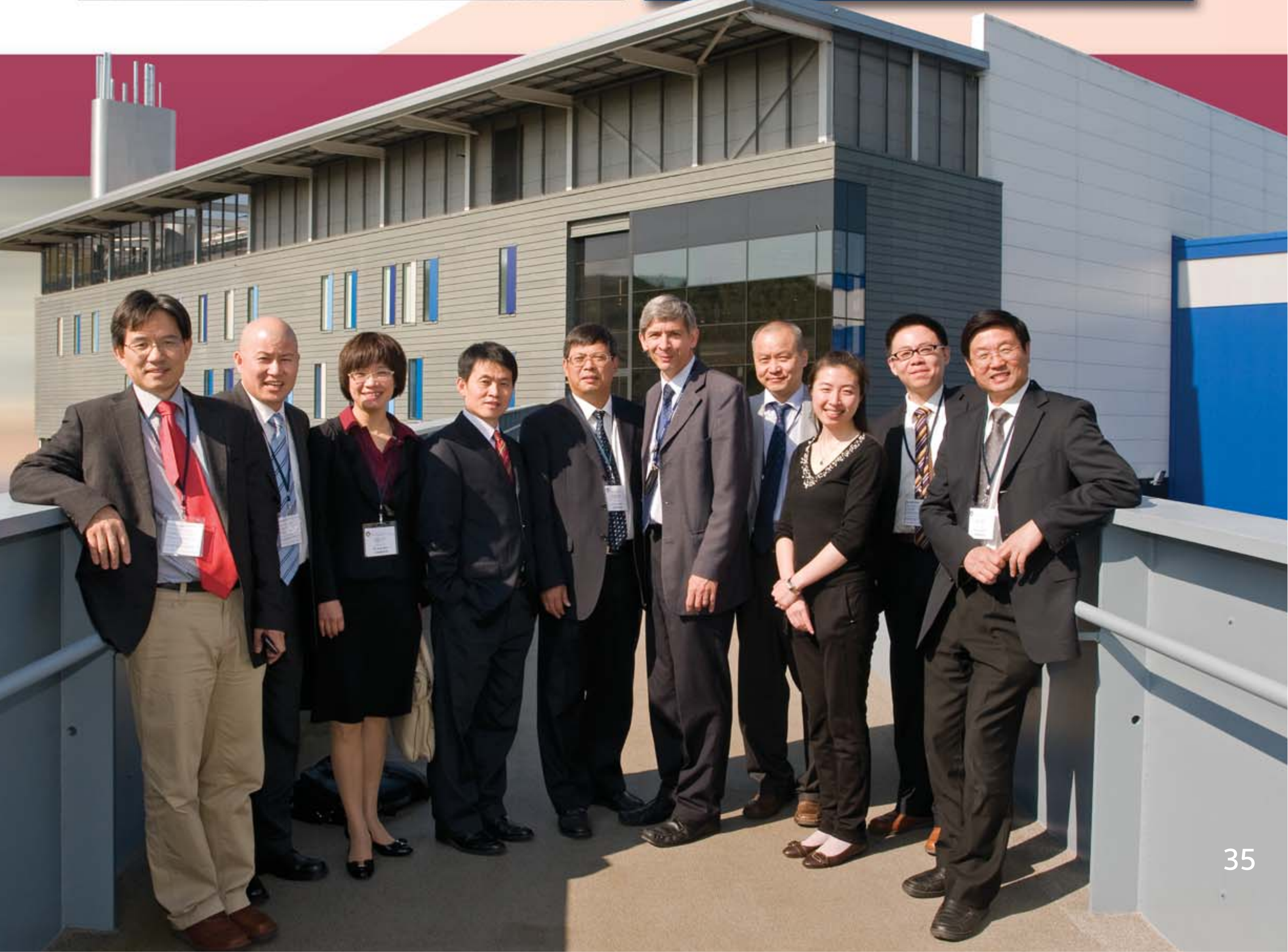
Below: Students attending the RAL Particle Physics Masterclass in March being shown the ISIS Second Target Station by James Lord (ISIS).

New Xpress services

Xpress services have existed on some ISIS instruments for quite a while. They enable a 'measure-by-courier' service that is suitable when only very limited neutron time is needed or for very new or infrequent users. The Xpress services have now been broadened to include the quasi-elastic instruments (Iris and Osiris) together with the muon spectrometers. They are an ideal way to do an initial characterisation of a sample or check a sample's feasibility for future experiments. Full details can be found in the 'Applying for beamtime' section of the ISIS website.

Elastic intensity vs temperature for a dry protein measured on the Osiris spectrometer – an example of a typical measurement that can be performed via QENS Xpress.





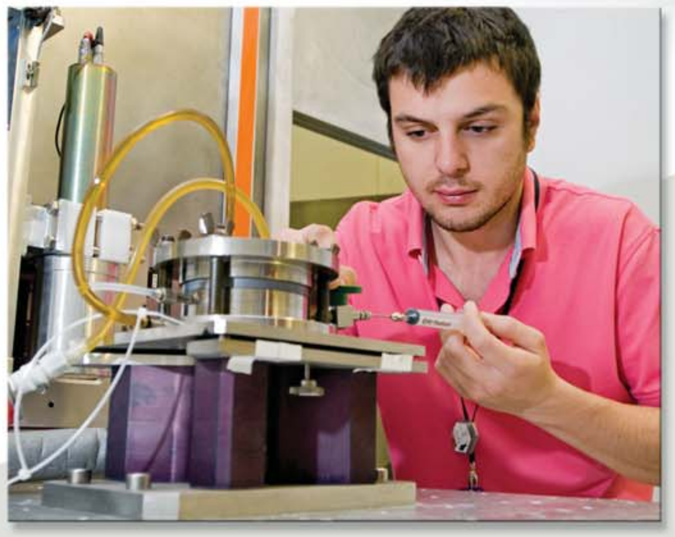
Liz Rodriguez, Lucy Rayner, Steve Perkins and Keying Li (UCL) using Sans2d to study the solution structures of immunologically important proteins.

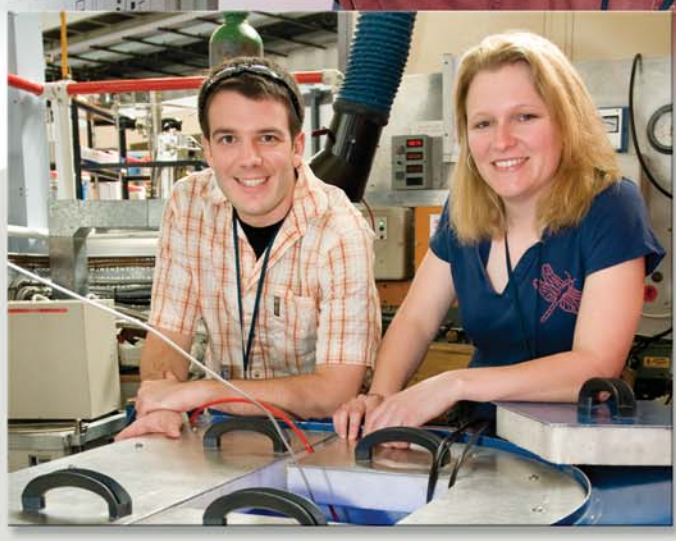
ISIS users at work

Right: Johannes Moller and Stephen Blundell (University of Oxford) exploring a field-induced spin Luttinger liquid phase in a spin ladder using HiFi.

Below right: Matt Hudson and Wendy Queen (university of Maryland, USA) conducting neutron scattering studies of hydrogen rotational transitions in metal organic frameworks for gas storage applications.

Below: Mario Campana (Queen Mary University London) using Inter to conduct a structural study of the hexadecane – water interface.





There are seven ISIS 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.

Far left: Tommy Nylander (University of Lund, Sweden) reading a proposal during the Large Scale Structures panel.

Centre left: Howard Stone (Cambridge), Anna Paradowska (ISIS) and Axel Steuer (ILL, France) considering Engineering applications.

Near left: Duncan Gregory (Glasgow) chairing the Crystallography FAP.

ISIS facility access panels (FAPs)

Far left: Isao Watanabe (RIKEN, Japan), Ian Terry (Durham), Rod Macrae (Marian College, USA) and Alan Drew (Queen Mary University London) discussing muon proposals.

Left: Des McMorrow (Univesity College London) reflecting on an Excitations proposal.

Neal Skipper (University College London) reviewing proposals with other members of the Molecular Spectroscopy FAP.

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 2010.

ISIS publications 2010

Stephen Cummings, Azmi Mohamed, Masanubo Sagisaka (University of Bristol) and Sarah Rogers (ISIS) using Sans2d for studies of surfactant modifiers of CO_2 solvent properties.

Abes M, Atkinson D, Tanner B K, Charlton T R, Langridge S, Hase T P A, Ali M, Marrows C H, Hickey B J, Neudert A, Hicken R J, Arena D, Wilkins S B, Mirone A, and Lebegue S
Spin polarization and exchange coupling of Cu and Mn atoms in paramagnetic CuMn diluted alloys induced by a Co layer
Physical Review B Vol: 82 (2010)

Abrahams I, Liu X, Hull S, Norberg S T, Krok F, Kozanecka-Szmigiel A, Islam M S and Stokes S J
A combined total scattering and simulation approach to analyzing defect structure in Bi_3YO_6
Chemistry of Materials Vol: 22 4435-4445 (2010)

Adam M S, Gutmann M J, Leech CK, Middlemiss D S, Parkin A, Thomas L H and Wilson C C
Stability and cooperativity of hydrogen bonds in dihydroxybenzoic acids
New Journal of Chemistry Vol: 34 85-91 (2010)

Adroja D T, Hillier A D, Deen P P, Strydom A M, Muro Y, Kajino J, Kockelmann W A, Takabatake Anand V K, Stewart J R and Taylor J
Long-range ordering of reduced magnetic moments in the spin-gap compound $CeOs_2Al_{10}$ as seen via muon spin relaxation and neutron scattering
Physical Review B Vol: 82 (2010)

Ahmed, H M, Mis M, El-Geassy A H A and Seetharanran S
Reduction-carburization of the oxides of Ni and W towards the synthesis of Ni-W-C carbides
Advanced Materials Forum V, Pt 1 and 2 Vol: 636-637 952-962 (2010)

Ahmed I, Kinyanjui F G, Rahman S M H, Steegstra P, Eriksson S G and Ahlberg E
Proton conductivity in mixed B-Site doped perovskite oxide $BaZr_{0.5}In_{0.25}Yb_{0.25}O_3$-delta
Journal of the Electrochemical Society Vol: 157 B1819-B1824 (2010)

Ahmed I, Kinyanjui F G, Steegstra P, Shen Z J, Eriksson S G and Nygren M
Improved proton conductivity in spark-plasma sintered cense ceramic $BaZr_{0.5}In_{0.5}O_3$-delta
Electrochemical and Solid State Letters Vol: 13 B130-B134 (2010)

Ahmed I, Rahman S M H, Steegstra P, Norberg S T, Eriksson S G, Ahlberg E, Knee C S and Hull S
Effect of co-doping on proton conductivity in perovskite oxides $BaZr_{0.9}In_{0.05}M_{0.05}O_3$-delta ($M = Yb^{3+}$ or Ga^{3+})
International Journal of Hydrogen Energy Vol: 35 6381-6391 (2010)

Ahmed R, Faisal N H, Knupfer S M, Paradowska A M, Fitzpatrick M E, Khor K A and Cizek J
Neutron diffraction residual strain measurements in plasma sprayed nanostructured hydroxyapatite coatings for orthopaedic implants
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol: 652 309-314 (2010)

Ahmed R, Faisal N, Reuben R, Paradowska A, Fitzpatrick M and Kitamura J
Neutron diffraction residual strain measurements of aluminium coatings
Journal of Physics: conference series Vol: 251 12051 1-4 (2010)

Akcora P, Kumar S K, Sakai V G, Li Y, Benicewicz B C and Schadler L S
Segmental dynamics in PMMA-grafted nanoparticle composites
Macromolecules Vol: 43 8275-8281 (2010)

Alba Venero D, Fernandez Barquin J, Alonso J, Svalov A, dez-Gubieda M L F
Magnetic disorder in nanostructured Fe_7Au_{93} films and $Fe_{14}Au_{86}$ powders
Journal of Physics: conference series vol: 200 072028 (2010)

Alberto H V, Weidinger A, Vilao R C, Duarte J P, Gil J M, Lord J S and Cox S F J
Mechanisms of electron polarization of shallow muonium in CdTe and CdS
Physical Review B Vol: 81 (2010)

Alessandroni S, Paradowska A M, Perelli Cippo E, Senesi R, Andreani C, and Montedoro P et al
Investigation of residual stress distribution of wheel rims using neutron diffraction
8th European Conference on Residual Stresses (ECRS8), Riva del Garda, Italy, 26-28 Jun 2010

Alexander G G, King S M, Richardson R M and Zimmermann H
Determination of the translational order parameter for smectic liquid crystals using small-angle neutron scattering
Liquid Crystals Vol: 37 961-968 (2010)

Allan D R, Marshall W G, Francis D J, Oswald I D H, Pulham C R and Spanswick C
The crystal structures of the low-temperature and high-pressure polymorphs of nitric acid
Dalton Transactions Vol: 39 3736-3743 (2010)

Arai T, Tani K and McGreevy R L
Reverse Monte Carlo modeling of amorphous structures in phase-change $In_{0.21}Sb_{0.79}$ thin film
Journal of Physics-Condensed Matter Vol: 22 (2010)

Arnalds U B, Papaioannou E T, Hase T P A, Raanaei H, Andersson G, Charlton T R, Langridge S and Hjorvarsson B
Magnetic structure and diffracted magneto-optics of patterned amorphous multilayers
Physical Review B Vol: 82 (2010)

Arnold D C, Knight K S, Catalan G, Redfern S A T, Scott J F, Lightfoot P and Morrison F D
The beta-to-gamma transition in $BiFeO_3$: a powder neutron diffraction study
Advanced Functional Materials Vol: 20 2116-2123 (2010)

Babkevich P, Prabhakaran D, Frost C D and Boothroyd A T
Magnetic spectrum of the two-dimensional antiferromagnet La_2CoO_4 studied by inelastic neutron scattering
Physical Review B Vol: 82 (2010)

Baikie T, Pramana S S, Ferraris C, Huang Y Z, Kendrick E, Knight K S, Ahmad Z and White T J
Polysomatic apatites
Acta Crystallographica Section B-Structural Science Vol: 66 1-16 (2010)

Baker P J, Lancaster T, Franke I, Hayes W, Blundell S J, Pratt F L, Jain P, Wang Z M and Kurmoo M
Muon spin relaxation investigation of magnetic ordering in the hybrid organic-inorganic perovskites $[(CH_3)2NH_2]M(HCOO)_3$ (M=Ni, Co, Mn, Cu)
Physical Review B Vol: 82 (2010)

Baker P J, Lewtas H J, Blundell S J, Lancaste, T, Franke I, Hayes W, Pratt F L, Bohaty L and Becker P
Muon-spin relaxation and heat capacity measurements on the magnetoelectric and multiferroic pyroxenes $LiFeSi_2O_6$ and $NaFeSi_2O_6$
Physical Review B Vol: 81 (2010)

Barbagallo M, Hine N D M, Cooper J F K, Steinke N J, Ionescu A, Barnes C H W, Kinan C J, Dalgliesh R M, Charlton T R and Langridge S
Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO
Physical Review B Vol: 81 (2010)

Barbour A M, Telling M T F and Larese J Z
Investigation of the behavior of ethylene molecular films using high resolution adsorption isotherms and neutron scattering
Langmuir Vol: 26 8113-8121 (2010)

Barcza A, Gercsi Z, Knight K S and Sandeman K G
Giant magnetoelastic coupling in a metallic helical metamagnet
Physical Review Letters Vol: 104 (2010)

Barney E R, Hannon A C, Laorodphan N, Dupree R and Holland D
A neutron diffraction and Tl-205 NMR study of the thallium germanate glass system
Journal of Non-Crystalline Solids Vol: 356 2517-2523 (2010)

Bateman J E, Dalgliesh R M, Duxbury D M, Holt S A, McPhail D J, Marsh A S, Rhodes N J, Schooneveld E M, Spill E J and Stephenson R
The FastGas detector
Nuclear Instruments & Methods in Physics Research Section a – Accelerators Spectrometers Detectors and Associated Equipment Vol: 616 59-64 (2010)

Bell A M T, Knight K S, Henderson C M B and Fitch A N
Revision of the structure of $Cs_2CuSi_5O_{12}$ leucite as orthorhombic Pbca
Acta Crystallographica Section B-Structural Science Vol: 66 51-59 (2010)

Bell C G, Breward C J W, Howell P D, Penfold J and Thomas R K
A theoretical analysis of the surface tension profiles of strongly interacting polymer-surfactant systems
Journal of Colloid and Interface Science Vol: 350 486-493 (2010)

Bennett T D, Goodwin A L, Dove M T, Keen D A, Tucker M G, Barney E R, Soper A K, Bithell E G, Tan J C and Cheetham A K
Structure and properties of an amorphous metal-organic framework
Physical Review Letters Vol: 104 (2010)

Berastegui P, Hull S and Eriksson S
A high temperature superionic phase of $CsSn_2F_5$
Journal of Solid State Chemistry Vol: 183 373-378 (2010)

Billette H, Wallraff T, Schwarz U, Smith R I and Ruschewitz U
Ternary transition metal acetylides $A_2(I)M(0)C_2$ (A(I) = K, Rb; M-0 = Pd, Pt): neutron diffraction studies and electronic properties
Zeitschrift Fur Anorganische Und Allgemeine Chemie Vol: 636 1834-1838 (2010)

Biswas P K, Balakrishnan G, Paul D M, Tomy C V, Lees M R and Hillier A D
Muon-spin-spectroscopy study of the penetration depth of $FeTe_{0.5}Se_{0.5}$
Physical Review B Vol: 81 (2010)

Blundell S J, Lancaster T, Pratt F, Baker P, Hayes W, Ansermet J, Comment A
Phase transition in the localized ferromagnet EuO probed by mu SR
Physical Review B Vol: 81 (2010)

Bocian A, C L Bull et al
Gas loading apparatus for the Paris-Edinburgh press
Review of Scientific Instruments 81(9) (2010)

Bordeneuve H, Tenailleau C, Guillemet-Fritsch S, Smith R, Suard E and Rousset A
Structural variations and cation distributions in $Mn_{3-x}Co_xO_4$ (0 <= x <= 3) dense ceramics using neutron diffraction data
Solid State Sciences Vol: 12 379-386 (2010)

Borgeschulte A, Gremaud R, Ramirez-cuesta A and Refson K
Evidence for hydrogen transport in deuterated $LiBH_4$
Advances in science and technology Vol: 72 150 -157 (2010)

Borowska-Centkowska A, Kario A, Krok F, Abrahams I, Chan S C M, Liu X, Wrobel W, Malys M, Hull S, Dygas J R and Suard E
Defect structure and electrical conductivity in the $Bi_{3+x}Nb_{0.8}W_{0.2}O_{71+3x/2}$ system
Solid State Ionics Vol: 181 1750-1756 (2010)

Bowron D T, D'Agostino C, Gladden L F, Hardacre C, Holbrey J D, Lagunas M C, McGregor J, Mantle M D, Mullan C L and Youngs T G A
Structure and dynamics of 1-ethyl-3-methylimidazolium acetate via molecular dynamics and neutron diffraction
Journal of Physical Chemistry B Vol: 114 7760-7768 (2010)

Bowron D T, Soper A K, Jones K, Ansell S, Birch S, Norris J, Perrott L, Riedel D, Rhodes N J, Wakefield S R, Botti A, Ricci M A, Grazzi F and Zoppi M
NIMROD: The Near and InterMediate Range Order Diffractometer of the ISIS second target station
Review of Scientific Instruments Vol: 81 (2010)

Branzoli F, Carretta P, Filibian M, Graf M J, Klyatskaya S, Ruben M, Coneri F and Dhakal P
Spin and charge dynamics in $[TbPc_2]^0$ and $[DyPc_2]^0$ = single-molecule magnets
Physical Review B Vol: 82 134401 (2010)

Brogan M A, Hughes R W, Smith R I and Gregory D H
Structural and compositional tuning of layered subnitrides; new complex nitride halides
Dalton Transactions Vol: 39 7153-7158 (2010)

Brooks N J, Gauthe B, Terrill N J, Rogers S E, Templer R H, Ces O and Seddon J M
Automated high pressure cell for pressure jump x-ray diffraction
Review of Scientific Instruments Vol: 81 (2010)

Bull C L, Guthrie M, Nelmes R J, Loveday J S, Komatsu K, Hamidov H and Gutmann M J
Time-of-flight single-crystal neutron diffraction to 10 GPa and above
High Pressure Research Vol: 30 219-219 (2010)

Bull D J, Weidner E, Shabalin I L, Telling M T F, Jewell C M, Gregory D H and Ross D K
Pressure-dependent deuterium reaction pathways in the Li-N-D system
Physical Chemistry Chemical Physics Vol: 12 2089-2097 (2010)

Bungau A, Cywinski R, Bungau C, King P and Lord J
GEANT4 validation studies a the ISIS Muon Facility
IPAC 2010 (2010)

Bungau A, Cywinski R, Bungau C, King P and Lord J
Geometry optimisation of the ISIS muon target
IPAC 2010 (2010)

Bungau A, Cywinski R, Bungau C, King P and Lord J
Impact of the energy of the proton driver on muon production
IPAC 2010 (2010)

Bungau A, Cywinski R, Bungau C, King P and Lord J
Material studies for the ISIS muon target
IPAC 2010 (2010)

Burton R C, Ferrari E S, Davey R J, Finney J L and Bowron D T
The relationship between solution structure and crystal nucleation: a neutron scattering study of supersaturated methanolic solutions of benzoic acid
Journal of Physical Chemistry B Vol: 114 8807-8816 (2010)

Calder S, Fennell T, Kockelmann W, Lau G C, Cava R J and Bramwell S T
Neutron scattering and crystal field studies of the rare earth double perovskite Ba_2ErSbO_6
Journal of Physics-Condensed Matter Vol: 22 (2010)

Calder S, Ke X, Bert F, Amato A, Baines C, Carboni C, Cava R J, Daoud-Aladine A, Deen P, Fennell T, Hillier A D, Karunadasa H, Taylor J W, Mendels P, Schiffer P and Bramwell S T
Magnetic properties of Ba_2ErSbO_6 with a frustrated lattice geometry
Physical Review B Vol: 81 (2010)

Candolfi C, Leszczynski J, Masschelein P, Chubilleau C, Lenoir B, Dauscher A, Guilmeau E, Hejtmanek J, Clarke S J and Smith R I
Crystal structure and high-temperature thermoelectric properties of the $Mo_{3-x}Ru_xSb_7$ compounds
Journal of Electronic Materials Vol: 39 2132-2135 (2010)

Carpenter M A, McKnight R E A, Howard C J and Knight K S
Symmetry and strain analysis of structural phase transitions in $Pr_{0.48}Ca_{0.52}MnO_3$
Physical Review B Vol: 82 (2010)

Carr S T, Quintanilla J and Betouras J J
Lifshitz transitions and crystallization of fully polarized dipolar fermions in an anisotropic two-dimensional lattice
Physical Review B Vol: 82 (2010)

Carroll B R, Lichti R L, King P J C, Celebi Y G, Yonenaga I and Chow K H
Muonium defect levels in Czochralski-grown silicon-germanium alloys
Physical Review B Vol: 82 205205 (2010)

Caspi E
Neutron diffraction study of levantine middle bronze age axes
Journal of Physics: conference series Vol: 251 12049 1-4 (2010)

Celli M, Colognesi D, Giannasi A, Ulivi L and Zoppi M
Simple and binary hydrogen clathrate hydrates
Advances in Science and Technology Vol: 72 196 -204 (2010)

Chahardehi A, Brennan F P and Steuwer A
The effect of residual stresses arising from laser shock peening on fatigue crack growth
Engineering Fracture Mechanics Vol: 77 2033-2039 (2010)

Chambrier M H, Ibberson R M and Goutenoire F
Structure determination of alpha-$La_6W_2O_{15}$
Journal of Solid State Chemistry Vol: 183 1297-1302 (2010)

Chatzidimitriou-Dreismann C A and Krzystynia M
Attosecond physics with neutrons and electrons: ultrafast entanglement and decoherence phenomena involving protons in condensed matter and molecules
Laser Physics Vol: 20 990-1000 (2010)

Chen B, Flewitt P E J and Smit D J
Microstructural sensitivity of 316H austenitic stainless steel: residual stress relaxation and grain boundary fracture
Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing Vol: 527 7387-7399 (2010)

Chen B, Smith D J, Flewitt P E J, Zhang S Y
Evaluating residual stress behaviour in 316H stainless steel using neutron diffraction
Proc 2010 International Symposium on Structural Integrity, Shanghai, China, 21-24 Oct 2010

Chen B, Spindler M W, Smith D J, Flewitt P E J
Effect of thermo-mechanical history on reheat cracking in 316H austenitic stainless steel weldments
Proc ASME 2010 Pressure Vessels & Piping, Bellevue, WA, 18-22 Jul 2010

Chen B, Smith D J, Flewitt P E J
Creep relaxation of residual stresses in the heat affected zone of type 316H austenitic stainless steel weldments
Proc 18th European Conference on Fracture, 30 Aug - 03 Sep 2010

Chen B, Flewitt P E J, Spindler M W, Smith D J,
Prediction of creep stress relaxation for 316H austenitic stainless steel at 550°C
Proc Int Conf of High Temperature Defect Assessment 5, Guildford, UK, 23-25 Jun 2010

Chen M L, Penfold J, Thomas R K, Smyth T J P, Perfumo A, Marchant R, Banat I M, Stevenson P, Parry A, Tucker I and Grillo I
Mixing behavior of the biosurfactant, rhamnolipid, with a conventional anionic surfactant, sodium dodecyl benzene sulfonate
Langmuir Vol: 26 17958-17968 (2010)

Chen M L, Penfold J, Thomas R K, Smyth T J P, Perfumo A, Marchant R, Banat I M, Stevenson P, Parry A, Tucker I and Grillo I
Solution self-assembly and adsorption at the air-water interface of the monorhamnose and dirhamnose rhamnolipids and their mixtures
Langmuir Vol: 26 18281-18292 (2010)

Ciftja O and Quintanilla J
Effective interaction potentials in the uppermost Landau level
Journal of Low Temperature Physics Vol: 159 189-192 (2010)

Cippo E P, Borella A, Gorini G, Kockelmann W, Pietropaolo A, Postma H, Rhodes N J, Schillebeeckx P, Schooneveld E M, Tardocchi M, Wynants R and Collaboration A C
A detector system for neutron resonance capture imaging
Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment Vol: 623 693-698 (2010)

Clark G N I, Hura G L, Teixeira J, Soper A K and Head-Gordon T
Small-angle scattering and the structure of ambient liquid water
Proceedings of the National Academy of Sciences of the United States of America Vol: 107 14003-14007 (2010)

Coldea R, Tennant D A, Wheeler E M, Wawrzynska E, Prabhakaran D, Telling M, Habicht K, Smeibidl P and Kiefer K
Quantum criticality in an Ising chain: experimental evidence for emergent E-8 symmetry
Science Vol: 327 177-180 (2010)

Colognesi D, Pietropaulo A, Ramirez-cuesta A, Catti M, Nale A and Zoppi M
Proton vibrations in $LiNH^+$ and $LiNH^+$ studies through incoherent INS
Advances in Science and Technology Vol: 72 158 - 163 (2010)

Coneri F, Sanna S, Zheng K, Lord, J and De Renzi R
Magnetic states of lightly hole-doped cuprates in the clean limit as seen via zero-field muon spin spectroscopy
Physical Review B Vol: 81 (2010)

Coronado E, Marti-Gastaldo C, Navarro-Moratalla E, Ribera A, Blundell S and Baker P
Coexistence of superconductivity and magnetism by chemical design
Nature Chemistry Vol: 2 1031-1036 (2010)

Cortes-Gil R, Parker D R, Pitcher M J, Hadermann J and Clarke S J
Indifference of superconductivity and magnetism to size-mismatched cations in the layered iron arsenides Ba+Na+Fe+As+
Chemistry of Materials Vol: 22 4304-4311 (2010)

Czapla M, Pelstrokka R, Zielinacuteski P M, Budziak A, Balstrokanda M, Makarewicz M, Pacyna A, Wasiutynacuteski T, Miyazaki Y, Nakazawa Y, Inaba A, Sorai M, Pratt F L, Podgajny R, Korzeniak T and Sieklucka B
Critical behavior of two molecular magnets probed by complementary experiments
Physical Review B Vol: 82 094446 (2010)

Damay F, Martin C, Hardy V, Maignan A, Andre G, Knight K, Giblin S R and Chapon L C
Zigzag ladders with staggered magnetic chirality in the S=3/2 compound beta-CaCr$_2$O$_4$
Physical Review B Vol: 81 (2010)

Davies C M, Wimpory R C, Paradowska A M and Nikbin K M
Residual stress measurements in large scale component sections
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol:652 321-326 (2010)

de Haan V O, Plomp J, Rekveldt M T, van Well A A, Dalgliesh R M, Langridge S, Bottger A J and Hendrikx R
Coherence approach in neutron, X-ray, and neutron spin-echo reflectometry
Physical Review B Vol: 81 (2010)

de Haan V O, Plomp J, Rekveldt T M, Kraan W H, van Well A A, Dalgliesh R M and Langridge S
Comment on "Observation of the Goos-Hanchen shift with neutrons" Reply
Physical Review Letters Vol: 105 (2010)

de Haan V-O, Plomp J, Rekveldt T M, Kraan W H, van Well A A, Dalgliesh R M and Langridge S
Observation of the Goos-Hanchen shift with neutrons
Phys Rev Lett Vol: 104 010401 (2010)

de la Fuente C, del Moral A, Adroja D T, Fraile A and Arnaudas J I
Study of 4f hybridization in CeNiX with X = Sn delta Ge$_{1-delta}$, 0 <=delta <= 1
Journal of Magnetism and Magnetic Materials Vol: 322 1059-1063 (2010)

de Vries M A, McLaughlin A C and Bos J W G
Valence bond glass on an fcc lattice in the double perovskite = Ba$_2$YMoO$_6$
Physical Review Letters Vol: 104 177202 (2010)

Deen P P, Strydom A M, Paschen S, Adroja D T, Kockelmann W and Rols S
Quantum fluctuations and the magnetic ground state of Ce$_3$Pd$_{20}$Si$_6$
Physical Review B Vol: 81 (2010)

Deen P P, O A Petrenko et al
Spin dynamics in the hyperkagome compound Gd$_3$Ga$_5$O$_{12}$
Physical Review B 82(17) (2010)

Demmel F, Howells S, Morkel C and Pilgrim W C
Slow dynamics in liquid metals as seen by QENS
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics Vol: 224 83-99 (2010)

Demont A, Dyer M S, Sayers R, Thomas M F, Tsiamtsouri M, Niu H N, Darling G R, Daoud-Aladine A, Claridge J B and Rosseinsky M J
Stabilization of a complex perovskite superstructure under ambient conditions: influence of cation composition and ordering, and evaluation as an SOFC cathode
Chemistry of Materials Vol: 22 6598-6615 (2010)

Deriu A, Di Bari M T and Gerelli Y
Dynamics of nanostructures for drug delivery: the potential of QENS
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics Vol: 224 227-242 (2010)

Diallo S O, Pratt D K, Fernandes R M, Tian W, Zarestk J L, Lumsden M, Perring T G, Broholm C L, Ni N, Bud'ko S L, Canfield P C, Li H F, Vaknin D, Kreyssig A, Goldman A I and McQueeney R J
Paramagnetic spin correlations in CaFe$_2$As$_2$ single crystals
Physical Review B Vol: 81 (2010)

Diyabalanage H V K, Nakagawa T, Shrestha R P, Semelsberger T A, Davis B L, Scott B L, Burrell A K, David W I F, Ryan K R, Jones M O and Edwards P P
Potassium(I) amidotrihydroborate: structure and hydrogen release
Journal of the American Chemical Society Vol: 132 11836-11837 (2010)

Doubble R, Hayden S M, Dai P C, Mook H A, Thompon J R and Frost C D
Direct observation of paramagnons in palladium
Physical Review Letters Vol: 105 (2010)

Dougan L, Crain J, Finney J L and Soper A K
Molecular self-assembly in a model amphiphile system
Physical Chemistry Chemical Physics Vol: 12 10221-10229 (2010)

Down R, Kozmenko G, Kirichek O, Wotherspoon R, Brown J and Bowden Z
Cryogen free high magnetic field sample environments for neutron scattering
Journal of Physics: conference series Vol: 251 12092 1-4 (2010)

Dreiser J, Waldmann O, Dobe C, Carver G, Ochsenbein S T, Sieber A, Gudel H U, van Duijn J, Taylor J and Podlesnyak A
Quantized antiferromagnetic spin waves in the molecular Heisenberg ring CsFe8
Physical Review B Vol: 81 (2010)

Dubreuil A, Zhang SY, Eve S, Korsunsky AM
A neutron-diffraction study of the low-cycle fatigue behaviour of an austenitic stainless steel 316
12th European Powder Diffraction Conference, Darmstadt, Germany, 27-30 Aug 2010

Duffy J A, Taylor J W, Dugdale S B, Shenton-Taylor C, Butchers M W, Giblin S R, Cooper M J, Sakurai Y and Itou M
Spin and orbital moments in Fe$_3$O$_4$
Physical Review B Vol: 81 (2010)

Dunbar A D F, Mokarian-Tabari P, Parnell A J, Martin S J, Skoda M W A and Jones R A L
A solution concentration dependent transition from self-stratification to lateral phase separation in spin-cast PS:d-PMMA thin films
European Physical Journal E Vol: 31 369-375 (2010)

Eblagon K M, Rentsch D, Friedrichs O, Remhof A, Zuettel A, Ramirez-Cuesta A J and Tsang S C
Hydrogenation of 9-ethylcarbazole as a prototype of a liquid hydrogen carrier
International Journal of Hydrogen Energy Vol: 35 11609-11621 (2010)

Eblagon K M, Tam K, Yu K M K, Zhao S L, Gong X Q, He H Y, Ye L, Wang L C, Ramirez-Cuesta A J and Tsang S C
Study of catalytic sites on ruthenium for hydrogenation of n-ethylcarbazole: implications of hydrogen storage via reversible catalytic hydrogenation
Journal of Physical Chemistry C Vol: 114 9720-9730 (2010)

Edler K J, Hawley A M, et al
Association of titania with nonionic block copolymers in ethanol: the early stages of templating and film formation
Chemistry of Materials 22(16): 4579-4590 (2010)

Ehlers G, Greedan J, Stewart J, Rule K, Fouquet P, Cornelius A, Adrino C, Pagliuso P, Qiu Y and Gardner J
High-resolution neutron scattering study of Tb$_2$Mo$_2$O$_7$: a geometrically frustrated spin glass
Physical Review B Vol: 81 (2010)

Emery N, Wildman E J, Skakle J M S, Giriat G, Smith R I and McLaughlin A C
Giant magnetoresistance in oxypnictides (La,Nd)OMnAs
Chemical Communications Vol: 46 6777-6779 (2010)

Eriksson A K, Eriksson S G, Chapon L C and Knee C S
Phase stability study of Bi$_{0.15}$Sr$_{0.85-x}$Ae$_x$CoO$_{3-delta}$ (x=0 and Ae = Ba-0.28; Ca-0.17) perovskites by in-situ neutron diffraction
Materials Research Bulletin Vol: 45 1875-1882 (2010)

Ewings R A, Freeman P G, Enderle M, Kulda J, Prabhakaran D and Boothroyd A T
Ferromagnetic excitations in La$_{0.82}$Sr$_{0.18}$CoO$_3$ observed using neutron inelastic scattering
Physical Review B Vol: 82 (2010)

Faircloth D C, Lawrie S, Letchford A P, Gabor C, Wise P, Whitehead M, Wood T, Westall M, Findlay D, Perkins M, Savage P J, Lee D A and Pozimski J K
The front end test stand high performance H$^-$ ion source at Rutherford Appleton Laboratory
Review of Scientific Instruments Vol: 81 (2010)

Faircloth D, Kronberger M, Kuchler D, Lettry J and Scrivens R
Finite element thermal study of the Linac4 plasma generator
Review of Scientific Instruments Vol: 81 (2010)

Fan R, Kinane C J, Charlton T R, Dorner R, Ali M, de Vries M A, Brydson R M D, Marrows C H, Hickey B J, Arena D A, Tanner B K, Nisbet G and Langridge S
Ferromagnetism at the interfaces of antiferromagnetic FeRh epilayers
Physical Review B Vol: 82 (2010)

Fan R, Lee S J, Goff J P, Ward R C C, Wang S G, Kohn A, Wang C, Wildes A R and Collins S P
The influence of interfacial roughness on the coherence of structure and magnetic coupling across barriers in Fe/MgO multilayers
Journal of Physics-Condensed Matter Vol: 22 (2010)

Fang J, Bull C L, Hamidov H, Loveday J S, Gutmann M J, Nelmes R J and Kamenev K V
A rotator for single-crystal neutron diffraction at high pressure
Review of Scientific Instruments Vol: 81 (2010)

Ferguson E L, De Luca E, Heenan R K, King S M and Griffiths P C
Time-resolved small-angle neutron scattering as a tool for studying controlled release from liposomes using polymer-enzyme conjugates
Macromolecular Rapid Communications Vol: 31 1685-1690 (2010)

Fernandez-AlonsoF, Bermejo F J, Saboungi M L
Molecular hydrogen in carbon nanostructures
Handbook of Nanophysics part VII 1-12, CRC Press, ISBN 1420075381

Fernandez-Rodriguez J, Scagnoli V, Mazzoli C, Fabrizi F, Lovesey S W, Blanco J A, Sivia D S, Knight K S, de Bergevin F and Paolasini L
Experimental evidence of anapolar moments in the antiferromagnetic insulating phase of V$_2$O$_3$ obtained from X-ray resonant Bragg diffraction
Physical Review B Vol: 81 (2010)

Festa G, Pietropaolo A, Reali E, Grazzi F and Schooneveld E M
A gamma-ray detector with a silicon photomultiplier (SiPM) readout for neutron diffraction experiments at spallation neutron sources
Measurement Science & Technology Vol: 21 (2010)

Fillaux F, Cousson A and Gutmann M J
Evidence of macroscopically entangled protons in a mixed isotope crystal of KHpD1-pCO$_3$
Journal of Physics-Condensed Matter Vol: 22 (2010)

Flewitt PEJ, Chen B, Smith D J
Relaxation of residual stresses and grain boundary fracture in 316H stainless steel
Proc 2010 International Symposium on Structural Integrity, Shanghai, China, 21-24 Oct 2010

Foglia F, M J Lawrence et al
On the hydration of the phosphocholine headgroup in aqueous solution
Journal of Chemical Physics 133(14) (2010)

Fortes A D, Wood I G and Knight K S
The crystal structure of perdeuterated methanol hemiammoniate (CD$_3$OD.0.5ND$_3$) determined from neutron powder diffraction data at 4.2 and 180 K
Journal of Applied Crystallography Vol: 43 328-336 (2010)

Francisco M C, Malliakas C D, Piccoli P M B, Gutmann M J, Schultz A J and Kanatzidis M G
Development and loss of ferromagnetism controlled by the interplay of Ge Concentration and Mn vacancies in structurally modulated Y$_4$Mn$_{1-x}$Ga$_{12-y}$Ge$_y$
Journal of the American Chemical Society Vol: 132 8998-9006 (2010)

Funnell N P, Dawson A, Francis D, Lennie A R, Marshall W G, Moggach S A, Warren J E and Parsons S
The effect of pressure on the crystal structure of L-alanine
Cry2stengcomm Vol: 12 2573-2583 (2010)

Gabor C, Faircloth D C, Lee D A, Lawrie S R, Letchford A P and Pozimski J K
Diagnostic experiments at a 3 MeV test stand at Rutherford Appleton Laboratory (United Kingdom)
Review of Scientific Instruments Vol: 81 (2010)

Gaj A, Bacmanski A, Joncour L, Panicaud B, Francois M and Braham C
Localisation of stresses in polycrystalline grains by neutron diffraction and modelling
Materials Science Forum Vol: 681 103 - 108 (2010)

Ganin A, Takabayashi Y, Jeglic P, Arcon D, Potocni A, et al
Polymorphism control of superconductivity and magnetism in Cs$_3$C$_{60}$ close to the Mott transition
Nature Vol: 466 221-U93 (2010)

Garcia-Barriocanal J, Cezar J C, Bruno F Y, Thakur P, Brookes N B, Utfeld C, Rivera-Calzada A, Giblin S R, Taylor J W, Duffy J A, Dugdale S B, Nakamura T, Kodama K, Leon C, Okamoto S and Santamaria J
Spin and orbital Ti magnetism at LaMnO$_3$/SrTiO$_3$ interfaces
Nature Communications Vol: 1 (2010)

Garcia-Munoz J L, Frontera C, Beran P, Bellido N, Hernandez-Velasco J and Ritter C
Consequences of embedding Ti^{4+} 3d^0 centers in Pr$_{0.50}$Ca$_{0.50}$MnO$_3$: phase competition in Pr$_{0.50}$Ca$_{0.50}$Mn$_{1-x}$TixO$_3$
Physical Review B Vol: 81 (2010)

Gardner J S, Gingras M J P and Greedan J E
Magnetic pyrochlore oxides
Reviews of Modern Physics Vol: 82 53-107 (2010)

Gaspar A M, Marques M A, Cabaco M I, Marques M I, Kolesnikov A I, Tomkinson J and Li J C
Structure and dynamics of concentrated aqueous solutions of aluminium chloride, beryllium chloride and aluminium bromide: Raman, inelastic neutron scattering and x-ray diffraction results
Journal of Physics-Condensed Matter Vol: 22 (2010)

Gereben O, Pusztai L and McGreevy R L
RMCSANS-modelling the inter-particle term of small angle scattering data via the reverse Monte Carlo method
Journal of Physics-Condensed Matter Vol: 22 (2010)

Ghugare S V, Chiessi E, Telling M T F, Deriu A, Gerelli Y, Wuttke J and Paradossi G
Structure and dynamics of a thermoresponsive microgel around its volume phase transition temperature
Journal of Physical Chemistry B Vol: 114 10285-10293 (2010)

Giannasi A, Colognesi D, Ulivi L, Zoppi M, Ramirez-Cuesta A J, Bardaji E G, Roehm E and Fichtner M
High resolution Raman and neutron investigation of Mg(BH$_4$)$_2$ in an extensive temperature range
Journal of Physical Chemistry A Vol: 114 2788-2793 (2010)

Gilbert G S, Howard E, Ayala-Orozco B, Bonilla-Moheno M, Cummings J, Langridge S, Parker I M, Pasari J, Schweizer D and Swope S
Beyond the tropics: forest structure in a temperate forest mapped plot
Journal of Vegetation Science Vol: 21 388-405 (2010)

Gliozzo E, Arletti R, Cartechini L, Imberti S, Kockelmann W A, Memmi I, Rinaldi R and Tykot R H
Non-invasive chemical and phase analysis of Roman bronze artefacts from Thamusida (Morocco)
Applied Radiation and Isotopes Vol: 68 2246-2251 (2010)

Goodwin A L, Michel F M, Phillips B L, Keen D A, Dove M T and Reeder R J
Nanoporous structure and medium-range order in synthetic amorphous calcium carbonate
Chemistry of Materials Vol: 22 3197-3205 (2010)

Goossens D J and Welberry T R
Approaches to modeling diffuse scattering from molecular crystals: para-terphenyl (C$_{18}$H$_{14}$)
Metallurgical and Materials Transactions a-Physical Metallurgy and Materials Science Vol: 41A 1119-1129 (2010)

Goremychkin E A, Osborn R, Sashin I L, Riseborough P, Rainford B D, Adroja D T and Lawrence J M
Transition from heavy-Fermion to mixed-balence behavior in Ce$_{1-x}$Y$_x$Al$_3$: a quantitative comparison with the Anderson impurity model
Physical Review Letters Vol: 104 (2010)

Gorria P, Martinez-Blanco D, Blanco J A and Smith R I
Neutron powder thermo-diffraction in mechanically alloyed Fe$_{64}$Ni$_{36}$ invar alloy
Journal of Alloys and Compounds Vol: 495 495-498 (2010)

Gray B M, Hector A L, Levason W, Reid G, Webster M, Zhang W J and Jura M
Synthesis, spectroscopic and structural characterisation of vanadium(IV) and oxovanadium(IV) complexes with arsenic donor ligands
Polyhedron Vol: 29 1630-1638 (2010)

Grazzi F, Bartoli L, Civita F, Paradowska A M, Scherillo A and Zoppi M
Non destructive characterization of phase distribution and residual strain/stress map of two ancient (Koto) age Japanese swords
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol: 652 167-173 (2010)

Grazzi F, Bartoli L, Siano S and Zoppi M
Characterization of copper alloys of archaeometallurgical interest using neutron diffraction: a systematic calibration study
Analytical and Bioanalytical Chemistry Vol: 397 2501-2511 (2010)

Greving I, Dicko C, Terry A, Callow P and Vollrath F
Small angle neutron scattering of native and reconstituted silk fibroin
Soft Matter Vol: 6 4389-4395 (2010)

Griffiths P C, Fallis I A, James C, Morgan I R, Brett G, Heenan R K, Schweins R, Grillo I and Paul A
Structure-property relationships in metallosurfactants
Soft Matter Vol: 6 1981-1989 (2010)

Griffiths P C, Knight D W, Morgan I R, Ford A, Brown J, Davies B, Heenan R K, King S M, Dalgliesh R M, Tomkinson J, Prescott S, Schweins R and Paul A
Gelation or molecular recognition; is the bis-(alpha,beta-dihydroxy ester)s motif an omnigelator?
Beilstein Journal of Organic Chemistry Vol: 6 1079-1088 (2010)

Griffiths P C, Nilmini R, Carter E, Dodds P, Murphy D M, Khayat Z, Lattanzio E, Griffiths P, Heenan R K, King S M and Duncan R
Interaction of an endosomolytic polyamidoamine ISA23 with vesicles mimicking intracellular membranes: a SANS/EPR study
Macromolecular Bioscience Vol: 10 963-973 (2010)

Griffiths P C, Occhipinti P, Morris C, Heenan R K, King S M and Gumbleton M
PGSE-NMR and SANS studies of the interaction of model polymer therapeutics with mucin
Biomacromolecules Vol: 11 120-125 (2010)

Guignard M, Cormier L, Montouillout V, Menguy N, Massiot D, Hannon A C and Beuneu B
Rearrangement of the structure during nucleation of a cordierite glass doped with TiO$_2$
Journal of Physics-Condensed Matter Vol: 22 (2010)

Guthrie M, Tucker M G, Tulk C A, Santos A and Molaison J
Neutron diffraction studies of liquids at high pressure
Geochimica Et Cosmochimica Acta Vol: 74 A368-A368 (2010)

Gutmann M J
Accelerated computation of diffuse scattering patterns and application to magnetic neutron scattering
Journal of Applied Crystallography Vol: 43 250-255 (2010)

Hagita K, McGreevy R L, Arai T, Inui M, Matsuda K and Tamura K
First example of multi-scale reverse Monte Carlo modeling for small-angle scattering experimental data using reverse mapping from coarse-grained particles to atoms
Journal of Physics-Condensed Matter Vol: 22 (2010)

Hakimi A, Schoofs F, Bali R, Stelmashenko N A, Blamire M G, Langridge S, Cavill S A, van der Laan G and Dhesi S S
Origin of magnetism in cobalt-doped indium tin oxide thin films
Physical Review B Vol: 82 (2010)

Hall D A, Evans J D S, Covey-Crump S J, Holloway R F, Oliver E C, Mori T and Withers P J
Effects of superimposed electric field and porosity on the hydrostatic pressure-induced rhombohedral to orthorhombic martensitic phase transformation in PZT 95/5 ceramics
Acta Materialia Vol: 58 6584-6591 (2010)

Hannon A C
Adrian C Wright: glasses, neutrons, borates!
Physics and Chemistry of Glasses-European Journal of Glass Science and Technology Part B Vol: 51 40-51 (2010)

Hardacre C, Holbrey J D, Mullan C L, Nieuwenhuyzen M, Youngs T G A, Bowron D T and Teat S J
Solid and liquid charge-transfer complex formation between 1-methylnaphthalene and 1-alkyl-cyanopyridinium bis{(trifluoromethyl)sulfonyl}imide ionic liquids
Physical Chemistry Chemical Physics Vol: 12 1842-1853 (2010)

Hardacre C, Holbrey J D, Mullan C L, Youngs T G A and Bowron D T
Small angle neutron scattering from 1-alkyl-3-methylimidazolium hexafluorophosphate ionic liquids (C(n)mim PF6 , n=4, 6, and 8)
Journal of Chemical Physics Vol: 133 (2010)

Hayes R, Norberg S, Ericksson S, Chawdhury M and Goodway C
New high temperature gas flow cell developed at ISIS
Journal of Physics: conference series Vol: 251 12090 1-4 (2010)

Headen T F, Howard C A, Skipper N T, Wilkinson M A, Bowron D T and Soper A K
Structure of pi-pi Interactions in aromatic liquids
Journal of the American Chemical Society Vol: 132 5735-5742 (2010)

Headings N S, Hayden S M, Coldea R and Perring T G
Anomalous high-energy spin excitations in the high-T_c superconductor-parent antiferromagnet La_2CuO_4
Physical Review Letters Vol: 105 (2010)

Hibble S J, Wood G B, Bilbe E J, Pohl A H, Tucker M G, Hannon A C and Chippindale A M
Structures and negative thermal expansion properties of the one-dimensional cyanides, CuCN, AgCN and AuCN
Zeitschrift Fur Kristallographie Vol: 225 457-462 (2010)

Hill A H, Harrison A, Dickinson C, Zhou W Z and Kockelmann W
Crystallographic and magnetic studies of mesoporous eskolaite, Cr_2O_3
Microporous and Mesoporous Materials Vol: 130 280-286 (2010)

Hillier A D, Manuel P, Adroja D T, Taylor J W, Azad A K and Irvine J T S
Probing the superconducting ground state near the charge density wave phase transition in $Cu_{0.06}TiSe_2$
Physical Review B Vol: 81 (2010)

Hillier A D, Quintanilla J and Cywinski R
Evidence for time-reversal symmetry breaking in the noncentrosymmetric superconductor $LaNiC_2$
Physical Review Letters Vol: 105 (2010)

Hillman A R, Ryder K S, Madrid E, Burley A W, Wiltshire R J, Merotra J, Grau M, Horswell S L, Glidle A, Dalgliesh R M, Hughes A, Cubitt R and Wildes A
Structure and dynamics of phospholipid bilayer films under electrochemical control
Faraday Discussions Vol: 145 357-379 (2010)

Hollamby M J, Eastoe J, Chemelli A, Glatter O, Rogers S, Heenan R K and Grillo I
Separation and purification of nanoparticles in a single step
Langmuir Vol: 26 6989-94 (2010)

Hollamby M J, Eastoe J, Mutch K J, Rogers S and Heenan R K
Fluorinated microemulsions as reaction media for fluorous nanoparticles
Soft Matter Vol: 6 971-976 (2010)

Hoser A A, Dobrzycki L, Gutmann M J and Wozniak K
Charge densities of two polymorphs of hydrated 1,8-bis(dimethylamino)naphthalene hydrochloride - similarities and differences
Crystal Growth & Design Vol: 10 5092-5104 (2010)

Hudsou M R, Allis D G and Hudson B S
The vibrational spectrum of parabanic acid by inelastic neutron scattering spectroscopy and simulation by solid-state DFT
Journal of Physical Chemistry A Vol: 114 3630-3641 (2010)

Hunter S M, McKay D, Smith R I, Hargreaves J S J and Gregory D H
Topotactic nitrogen transfer: structural transformation in cobalt molybdenum nitrides
Chemistry of Materials Vol: 22 2898-2907 (2010)

Hutchings L R, Douglas C J R, Rhodes C L, Carswell W D, Skoda M W A, Webster J R P and Thompson R L
Nonsolvent annealing polymer films with ionic liquids
Langmuir Vol: 26 15486-15493 (2010)

Ianeselli L, Zhang F J, Skoda M W A, Jacobs R M J, Martin R A, Callow S, Prevost S and Schreiber F
Protein-protein interactions in ovalbumin solutions studied by small-angle scattering: effect of ionic strength and the chemical nature of cations
Journal of Physical Chemistry B Vol: 114 3776-3783 (2010)

Imberti S and Bowron D T
Formic and acetic acid aggregation in the liquid state
Journal of Physics-Condensed Matter Vol: 22 (2010)

Irie Y, Fukumoto S, Muto K, Nakanishi H, Oki T, Takagi A et al
Wodeband low-output impedance RF system for the ISIS Second Harmonic Cavity
Proc 1st International Particle Accelerator Conference (IAPC'10), Kyoto, Japan, 23-28 May 2010

Ishii Y, Nagasawa M, Suzuki T, Watanabe I, Matsuzaki T, Yamamoto H M and Kato R
Zero field- and longitudinal field-mu SR studies of quasi-one-dimensional organic conductor, $TMTTF_2PF_6$
Physica B-Condensed Matter Vol: 405 S98-S100 (2010)

James J, Zhang S-Y
Residual stress distribution in welds measured by neutron diffraction, visualisation and optimisation of experiments using SSCANSS
International Conference of the International Institute of Welding (IIW2010), Istanbul, Turkey, 11-16 Jul 2010

Jarvie H P and King S M
Just scratching the surface? New techniques show how surface functionality of nanoparticles influences their environmental fate
Nano Today Vol: 5 248-250 (2010)

Jarvie H P, Al-Obaidi H, King S M, Bowes M J, Lawrence M J, Drake A F, Green M A and Dobson P J
Effects of surfactant coating on the fate of engineered oxide nanoparticles in simulated wastewater treatment
Geochimica Et Cosmochimica Acta Vol: 74 A460-A460 (2010)

Johnson R D, Frawley T, Manuel P, Khalyavin D D, Adriano C, Giles C, Pagliuso P G and Hatton P D
Magnetic structures of the anisotropic intermetallic compounds Er_2CoGa_8 and Tm_2CoGa_8
Physical Review B Vol: 82 (2010)

Johnston K E, Tang C C, Parker J E, Knight K S, Lightfoot P and Ashbrook S E
The polar phase of $NaNbO_3$, a combined study by powder diffraction, solid-state NMR, and first-principles calculations
Journal of the American Chemical Society Vol: 132 8732-8746 (2010)

Johnstone R D L, Lennie A R, Parker S F, Parsons S, Pidcock E, Richardson P R, Warren J E and Wood P A
High-pressure polymorphism in salicylamide
Crystengcomm Vol: 12 1065-1078 (2010)

Juarez R, Parker S F, Concepcion P, Corma A and Garcia H
Heterolytic and heterotopic dissociation of hydrogen on ceria-supported gold nanoparticles Combined inelastic neutron scattering and FT-IR spectroscopic study on the nature and reactivity of surface hydrogen species
Chemical Science Vol: 1 731-738 (2010)

Jun T, Song X, Rotundo F, Ceschini A, Morri L and Threadgill P
Numerical and experimental study of residual stresses in a linear friction weld
Advanced Materials Research Vol: 89 - 91 268 -274 (2010)

Jura M, Levason W, Petts E, Reid G, Webster M and Zhang W J
Taking TiF4 complexes to extremes - the first examples with phosphine co-ligands
Dalton Transactions Vol: 39 10264-10271 (2010)

Jura M, Levason W, Ratnani R, Reid G and Webster M
Six- and eight-coordinate thio- and seleno-ether complexes of NbF_5 and some comparisons with $NbCl_5$ and $NbBr_5$ adducts
Dalton Trans Vol: 39 883-91 (2010)

Kawamura N, Ishida K, Matsuzaki T, Imao H and Nagamine K
Muonic molecule formation in muon-catalyzed fusion
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Keen D A and Pusztai L
The first 21 years of reverse Monte Carlo modelling-a workshop held in Budapest, Hungary (1-3 October 2009) Preface
Journal of Physics-Condensed Matter Vol: 22 (2010)

Keen D A, Dove M T, Evans J S O, Goodwin A L, Peters L and Tucker M G
The hydrogen-bonding transition and isotope-dependent negative thermal expansion in $H_3Co(CN)_6$
Journal of Physics-Condensed Matter Vol: 22 (2010)

Kelleher J F, Lopez-Crespo P, Yusof F and Withers P J
The use of fiffraction to study fatigue crack tip mechanics
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol: 652 216-221 (2010)

Kelleher J, Paradowska A and Zhang S
In-situ loading on the neutron diffractiometer Engin-x
TMS 2010 (2010)

Kendrick E, Knight K S, Islam M S and Slater P R
Combined experimental and modelling studies of proton conducting $La_{1-x}Ba_{1+x}GaO_{4-x/2}$: proton location and dopant site selectivity
Journal of Materials Chemistry Vol: 20 10412-10416 (2010)

Khalyavin D D, Hillier A D, Adroja D T, Strydom A M, Manuel P, Chapon L C, Peratheepan P, Knight K, Deen P, Ritter C, Muro Y and Takabatake T
Long-range magnetic order in $CeRu_2Al_{10}$ studied via muon spin relaxation and neutron diffraction
Physical Review B Vol: 82 100405 (2010)

Khalyavin D D, Manuel P, Mitchell J F and Chapon L C
Spin correlations in the geometrically frustrated $RBaCo_4O_7$ antiferromagnets: Mean-field approach and Monte Carlo simulations
Physical Review B Vol: 82 (2010)

King M D, Rennie A R, Pfrang C, Hughes A V and Thompson K C
Interaction of nitrogen dioxide (NO_2) with a monolayer of oleic acid at the air-water interface – simple proxy for atmospheric aerosol
Atmospheric Environment Vol: 44 1822-1825 (2010)

King P D C, McKenzie I and Veal T D
Observation of shallow-donor muonium in Ga_2O_3: Evidence for hydrogen-induced conductivity
Applied Physics Letters Vol: 96 (2010)

Kirichek O, Down R B E, Kouzmenko G, Keeping J, Bunce D, Wotherspoon R and Bowden Z A
Operation of superconducting magnet with dilution refrigerator insert in zero boil-off regime
Cryogenics Vol: 50 666-669 (2010)

Kirstein O, Zhang J F, Kisi E H, Riley D P, Styles M J and Paradowska A
Single crystal elastic constants of the MAX phase Ti_3AlC_2 determined by neutron diffraction
Thermec 2009, Pts 1-4 Vol: 638-642 2417-2422 (2010)

Kisi E H, Zhang J F, Kirstein O, Riley D P, Styles M J and Paradowska A M
Shear stiffness in nanolaminar Ti_3SiC_2 challenges ab initio calculations
Journal of Physics-Condensed Matter Vol: 22 (2010)

Knight K S
Analytical expressions to determine the isothermal compressibility tensor and the isobaric thermal expansion tensor for monoclinic crystals: application to determine the direction of maximum compressibility in jadeite
Physics and Chemistry of Minerals Vol: 37 529-533 (2010)

Knight K S, Henderson C M B and Clark S M
Structural variations in the wesselsite-effenbergite $(Sr_{1-x}Ba_xCuSi_4O_{10})$ solid solution
European Journal of Mineralogy Vol: 22 411-423 (2010)

Knupfer S, Paradowska A M, Kirstein O and Moore A
Investigation of residual stress in laser formed mild steel plates using neutron diffraction
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol: 652 123-128 (2010)

Kovalevsky A Y, Hanson L, Fisher S Z, Mustyakimov M, Mason S A, Forsyth V T, Blakeley M P, Keen D A, Wagner T, Carrell H L, Katz A K, Glusker J P and Langan P
Metal ion roles and the movement of hydrogen during reaction catalyzed by d-xylose isomerase: a joint X-ray and neutron diffraction study
Structure Vol: 18 688-699 (2010)

Krzystyniak M
Nuclear momentum distribution in solid and liquid HF from ab initio calculation
Journal of Chemical Physics Vol: 133 (2010)

Krzystyniak M and Abdul-Redah T
Proton momentum distribution in solid and liquid HF
Physical Review B Vol: 82 (2010)

Krzystyniak M, Lopez-Anton R, Chatzidimitriou-Dreismann A, Lerch M and Fernandez-Alonso F
Dynamics of caged hydronium ions and super-protonic conduction in $(H_3O)SbTeO_6$
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics Vol: 224 279-287 (2010)

Kulterer M R and Hudson B S
Raman spectra and vibrational analysis of cis- and trans-cyclooctene for conformational analysis compared to inelastic neutron scattering
Journal of Raman Spectroscopy Vol: 41 1211-1215 (2010)

Kurban Z, Lovell A, Bennington S M, Jenkins D W K, Ryan K R, Jones M O, Skipper N T and David W I F
A solution selection model for coaxial electrospinning and its application to nanostructured hydrogen storage materials
Journal of Physical Chemistry C Vol: 114 21201-21213 (2010)

Kurban Z, Lovell A, Jenkins D, Bennington S, Loader I, Schober A and Skipper N
Turbostratic graphite nanofibres from electrospun solutions of PAN in dimethylsulphoxide
European Polymer Journal Vol: 46 1194-1202 (2010)

Lake B, Tsvelik A M, Notbohm S, Tennant D A, Perring T G, Reehuis M, Sekar C, Krabbes G and Buchner B
Confinement of fractional quantum number particles in a condensed-matter system
Nature Physics Vol: 6 50-55 (2010)

Lancaster T, Blundell S J, Pratt F L, Franke I, Steele A J, Baker P J, Salman Z, Baines C, Watanabe I, Carretta S, Timco G A and Winpenny R E P
Relaxation of muon spins in molecular nanomagnets
Physical Review B Vol: 81 140409 (2010)

Lathiotakis N N, Gidopoulos N I and Helbig N
Size consistency of explicit functionals of the natural orbitals in reduced density matrix functional theory
Journal of Chemical Physics Vol: 132 (2010)

Lawrie S R, Faircloth D C, Letchford A P, Gabor C and Pozimski J K
Plasma meniscus and extraction electrode studies of the ISIS H^- ion source
Review of Scientific Instruments Vol: 81 (2010)

Lawrie S, Faircloth D, Letchford A, Perkins M and Pozimski P
Assessing the transmission of the H^- ion beam on the front end test stand
IPAC 2010 (2010)

Lawrie S, Letchford A, Pozimski J and Savage P
Combined electromagnetic-thermal-structural simulation of the four meter radio frquency quadrupole to be installed on the front end test stand
IPAC 2010 (2010)

Lazim A M, Eastoe J, Bradley M, Trickett K, Mohamed A and Rogers S E
Recovery of gold nanoparticles using pH-sensitive microgels
Soft Matter Vol: 6 2050-2055 (2010)

Le Joncour L, Panicaud B, Baczmanski A, Francois M, Braham C and Paradowska A
Large deformation and mechanical effects of damage in aged duplex stainless steel
Mechanical Stress Evaluation by Neutrons and Synchrotron Radiation Vol: 652 155-160 (2010)

Le Joncour L, Panicaud B, Baczmanski A, Francois M, Braham C, Paradowska A, Wronski S and Chiron R
Damage in duplex steels studied at mesoscopic and macroscopic scales
Mechanics of Materials Vol: 42 1048-1063 (2010)

Lee J S, Arena D A, Yu P, Nelson C S, Fan R, Kinane C J, Langridge S, Rossell M D, Ramesh R and Kao C C
Hidden magnetic configuration in epitaxial $La_{1-x}Sr_xMnO_3$ films
Physical Review Letters Vol: 105 (2010)

Lepadatu S, Claydon J S, Ciudad D, Kinane C J, Langridge S, Cavill S, Dhesi S S and Marrows C H
Determination of domain wall depinning and driving currents in doped permalloy structures
IEEE Transactions on Magnetics Vol: 46 1759-1761 (2010)

Lepadatu S, Claydon J S, Ciudad D, Kinane C J, Langridge S, Dhesi S S and Marrows C H
Tuning of current-induced domain wall resonance frequency using Gd doping
Applied Physics Letters Vol: 97 (2010)

Lepadatu S, Claydon J, Ciudad D, Naylor A, Kinane C, Langridge S, Dhesi S S and Marrows C
Reduction of threshold current for domain wall depinning using Gd doping of permalloy
Applied Physics Express Vol: 3 (2010)

Lepadatu S, Wessely O, Vanhaverbeke A, Allenspach R, Potenza A, Marchetto H, Charlton T R, Langridge S, Dhesi S S and Marrows C H
Domain-wall spin-torque resonators for frequency-selective operation
Physical Review B Vol: 81 (2010)

Lepadau S, Claydon J S, Kinane C J, Charlton T R, Langridge S, Potenza A, Dhesi S S, Keatley P S, Hicken R J, Hickey B J and Marrows C H
Domain-wall pinning, nonadiabatic spin-transfer torque, and spin-current polarization in permalloy wires doped with vanadium
Physical Review B Vol: 81 (2010)

Lester C, Chu J H, Analytis J G, Perring T G, Fisher I R and Hayden S M
Dispersive spin fluctuations in the nearly optimally doped superconductor $Ba(Fe_{1-x}Co_x)2As_2$ (x=0.065)
Physical Review B Vol: 81 (2010)

Lettry J, Kronberger M, Scrivens R, Chaudet E, Faircloth D, Favre G, Geisser J M, Kuchler D, Mathot S, Midttun O, Paoluzzi M, Schmitzer C and Steyaert D
High duty factor plasma generator for CERN's superconducting proton linac
Review of Scientific Instruments Vol: 81 (2010)

Levin I, Karimi S, Provenzano V, Dennis C L, Wu H, Comyn T P, Stevenson T J, Smith R I and Reaney I M
Reorientation of magnetic dipoles at the antiferroelectric-paraelectric phase transition of $Bi_{1-x}Nd_xFeO_3$ (0.15 <= x <= 0.25)
Physical Review B Vol: 81 (2010)

Levin I, Woicik J C, Llobet A, Tucker M G, Krayzman V, Pokorny J and Reaney I M
Displacive ordering yransitions in perovskite-like $AgNb_{1/2}Ta_{1/2}O_3$
Chemistry of Materials Vol: 22 4987-4995 (2010)

Lewtas H, Lancaster T, Baker P, Blundell S Prabhakaran D, Pratt F
Local magnetism and magnetoelectric effect in $HoMnO_3$ studied with muon-spin relaxation
Physical Review B Vol: 81 (2010)

Lord T D, Hobbs J K, Terry A E, Kvick A and Hanna S
Variation of lattice parameters with fold state in the ultralong n-alkanes
Macromolecules Vol: 43 3365-3375 (2010)

Lumsden M D, Christianson A D, Goremychkin E A, Nagler S E, Mook H A, Stone M B, Abernathy D L, Guidi T, MacDougall G J, de la Cruz C, Sefat A S, McGuire M A, Sales B C and Mandrus D
Evolution of spin excitations into the superconducting state in $FeTe_{1-x}Se_x$
Nature Physics Vol: 6 182-186 (2010)

Macchi P, Casati N, Marshall W G and Sironi A
The alpha and beta forms of oxalic acid di-hydrate at high pressure: a theoretical simulation and a neutron diffraction study
Crystengcomm Vol: 12 2596-2603 (2010)

MacLaughlin D E, Hillier A D, Mackie J M, Shu L, Aoki Y, Kikuchi D, Sato H, Tunashima Y and Sugawara H
Comment on "Pronounced enhancement of the lower critical field and critical current deep in the superconducting state of PrOs4Sb12"
Phys Rev Lett Vol: 105 019701; author reply 019702 (2010)

Madhuku M, Gxawu D, Connell S H, Machi I Z, Keartland J M and King P J C
Muon spin relaxation in synthetic type IIa diamond grown by high-pressure and high-temperature (HPHT) synthesis
Physica B-Condensed Matter Vol: 405 41-44 (2010)

Maier B J, Angel R J, Marshall W G, Mihailova B, Paulmann C, Engel J M, Gospodinov M, Welsch A M, Petrova D and Bismayer U
Octahedral tilting in Pb-based relaxor ferroelectrics at high pressure
Acta Crystallographica Section B-Structural Science Vol: 66 280-291 (2010)

Malardier-Jugroot C, Bowron D T, Soper A K, Johnson M E and Head-Gordon T
Structure and water dynamics of aqueous peptide solutions in the presence of co-solvents
Physical Chemistry Chemical Physics Vol: 12 382-392 (2010)

Mancinelli R
The effect of confinement on water structure
Journal of Physics-Condensed Matter Vol: 22 (2010)

Mancinelli R, Bruni F and Ricci M A
Controversial evidence on the point of minimum density in deeply supercooled confined water
Journal of Physical Chemistry Letters Vol: 1 1277-1282 (2010)

Manson J L, Lancaster T, Blundell S J, Qiu Y M, Singleton J, Sengupta P, Pratt F L, Kang J, Lee C and Whangbo M H
Spin fluctuations and orbital ordering in quasi-one-dimensional alpha-$Cu(dca)_2(pyz)$ {dca = dicyanamide = $N(CN)_2(-)$; pyz = pyrazine}, a molecular analogue of $KCuF_3$
Polyhedron Vol: 29 514-520 (2010)

Manuel P, Chapon L C, Todorov I S, Chung D Y, Castellan J P, Rosenkranz S, Osborn R, Toledano P and Kanatzidis M G
Incommensurate spin-density wave and magnetic lock-in transition in $CaFe_4As_3$
Physical Review B Vol: 81 (2010)

Markvardsen A J and David W I F
Diffusion-equation method for crystallographic figure of merits
Acta Crystallographica Section A Vol: 66 591-596 (2010)

Maynard-Casely H E, C L Bull et al
The distorted close-packed crystal structure of methane A
Journal of Chemical Physics 133(6) (2010)

McFarlane A, McMillan L, Silverwood I, Hamilton N G, Siegel D, Parker S F, Lundie D T and Lennon D
The observation of equilibria present in stepwise gas phase hydrogenation reactions
Catalysis Today Vol: 155 206-213 (2010)

McKenzie I
DFT study of paramagnetic adducts of tris-(8-hydroxyquinoline)aluminum (III)
Journal of Physical Chemistry A Vol: 114 12759-12763 (2010)

McKenzie I, Cammidge A N, Dilger H, Gopee H, Scheuermann R, Stoykov A and Jayasooriya U A
Muon spin spectroscopy of the discotic liquid crystal HAT6
Physical Chemistry Chemical Physics Vol: 12 9900-9908 (2010)

McKenzie I, Dilger H, Scheuermann R and Stoykov A
Muon spin spectroscopy of the rod-like liquid crystal 4-n-octyl-4 '-cyanobiphenyl (8CB)
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Meersman F, Bowron D, Soper A K and Koch M H J
Counteraction of urea by trimethylamine N-oxide is due to direct interaction
Biophysical Journal Vol: 98 174-174 (2010)

Mendels P and Bert F
Quantum Kagome Antiferromagnet $ZnCu_3(OH)_6Cl_2$
Journal of the Physical Society of Japan Vol: 79 (2010)

Middleton C A, Wood I G W, Grindrod P M, Fortes A D, Hunt S A, Zhang S Y et al
The use of neutron diffraction in studies of planetary ice-rock analogue mixtures
Proc International Mineralogical Association, 20th General Meeting, Budapest, 21-27 Aug 2010

Millar D I A, Marshall W G, Oswald I D H and Pulham C R
High-pressure structural studies of energetic materials
Crystallography Reviews Vol: 16 115-132 (2010)

Millar D I A, Maynard-Casely H E, Kleppe A K, Marshall W G, Pulham C R and Cumming A S
Putting the squeeze on energetic materials-structural characterisation of a high-pressure phase of CL-20
Crystengcomm Vol: 12 2524-2527 (2010)

Millar D I A, Oswald I D H, Barry C, Francis D J, Marshall W G, Pulham C R and Cumming A S
Pressure-cooking of explosives-the crystal structure of epsilon-RDX as determined by X-ray and neutron diffraction
Chemical Communications Vol: 46 5662-5664 (2010)

Moglianetti M, Webster J R P, Edmondson S, Armes S P and Titmuss S
Neutron reflectivity study of the structure of pH-responsive polymer brushes grown from a macroinitiator at the sapphire-water interface
Langmuir Vol: 26 12684-12689 (2010)

Mohamed A, Trickett K, Chin S Y, Cummings S, Sagisaka M, Hudson L, Nave S, Dyer R, Rogers S E, Heenan R K and Eastoe J
Universal surfactant for water, oils, and CO_2
Langmuir Vol: 26 13861-13866 (2010)

Moser D, Bull D J, Cowpe J S, Roach D L, Ross D K, Noreus D and Tucker M G
An in situ neutron diffraction measurement of the pressure-temperature evolution of a MgD_2:TiD_2 mixture
High Pressure Research Vol: 30 643-652 (2010)

Moss R M, Abou Neel E A, Pickup D M, Twyman H L, Martin R A, Henson M D, Barney E R, Hannon A C, Knowles J C and Newport R J
The effect of zinc and titanium on the structure of calcium-sodium phosphate based glass
Journal of Non-Crystalline Solids Vol: 356 1319-1324 (2010)

Mulder F M, Assfour B, Huot J, Dingemans T J, Wagemaker M and Ramirez-Cuesta A J
Hydrogen in the metal-organic framework Cr MIL-53
Journal of Physical Chemistry C Vol: 114 10648-10655 (2010)

Muransky O, Barnett M R, Carr D G, Vogel S C and Oliver E C
Investigation of deformation twinning in a fine-grained and coarse-grained ZM20Mg alloy: Combined in situ neutron diffraction and acoustic emission
Acta Materialia Vol: 58 1503-1517 (2010)

Mutch K J, van Duijneveldt J S, Eastoe J, Grillo I and Heenan R K
Scaling the structure factors of protein limit colloid-polymer mixtures
Langmuir Vol: 26 1630-1634 (2010)

Myakonkaya O, Deniau B, Eastoe J, Rogers S E, Ghigo A, Hollamby M, Vesperinas A, Sankar M, Taylor S H, Bartley J K and Hutchings G J
Recovery and reuse of nanoparticles by tuning solvent quality
Chemsuschem Vol: 3 339-341 (2010)

Nakano T, Suehiro R, Hanazawa A, Watanabe K, Watanabe I, Amato A, Pratt F L and Nozue Y
muSR study on antiferromagnetism of alkali-metal clusters incorporated in zeolite sodalite
Journal of the Physical Society of Japan Vol: 79 (2010)

Nanu D E, Tucker M G, Haije W G, Vente J F and Bottger A J
Atom configurations in Pd-Au and Pd-Au-D alloys: a neutron total scattering and Reverse Monte Carlo study
Acta Materialia Vol: 58 5502-5510 (2010)

Nemkovski K S, Alekseev P A, Mignot J M, Goremychkin E A, Nikonov A A, Parfenov O E, Lazukov V N, Shitsevalova N Y and Dukhnenko A V
Spin dynamics in the electron-doped Kondo insulator $Yb_{1-x}Zr_xB_{12}$ $(x=_{0.2})$
Physical Review B Vol: 81 (2010)

Norberg S T, Hull S, Mathieu R and Eriksson S G
Local structural properties of $05BiMnO_3$-$05ATiO_3$ (A = Ba or Sr)
Chemical Communications Vol: 46 1455-1457 (2010)

O'Callaghan J M, McNamara H, Copley M P, Hanrahan J P, Morris M A, Steytler D C, Heenan R K and Holmes J D
Swelling of ionic and nonionic surfactant micelles by high pressure gases
Langmuir Vol: 26 7725-31 (2010)

Ohta H, Mansson M, Ikedo Y, Sugiyama J, Michioka C, Yoshimura K, Brewer J H, Ansaldo E J, Stubbs S L, Chow K H and Lord J S
Microscopic magnetic nature of water absorbed $Na_{0.35}CoO_2$ investigated by NMR, NQR and muSR
Physica C-Superconductivity and Its Applications Vol: 470 S755-S757 (2010)

Ok K M, O'Hare D, Smith R I, Chowdhury M and Fikremariam H
New large volume hydrothermal reaction cell for studying chemical processes under supercritical hydrothermal conditions using time-resolved in situ neutron diffraction
Review of Scientific Instruments Vol: 81 (2010)

Oka K, Azuma M, Chen W T, Yusa H, Belik A A, Takayama-Muromachi E, Mizumaki M, Ishimatsu N, Hiraoka N, Tsujimoto M, Tucker M G, Attfield J P and Shimakawa Y
Pressure-Induced Spin-State Transition in $BiCoO_3$
Journal of the American Chemical Society Vol: 132 9438-9443 (2010)

Omoto K, Norberg S T, Hull S, Aoto A and Hashimoto T
Neutron diffraction study of the crystal structure and structural phase transition of $La_{0.7}Ca_{0.3-x}Sr_xCrO_3$ (0 <= x <= 0.3) The relationship between thermodynamic behavior and crystal structure changes at the phase transition
Journal of Solid State Chemistry Vol: 183 392-401 (2010)

Oswald I D H, Millar D I A, Davidson A J, Francis D J, Marshall W G, Pulham C R, Cumming A S, Lennie A R and Warren J E
High-pressure structural studies of energetic compounds
High Pressure Research Vol: 30 280-291 (2010)

S Paddea JA Francis AM Paradowska PJ Bouchard IA Shibli
Characterisation of residual stresses in a welded P91 pipe section using neutron diffraction
High Temperature Defect Assesment 5 (HIDA-5), Surrey,UK, 25-28 Jun 2010

Paddea S, Francis J A, Paradowska AM, BouchardP J, Shibli I A
Residual stresses in as-welded P91 steel pipe
8th European Conference on Residual Stresses (ECRS8), 26-28 Jun 2010

Pagnotta S E, McLain S E, Soper A K, Bruni F and Ricci M A
Water and trehalose: How much do they interact with each other?
Journal of Physical Chemistry B Vol: 114 4904-4908 (2010)

Pan F, Zhao X B, Perumal S, Waigh T A, Lu J R and Webster J R P
Interfacial dynamic adsorption and structure of molecular layers of peptide surfactants
Langmuir Vol: 26 5690-5696 (2010)

Pang W K, Low I M, Kennedy S J and Smith R I
In situ diffraction study on decomposition of Ti_2AlN at 1500-1800 degrees C in vacuum
Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing Vol: 528 137-142 (2010)

Paradowska A M, Price J W H, Finlayson T R, Lienert U and Ibrahim R
Comparison of neutron and synchrotron diffraction measurements of residual stress in bead-on-plate weldments
Journal of Pressure Vessel Technology-Transactions of the Asme Vol: 132 (2010)

Paradowska A M, Price J W H, Kerezsi B, Dayawansa P and Zhao X L
Stress relieving and its effect on life of welded tubular joints
Engineering Failure Analysis Vol: 17 320-327 (2010)

Paradowska A, Price J, Finlayson T and Ibrahim R
Evaluation of residual stress measurements before and after post-weld heat treatment in the weld repairs
Journal of Physics: conference series Vol: 251 12050 1-4 (2010)

Paradowska A, Suder W and Williams S
Neutron diffraction residual stress measurements in key-hole laser formed weldments
Journal of Physics: conference series Vol: 251 12049 1-4 (2010)

Paradowska AM, Zhang S
In-situ loading on the neutron diffractometer Engin-X
TMS 2010 Annual Meeting & Exhibition (TMS 2010), Seattle, USA, 14-18 Feb 2010

Paradowska A, James J and Zhang S
Residual stress distribution in welds by neutron diffraction, visualisation and optimisation using SSCANSS
IIW 2010 (2010)

Paradowska AM
Investigation of residual stress in welds
LAP Lambert Academic Publishing AG & CO KG , ISBN 978-3-8383-69

Parker D, Smith M, Lancaster T, Steele A, Franke I, Baker P, Pratt F, Pitcher M, Blundell S, Clarke S
Control of the competition between a magnetic phase and a superconducting phase in cobalt-doped and nickel-doped NaFeAs using electron count
Physical Review Letters Vol: 104 (2010)

Parker S F
Reactions of iron atoms with benzene
Journal of Physical Chemistry A Vol: 114 1657-1664 (2010)

Parker S F
Spectroscopy and bonding in ternary metal hydride complexes-Potential hydrogen storage media
Coordination Chemistry Reviews Vol: 254 215-234 (2010)

Parker S F, Bowron D T, Imberti S, Soper A K, Refson K, Lox E S, Lopez M and Albers P
Structure determination of adsorbed hydrogen on a real catalyst
Chemical Communications Vol: 46 2959-2961 (2010)

Parker S F, Refson K, Hannon A C, Barney E R, Robertson S J and Albers P
Characterization of hydrous palladium oxide: implications for low-temperature carbon monoxide oxidation
Journal of Physical Chemistry C Vol: 114 14164-14172 (2010)

Parnell A J, Dunbar A D F, Pearson A J, Staniec P A, Dennison A J C, Hamamatsu H, Skoda M W A, Lidzey D G and Jones R A L
Depletion of PCBM at the cathode interface in P3HT/PCBM thin films as quantified via neutron reflectivity measurements
Advanced Materials Vol: 22 2444 (2010)

Parnell S R, Deppe M H, Ajraoui S, Parra-Robles J, Boag S and Wild J M
Measurement of laser heating in spin exchange optical pumping by NMR diffusion sensitization gradients
Journal of Applied Physics Vol: 107 (2010)

Pascual E C, Amores J M G, Puche R S, Castro M, Taira N, de Paz J R and Chapon L C
Zircon to scheelite phase transition induced by pressure and magnetism in $TbCrO_4$
Physical Review B Vol: 81 (2010)

Patwardhan S V, Holt S A, Kelly S M, Kreiner M, Perry C C and van der Walle C F
Silica condensation by a silicatein alpha homologue involves surface-induced transition to a stable structural intermediate forming a saturated monolayer
Biomacromolecules Vol: 11 3126-3135 (2010)

Paul A, Fallis I, Cooper C, Wess T, Thomas K, Heenan R, King S and Griffiths P
A contrast variation small-angle scattering study of the microstructure of 2,5-dimethyl-7-hydroxy-2,5-diazaheptadecane-toluene-butanol oil-in-water metallomicroemulsions
Soft Matter Vol: 6 2552-2556 (2010)

Paul A, James C, Heenan R K and Schweins R
Drug mimic induced conformational changes in model polymer-drug conjugates characterized by small-angle neutron scattering
Biomacromolecules Vol: 11 1978-1982 (2010)

Pelley C, Kargl F, Garcia-sakai V, Telling M, Fernandez-Alonso F and Demmel F
Guide design study for the high resolution backscattering spectrometer FIRES
Journal of Physics: conference series Vol: 251 12063 1-4 (2010)

Peterson V K, Kearley G J, Wu Y, Ramirez-Cuesta A J, Kemner E and Kepert C J
Local vibrational mechanism for negative thermal expansion: a combined neutron scattering and first-principles study
Angewandte Chemie-International Edition Vol: 49 585-588 (2010)

Petkov J T, Tucker I M, Penfold J, Thomas R K, Petsev D N, Dong C C, Golding S and Grillo I
The Impact of multivalent counterions, Al^{3+}, on the surface adsorption and self-assembly of the anionic surfactant alkyloxyethylene sulfate and anionic/nonionic surfactant mixtures
Langmuir Vol: 26 16699-16709 (2010)

Pieper O, Guidi T, Carretta S, van Slageren J, El Hallak F, Lake B, Santini P, Amoretti G, Mutka H, Koza M, Russina M, Schnegg A, Milios C J, Brechin E K, Julia A and Tejada J
Inelastic neutron scattering and frequency-domain magnetic resonance studies of S=4 and S=12 Mn_6 single-molecule magnets
Physical Review B Vol: 81 (2010)

Pietropaolo A, Andreani C, Rebai M, Giacomelli L, Gorini G, Cippo E P, Tardocchi M, Fazzi A, Rinati G V, Verona C, Marinelli M, Milani E, Frost C D and Schooneveld E M
Single-crystal diamond detector for time-resolved measurements of a pulsed fast-neutron beam
Epl Vol: 92 (2010)

Pietropaolo A, Gorini G, Festa G, Reali E, Grazzi F and Schooneveld E M
A neutron resonance capture analysis experimental station at the ISIS spallation source
Applied Spectroscopy Vol: 64 1068-1071 (2010)

Pitcher M, Lancaster T, Wright J, Franke I, Steele A, Baker P, Pratt F, Thomas W, Parker D, Blundell S, Clarke S
Compositional Control of the Superconducting Properties of LiFeAs
Journal of the American Chemical Society Vol: 132 10467-10476 (2010)

Postma H, Amkreutz L, Borella A, Clarijs M, Kamermans H, Kockelmann W, Paradowska A, Schillebeeckx P and Visser D
Non-destructive bulk analysis of the Buggenum sword by neutron resonance capture analysis and neutron diffraction
Journal of Radioanalytical and Nuclear Chemistry Vol: 283 641-652 (2010)

Pratt F L
Using Shubnikov-de Haas data to estimate the magnetic frustration parameter t '/t in the spin-liquid system kappa-ET$_2$Cu$_2$(CN)$_3$
Physica B-Condensed Matter Vol: 405 S205-S207 (2010)

Preuss M, da Fonseca J Q, Allen V, Prakash D G L and Daymond M R
Twinning in structural material with a hexagonal close-packed crystal structure
Journal of Strain Analysis for Engineering Design Vol: 45 377-389 (2010)

Pulham C R, Millar D I A, Oswald I D H and Marshall W G
High-pressure studies of energetic materials
High-Pressure Crystallography: from Fundamental Phenomena to Technological Applications Vol: 447-457 (2010)

Quintanilla J, Hillier A D, Annett J F and Cywinski R
Relativistic analysis of the pairing symmetry of the noncentrosymmetric superconductor LaNiC$_2$
Physical Review B Vol: 82 (2010)

Quintero-Castro D L, Lake B, Wheeler E M, Islam A, Guidi T, Rule K C, Izaola Z, Russina M, Kiefer K and Skourski Y
Magnetic excitations of the gapped quantum spin dimer antiferromagnet Sr$_3$Cr$_2$O$_8$
Physical Review B Vol: 81 (2010)

Reeder R J, Goodwin A L, Michel M, Phillips B L, Keen D A and Dove M T
Structure model of synthetic amorphous calcium carbonate
Geochimica Et Cosmochimica Acta Vol: 74 A855-A855 (2010)

Reiter G F, Senesi R and Mayers J
Changes in the zero-point energy of the protons as the source of the binding energy of water to a-phase DNA
Physical Review Letters Vol: 105 (2010)

Remhof A, Gremaud R, Buchter F, Lodziana Z, Embs J P, Ramirez-Cuesta T A J, Borgschulte A and Zuttel A
Hydrogen dynamics in lightweight tetrahydroborates
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics Vol: 224 263-278 (2010)

Risdiana Adachi T, Oki N, Koike Y, Suzuki T and Watanabe I
Muon spin relaxation study of the Cu spin dynamics in electron-doped high-T$_c$ superconductor Pr$_{0.86}$LaCe$_{0.14}$Cu$_{1-y}$ Zn$_y$O$_4$
Physical Review B Vol: 82 014506 (2010)

Risdiana Fitrilawati Hidayat R, Nugroho A A, Siregar R E, Tjia M O and Watanabe I
Intra- and inter-chain polaron diffusion in regio-random polythiophene studied by muon spin relaxation
Physica B-Condensed Matter Vol: 405 S381-S383 (2010)

Risdiana Fitrilawati Siregar R E, Hidayat R, Nugroho A A, Tjia M O, Ishii Y and Watanabe I
Field and temperature dependent charge transport characteristics in regio-regular poly(3-octylthiophene-2,5-diyl) studied by muon spin relaxation
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Roosen-Runge F, Hennig M, Seydel T, Zhang F J, Skoda M W A, Zorn S, Jacobs R M J, Maccarini M, Fouquet P and Schreiber F
Protein diffusion in crowded electrolyte solutions
Biochimica Et Biophysica Acta-Proteins and Proteomics Vol: 1804 68-75 (2010)

Ross N L, Spencer E C, Parker S F, Kolesnikov A I, Boerio-Goates J, Woodfield B F and Navrotsky A
Influence of adsorbed water on energetics of cassiterite nanoparticles
Geochimica Et Cosmochimica Acta Vol: 74 A884-A884 (2010)

Salman Z, Giblin S R, Lan Y, Powell A K, Scheuermann R, Tingle R and Sessoli R
Probing the magnetic ground state of the molecular dysprosium triangle with muon spin relaxation
Physical Review B Vol: 82 (2010)

Sanna S, Coneri F, Rigoldi A, Concas G, Giblin S R and De Renzi R
Competing orders suppressed by disorder around a hidden quantum critical point in high-T$_c$ cuprate superconductors
Physical Review B Vol: 82 (2010)

Sanna S, De Renzi R, Shiroka T, Lamura G, Prando G, Carretta P, Putti M, Martinelli A, Cimberle M R, Tropeano M and Palenzona A
Nanoscopic coexistence of magnetic and superconducting states within the FeAs layers of CeFeAsO$_{1-x}$F$_x$
Physical Review B Vol: 82 (2010)

Sardar K, Playford H Y, Darton R J, Barney E R, Hannon A C, Tompsett D, Fisher J, Kashtiban R J, Sloan J, Ramos S, Cibin G and Walton R I
Nanocrystalline cerium-bismuth oxides: synthesis, structural characterization, and redox properties
Chemistry of Materials Vol: 22 6191-6201 (2010)

Sartbaeva A, Wells S, Sommariva M, Lodge M, Jones M, Ramirez-Cuesta A, Li G and Edwards P
Formation of crystalline sodium hydride nanoparticles encapsulated within an amorphous framework
Journal of Cluster Science Vol: 21 543-549 (2010)

Schoofs F, Fix T, Hakimi A, Dhesi S S, van der Laan G, Cavill S A, Langridge S, MacManus-Driscoll J L and Blamire M G
Strain dependent defect mediated ferromagnetism in Mn-doped and undoped ZnO thin films
Journal of Applied Physics Vol: 108 (2010)

Seel A G, Sartbaeva A, Rammirez-Cuesta A J and Edwards P P
Inelastic neutron scattering of Na-zeolite A with in situ ammoniation: an examination of initial coordination
Physical Chemistry Chemical Physics Vol: 12 9661-9666 (2010)

Sefrioui Z, Visani C, Calderon M J, March K, Carretero C, Walls M, Rivera-Calzada A, Leon C, Anton R L, Charlton T R, Cuellar F A, Iborra E, Ott F, Imhoff D, Brey L, Bibes M, Santamaria J and Barthelemy A
All-manganite tunnel junctions with interface-induced barrier magnetism
Advanced Materials Vol: 22 5029 (2010)

Senkov O N, Miracle D B, Barney E R, Hannon A C, Cheng Y Q and Ma E
Local atomic structure of Ca-Mg-Zn metallic glasses
Physical Review B Vol: 82 (2010)

Shankland K, Markvardsen A J, Rowlatt C, Shankland N and David W I F
A benchmark method for global optimization problems in structure determination from powder diffraction data
Journal of Applied Crystallography Vol: 43 401-406 (2010)

Sharma J, King S M, Bohlin L and Clarke N
Apparatus for simultaneous rheology and small-angle neutron scattering from high-viscosity polymer melts and blends
Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment Vol: 620 437-444 (2010)

Sharma V K, Mitra S, Verma G, Hassan P A, Sakai V G and Mukhopadhyay R
Internal dynamics in SDS micelles: neutron scattering study
Journal of Physical Chemistry B Vol: 114 17049-17056 (2010)

Shen H H, Thomas R K, Penfold J and Fragneto G
Destruction and solubilization of supported phospholipid bilayers on silica by the biosurfactant surfactin
Langmuir Vol: 26 7334-7342 (2010)

Shimomura K, Bakule P, Pratt F L, Ohishi K, Ishida K, Watanabe I, Matsuda Y, Nishiyama K, Torikai E and Nagamine K
Pilot experiment for muonium photo ionization in GaAs
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Silverwood I P, Hamilton N G, Laycock C J, Staniforth J Z, Ormerod R M, Frost C D, Parker S F and Lennon D
Quantification of surface species present on a nickel/alumina methane reforming catalyst
Physical Chemistry Chemical Physics Vol: 12 3102-3107 (2010)

Silverwood I P, Hamilton N G, Staniforth J Z, Laycock C J, Parker S F, Ormerod R M and Lennon D
Persistent species formed during the carbon dioxide reforming of methane over a nickel-alumina catalyst
Catalysis Today Vol: 155 319-325 (2010)

Sirsch P, Clark N L N, Onut L, Burchell R P L, Decken A, McGrady G S, Daoud-Aladine A and Gutmann M J
Insights into metal borohydride and aluminohydride bonding: x-ray and neutron diffraction structures and a DFT and charge density study of Na(15-crown-5) EH4 (E = B, Al)
Inorganic Chemistry Vol: 49 11395-11402 (2010)

Smrcok L, Tunega D, Ramirez-Cuesta A J and Scholtzova E
The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite
Physics and Chemistry of Minerals Vol: 37 571-579 (2010)

Smrcok L, Tunega D, Ramirez-Cuesta A, Ivanov A and Valuchova J
The combined inelastic neutron scattering (INS) and solid-state study of hydrogen atoms dynamics in kaolinite dimethylsufloxide intercalate T
Clays and Clay Minerals Vol: 58 52-61 (2010)

Smyth T J, Perfumo A, Marchant R, Banat I M, Chen M L, Thomas R K, Penfold J, Stevenson P S and Parry N J
Directed microbial biosynthesis of deuterated biosurfactants and potential future application to other bioactive molecules
Applied Microbiology and Biotechnology Vol: 87 1347-1354 (2010)

Song X, Zhang S Y and Korsunsky A M
Strain gradient polycrystal plasticity analysis: Fe modelling and synchrotron X-ray diffraction
International Journal of Modern Physics B Vol: 24 10-17 (2010)

Soper A K
Network structure and concentration fluctuations in a series of elemental, binary, and tertiary liquids and glasses
Journal of Physics-Condensed Matter Vol: 22 (2010)

Soper A K
Recent water myths
Pure and Applied Chemistry Vol: 82 1855-1867 (2010)

Soper A K, Teixeira J and Head-Gordon T
Is ambient water inhomogeneous on the nanometer-length scale?
Proceedings of the National Academy of Sciences of the United States of America Vol: 107 E44-E44 (2010)

Springell R, Langridge S, Wildes A, Wilkins S B, Sanchez-Hanke C, Moore K T, Butterfield M T, Chivall J, Ward R C C, Wells M R and Lander G H
Chemical and magnetic structure of uranium/gadolinium multilayers studied by transmission electron microscopy, neutron scattering, and X-ray reflectivity
Physical Review B Vol: 81 (2010)

Srinivas G, Lovell A, Howard C A, Skipper N T, Ellerby M and Bennington S M
Structure and phase stability of hydrogenated first-stage alkali- and alkaline-earth metal-graphite intercalation compounds
Synthetic Metals Vol: 160 1631-1635 (2010)

Srinivas G, Lovell A, Skipper N T, Bennington S M, Kurban Z and Smith R I
Ammonia absorption in calcium graphite intercalation compound: in situ neutron diffraction, Raman spectroscopy and magnetization
Physical Chemistry Chemical Physics Vol: 12 6253-6259 (2010)

Srinivas G, M Ellerby et al
Magnetic behaviour in Dy$_{1-x}$Mm$_x$Co$_2$ compounds
Journal of Physics-Condensed Matter 22(43) (2010)

Stadler A M
Dynamics in Biological Systems as seen by QENS
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics Vol: 224 201-214 (2010)

Stevenson T, Comyn T P, Daoud-Aladine A and Bell A J
Change in periodicity of the incommensurate magnetic order towards commensurate order in bismuth ferrite lead titanate
Journal of Magnetism and Magnetic Materials Vol: 322 L64-L67 (2010)

Stewart J R, Hillier A D, Hillier J M and Cywinski R
Structural and dynamical study of moment localization in beta-Mn$_{1-x}$In$_x$
Physical Review B Vol: 82 144439 (2010)

Stock C, Cowley R A, Buyers W J L, Frost C D, Taylor J W, Peets D, Liang R, Bonn D and Hardy W N
Effect of the pseudogap on suppressing high energy inelastic neutron scattering in superconducting YBa$_2$Cu$_3$O$_{6.5}$
Physical Review B Vol: 82 (2010)

Stock C, Cowley R A, Taylor J W and Bennington S M
High-energy neutron scattering from hydrogen using a direct geometry spectrometer
Physical Review B Vol: 81 (2010)

Stock C, L Van Eijck et al
Interplay between static and dynamic polar correlations in relaxor Pb(Mg$_{1/3}$Nb$_{2/3}$)O$_3$
Physical Review B 81(14) (2010)

Sugano T, Blundell S J, Lancaster T, Pratt F L and Mori H
Magnetic order in the purely organic quasi-one-dimensional ferromagnet 2-benzimidazolyl nitronyl nitroxide
Physical Review B Vol: 82 (2010)

Sugiyama J, Ikedo Y, Mansson M, Brewer J H, Stubbs S L, Ansaldo E J, Chow K H, Lord J S, Ohta H, Michioka C and Yoshimura K
Magnetic and superconducting nature of Na$_{0.35}$CoO$_2$ .yH$_2$O and Na$_{0.35}$CoO$_2$ .yD$_2$O investigated by muon-spin spectroscopy
Physical Review B Vol: 82 214505 (2010)

Sugiyama J, Ikedo Y, Mukai K, Nozaki H, Mansson M, Ofer O, Harada M, Kamazawa K, Miyake Y, Brewer J H, Ansaldo E J, Chow K H, Watanabe I and Ohzuku T
Low-temperature magnetic properties and high-temperature diffusive behavior of LiNiO$_2$ investigated by muon-spin spectroscopy
Physical Review B Vol: 82 (2010)

Suzuki K, Adachi T, Tanabe Y, Koike Y, Kawamata T, Risdiana Suzuki T and Watanabe I
Hole trapping by Ni, Kondo effect, and electronic phase diagram in nonsuperconducting Ni-substituted La$_{2-x}$Sr$_x$Cu$_{1-y}$NiyO$_4$
Physical Review B Vol: 82 (2010)

Suzuki T, Watanabe I, Yamada F, Yamada M, Ishii Y, Kawamata T, Goto T and Tanaka H
Pressure-induced new magnetic phase in Tl(Cu$_{0.985}$Mg$_{0.015}$)Cl$_3$ probed by muon spin rotation
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Suzuki T, Yamada F, Yamada M, Kawamata T, Ishii Y, Watanabe I, Goto T and Tanaka H
Low-energy spin dynamics in randomness-introduced spin-gap systems Tl$_{1-x}$K$_x$CuCl$_3$ (0.40 <= x <= 0.65) probed by zero-and longitudinal-field muon spin relaxation
Physical Review B Vol: 82 (2010)

Swenson J, Sjostrom J and Fernandez-Alonso F
Reduced mobility of di-propylene glycol methylether in its aqueous mixtures by quasielastic neutron scattering
Journal of Chemical Physics Vol: 133 (2010)

Tabor R F, Eastoe J, Dowding P J, Grillo I and Rogers S E
Bidisperse colloids: Nanoparticles and microemulsions in coexistence
Journal of Colloid and Interface Science Vol: 344 447-450 (2010)

Tanabe Y, Suzuki K, Adachi T, Koike Y, Kawamata T, Risdiana Suzuki T and Watanabe I
Change of the ground state upon hole doping unveiled by Ni impurity in high-T$_c$ cuprates
Journal of the Physical Society of Japan Vol: 79 (2010)

Tanaka Y, Kojima T, Takata Y, Chainani A, Lovesey S W, Knight K S, Takeuchi T, Oura M, Senba Y, Ohashi H and Shin S
Determination of structural chirality of berlinite and quartz using resonant X-ray diffraction with circularly polarized X-rays
Physical Review B Vol: 81 (2010)

Tassel C, Kang J, Lee C, Hernandez O, Qiu Y, Paulus W, Collet E, Lake B, Guidi T, Whangbo M H, Ritter C, Kageyama H and Lee S H
Ferromagnetically coupled Shastry-Sutherland quantum spin singlets in (CuCl)LaNb$_2$O$_7$
Physical Review Letters Vol: 105 (2010)

Thomas L H, Blagden N, Gutmann M J, Kallay A A, Parkin A, Seaton C C and Wilson C C
Tuning proton behavior in a ternary molecular complex
Crystal Growth & Design Vol: 10 2770-2774 (2010)

JWG Thomason DJ Adams DJS Findlay ISK Gardner SJS Jago B Jones et al
Injection upgrades for the ISIS synchrotron
Proc 1st International Particle Accelerator Conference (IPAC'10), Kyoto, Japan, 23-28 May 2010

Todorov I, Chung D Y, Claus H, Gray K E, Li Q A, Schleuter J, Bakas T, Douvalis A P, Gutmann M and Kanatzidis M G
Selective Substitution of Cr in CaFe$_4$As$_3$ and Its Effect on the spin density wave
Chemistry of Materials Vol: 22 4996-5002 (2010)

Tomiyasu K, Kageyama H, Lee C, Whangbo M H, Tsujimoto Y, Yoshimura K, Taylor J W, Llobet A, Trouw F, Kakurai K and Yamada K
Magnetic excitations in infinite-layer antiferromagnetic insulator
Journal of the Physical Society of Japan Vol: 79 (2010)

Tomkinson J
Comment on: "FTIR and FTRaman spectra, assignments, ab initio HF and DFT analysis of 4-nitrotoluene" by S Ramalingam et al, Spectrochemica Acta A 75 (2010) 1308-1314
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy Vol: 77 539-540 (2010)

Tomkinson J
Comment on: "FTIR, FT-Raman, scaled quantum chemical studies of the structure and vibrational spectra of 1,5-dinitronaphthalene" by Arivazhaga et al Spectrochim Acta A72 (2009) 941-946
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy Vol: 75 1377-1379 (2010)

Tomkinson J and Parker S F
Vibrational spectra of benzene chromium tricarbonyl and its mesityl analogue: a study by neutron spectroscopy
Journal of Physical Chemistry A Vol: 114 12605-12612 (2010)

Tomkinson J, Parker S F and Lennon D
No evidence for Evans' holes in the A, B, C vibrational structure of potassium dihydrogen arsenate
Journal of Chemical Physics Vol: 133 (2010)

Tomono D, Kawamata T, Hirayama Y, Iwasaki M, Watanabe I, Ishida K and Matsuzaki T
Progress in development of new muSR spectrometer at RIKEN-RAL
Advanced Science Research Symposium 2009: Positron, Muon and Other Exotic Particle Beams for Materials and Atomic/Molecular Sciences Vol: 225 (2010)

Tran V H, Hillier A D and Adroja D T
Reply to "Comment on 'Muon-spin-rotation study of the superconducting properties of Mo$_3$Sb$_7$'"
Physical Review B Vol: 82 (2010)

Tran V H, Hillier A D, Adroja D T and Kaczorowski D
Muon spin rotation and relaxation studies of the filled skutterudite superconductor ThPt$_4$Ge$_{12}$
Journal of Physics-Condensed Matter Vol: 22 (2010)

Tremsin A S, McPhate J B, Vallerga J V, Siegmund O H W, Kockelmann W, Steuwer A and Feller W B
A high resolution neutron counting sensors in strain mapping through a transmission Bragg edge diffraction
2010 IEEE Sensors Vol: 2316-2318 (2010)

Trickett K, Brice H, Myakonkaya O, Eastoe J, Rogers S E, Heenan R K and Grillo I
Microemulsion-based organogels containing inorganic nanoparticles
Soft Matter Vol: 6 1291-1296 (2010)

Trickett K, Xing D Z, Enick R, Eastoe J, Hollamby M J, Mutch K J, Rogers S E, Heenan R K and Steytler D C
Rod-Like Micelles Thicken CO_2
Langmuir Vol: 26 83-88 (2010)

Trickett K, Xing D, Eastoe J, Enick R, Mohamed A, Hollamby M J, Cummings S, Rogers S E and Heenan R K
Hydrocarbon metallosurfactants for CO_2
Langmuir Vol: 26 4732-7 (2010)

Tucker I, Penfold J, Thomas R K, Dong C C, Golding S, Gibson C and Grillo I
Surface and solution properties of anionic/nonionic surfactant mixtures of alkylbenzene sulfonate and triethyleneglycol decyl ether
Langmuir Vol: 26 10614-10626 (2010)

Tucker I, Petkov J, Penfold J and Thomas R K
Adsorption of nonionic and mixed nonionic/cationic surfactants onto hydrophilic and hydrophobic cellulose thin films
Langmuir Vol: 26 8036-8048 (2010)

Utfeld C, Laverock J, Haynes T D, Dugdale S B, Duffy J A, Butchers M W, Taylor J W, Giblin S R, Analytis J G, Chu J H, Fisher I R, Itou M and Sakurai Y
Bulk electronic structure of optimally doped $Ba(Fe_{1-x}Co_x)_2As_2$
Physical Review B Vol: 81 (2010)

Vaknin D, Garlea V O, Demmel F, Mamontov E, Nojiri H, Martin C, Chiorescu I, Qiu Y, Kogerler P, Fielden J, Engelhardt L, Rainey C and Luban M
Level crossings and zero-field splitting in the Cr_8-cubane spin cluster studied using inelastic neutron scattering and magnetization
Journal of Physics-Condensed Matter Vol: 22 (2010)

Varga B, Migliardo F, Takacs E, Vertessy B, Magazu S and Telling M T F
Study of solvent-protein coupling effects by neutron scattering
Journal of Biological Physics Vol: 36 207-220 (2010)

Vaz P D, Nolasco M M, Gil F, Ribeiro-Claro P J A and Tomikinson J
Hydrogen-bond dynamics of C-H center O interactions: the chloroform acetone case
Chemistry-a European Journal Vol: 16 9010-9017 (2010)

Vecchini C, Poienar M, Damay F, Adamopoulos O, Daoud-Aladine A, Lappas A, Perez-Mato J, Chapon L and Martin C
Magnetoelastic coupling in the frustrated antiferromagnetic triangular lattice $CuMnO_2$
Physical Review B Vol: 82 (2010)

Vilminot S, Baker P, Blundell S, Sugano T, Andre G and Kurmoo M
Giant magnetic hardness in the synthetic mineral ferrimagnet $K_2Co3II(OH)_2(SO_4)_3(H_2O)_2$
Chemistry of Materials Vol: 22 4090-4095 (2010)

Waki T, Kajinami Y, Tabata Y, Nakamura H, Yoshida M, Takigawa M and Watanabe I
Spin-singlet state formation in the cluster Mott insulator $GaNb_4S_8$ studied by muSR and NMR spectroscopy
Physical Review B Vol: 81 (2010)

Wang C H, Christianson A D, Lawrence J M, Bauer E D, Goremychkin E A, Kolesnikov A I, Trouw F, Ronning F, Thompson J D, Lumsden M D, Ni N, Mun E D, Jia S, Canfield P C, Qiu Y and Copley J R D
Neutron scattering and scaling behavior in URu_2Zn_{20} and $YbFe_2Zn_{20}$
Physical Review B Vol: 82 (2010)

Wang C H, Lawrence J M, Christianson A D, Goremychkin E A, Fanelli V R, Gofryk K, Bauer E D, Ronning F, Thompson J D, de Souza N R, Kolesnikov A I and Littrell K C
Kondo behavior, ferromagnetic correlations, and crystal fields in the heavy-fermion compounds Ce_3X (X = In, Sn)
Physical Review B Vol: 81 (2010)

Wang S K, Mamontov E, Bai M, Hansen F Y, Taub H, Copley J R D, Sakai V G, Gasparovic G, Jenkins T, Tyagi M, Herwig K W, Neumann D A, Montfrooij W and Volkmann U G
Localized diffusive motion on two different time scales in solid alkane nanoparticles
Epl Vol: 91 (2010)

Wheeler E M, Lake B, Islam A, Reehuis M, Steffens P, Guidi T and Hill A H
Spin and orbital order in the vanadium spinel MgV_2O_4
Physical Review B Vol: 82 (2010)

Wilding M, Guthrie M, Bull C and Tucker M
Neutron diffraction studies of amorphous materials at high pressure
Geochimica Et Cosmochimica Acta Vol: 74 A1132-A1132 (2010)

Willers T, Hu Z, Hollmann N, Korner P O, Gegner J, Burnus T, Fujiwara H, Tanaka A, Schmitz D, Hsieh H H, Lin H J, Chen C T, Bauer E D, Sarrao J L, Goremychkin E, Koza M, Tjeng L H and Severing A
Crystal-field and Kondo-scale investigations of $CeMIn_5$ (M=Co, Ir, and Rh): a combined X-ray absorption and inelastic neutron scattering study
Physical Review B Vol: 81 (2010)

Wu C Z, Wu G T, Xiong Z T, David W I F, Ryan K R, Jones M O, Edwards P P, Chu H L and Chen P
Stepwise phase transition in the formation of lithium amidoborane
Inorganic Chemistry Vol: 49 4319-4323 (2010)

Xu P G, Oliver E C, Paradowska A M
In situ neutron diffraction during thermo-mechanically controlled process for low alloy steel
In-situ Studies with Photons, Neutrons and Electrons Scattering , Chapter 12 175-190, ISBN 9783642147937

Yan Y, Telepeni I, Yang S H, Lin X, Kockelmann W, Dailly A, Blake A J, Lewis W, Walker G S, Allan D R, Barnett S A, Champness N R and Schroder M
Metal-organic polyhedral frameworks: a high H_2 adsorption capacities and neutron powder diffraction studies
Journal of the American Chemical Society Vol: 132 4092 (2010)

Yang G D, Jiang Z, Shi H H, Jones M O, Xiao T C, Edwards P P and Yan Z F
Study on the photocatalysis of F-S co-doped TiO_2 prepared using solvothermal method
Applied Catalysis B-Environmental Vol: 96 458-465 (2010)

Yin C L, Li G B, Kockelmann W A, Liao F H, Attfield J P and Lin J H
Frustrated and unfrustrated magnetic orders in the 10H perovskite $Ba_5Sb_{1-x}Mn_{4+x}O_{15\text{-delta}}$
Chemistry of Materials Vol: 22 3269-3276 (2010)

Zaberchik M, Chashka K, Patlgan L, Maniv A, Baines C, King P and Kanigel A
Possible evidence of a two-gap structure for the Cu_xTiSe_2 superconductor
Physical Review B Vol: 81 220505 (2010)

Zaleski P, Szymanski K, Przewoznik J, Recko K, Cottrell S and Dobrzynski L
Cr_3Si doped by Co studied by muon spin relaxation and scanning electron microscopy techniques
Journal of Alloys and Compounds Vol: 498 5-12 (2010)

Zarbakhsh A, Campana M, Mills D and Webster J R P
Structural studies of aliphatic substituted phthalocyanine-lipid multilayers
Langmuir Vol: 26 15383-15387 (2010)

Zarbakhsh A, Campana M, Webster J R P and Wojciechowski K
Stabilization of alkylated azacrown ether by fatty acid at the air-water interface
Langmuir Vol: 26 18194-18198 (2010)

Zhang B, Kurmoo M, Mori T, Zhang Y, Pratt F L and Zhu D B
Polymorphism in hybrid organic-inorganic bilayered magnetic conductors $(BEDT\text{-}TTF)_3(FeCl_4)$-Cl-(III)$_2$. BEDT-TTF = bis(ethylenedithio)tetrathiafulvalene
Crystal Growth & Design Vol: 10 782-789 (2010)

Zhang F J, Weggler S, Ziller M J, Ianeselli L, Heck B S, Hildebrandt A, Kohlbacher O, Skoda M W A, Jacobs R M J and Schreiber F
Universality of protein reentrant condensation in solution induced by multivalent metal ions
Proteins-Structure Function and Bioinformatics Vol: 78 3450-3457 (2010)

Zhang , H, Baker P and Grantz P
Fabrication and electrical properties of bulk textured $LiCoO_2$
Journal of the American Ceramic Society Vol: 93 1856-1859 (2010)

Zhang Z M, Kennedy B J, Howard C J, Jang L Y, Knight K S, Matsuda M and Miyake M
X-ray absorption and neutron diffraction studies of $(Sr_{1-x}Ce_x)MnO_3$: transition from coherent to incoherent static Jahn-Teller distortions
Journal of Physics-Condensed Matter Vol: 22 (2010)

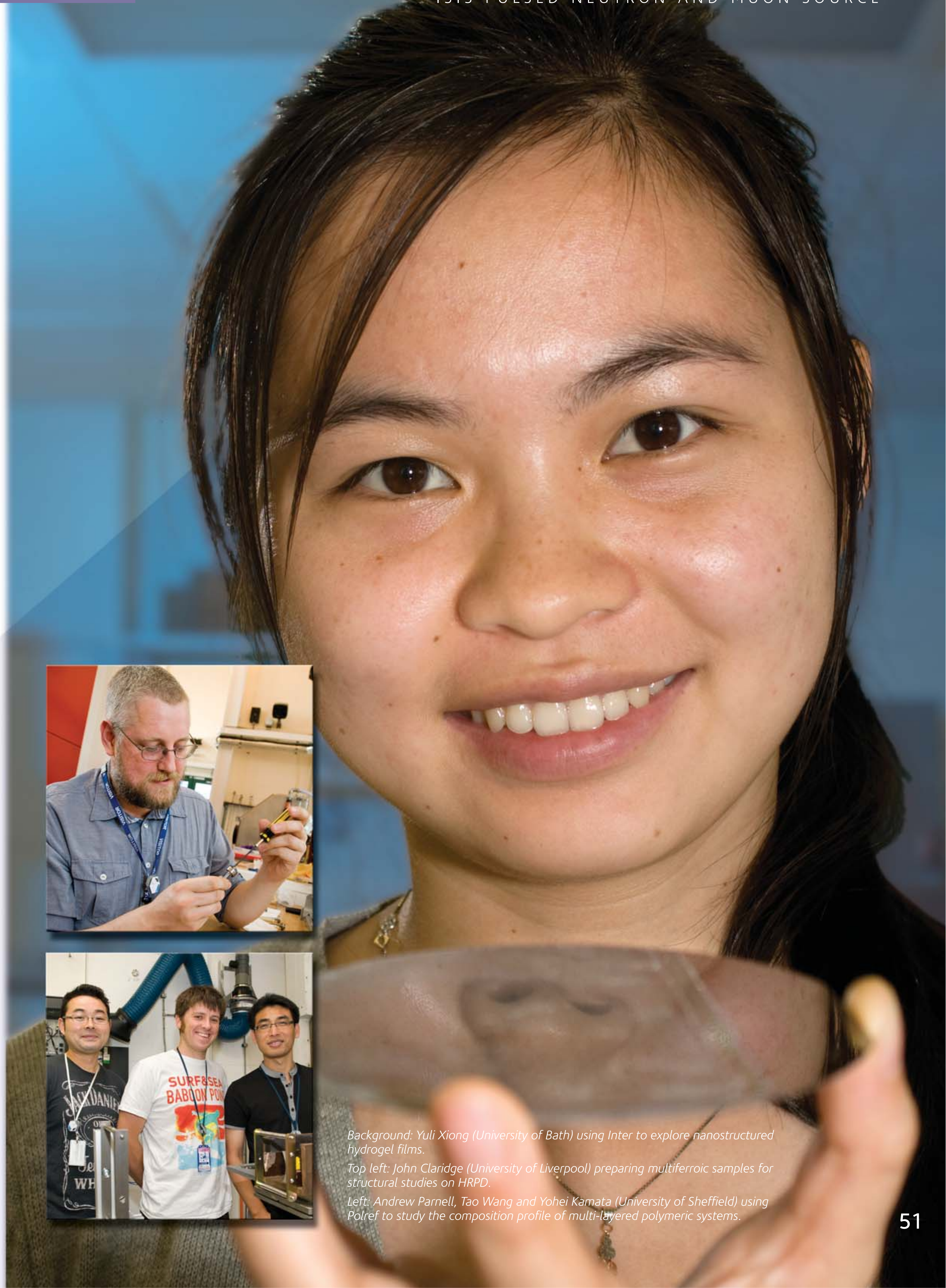
Zhang Z Y, Pen Y, Edyvean R G, Banwart S A, Dalgliesh R M and Geoghegan M
Adhesive and conformational behaviour of mycolic acid monolayers
Biochimica Et Biophysica Acta-Biomembranes Vol: 1798 1829-1839 (2010)

SY Zhang A Paradowska J Kelleher W Kockelmann
Neutrons for materials engineering at ISIS: present and future capabilities
The 8th European Conference on Residual Stresses , Riva del Garda, Italy, 26-28 Aug 2010

SY Zhang B Abbey W Vorster AM Korsunsky
Feasibility study of neutron strain tomography
12th European Powder Diffraction Conference, Darmstadt, Germany, 27-30 Aug 2010

Zhou H D, Jo Y J, Carpino J F, Munoz G J, Wiebe C R, Cheng J G, Rivadulla F and Adroja D T
Orbital fluctuations in the S=1/2 Mott insulator Sr_2VO_4
Physical Review B Vol: 81 (2010)

Zorko A, Bert F, Mendels P, Marty K and Bordet P
Ground state of the easy-axis rare-earth Kagome langasite $Pr_3Ga_5SiO_{14}$
Physical Review Letters Vol: 104 (2010)



Background: Yuli Xiong (University of Bath) using Inter to explore nanostructured hydrogel films.

Top left: John Claridge (University of Liverpool) preparing multiferroic samples for structural studies on HRPD.

Left: Andrew Parnell, Tao Wang and Yohei Kamata (University of Sheffield) using Polref to study the composition profile of multi-layered polymeric systems.

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

ISIS seminars 2010-2011

11 May 2010
Nicola Marzari (Oxford University)
Characterizing complex materials from first-principles

25 May 2010
Roger Pynn (Indiana University, USA)
Some recent progress with spin echo scattering angle measurement

8 June 2010
Dr Tomaso Aste (University of Kent)
Insights into disorder

6 July 2010
Evgenyi Shalaev (Groton Laboratories, USA)
Water relationships in solid pharmaceuticals - from small molecules to biological systems

13 July 2010
Brahim Elouadi (Universite de la Rochelle, France)
Correlation between the composition and ferroelectric phase transitions in Lithium niobate and related non stoichioemtric compounds

15 July 2010
Gabriel Kotliar (Rutgers University, USA)
Towards an ab-initio theory of correlated materials: the challenge of the iron pnictides

20 July 2010
Paola Verrucchi (Istituto dei Sistemi Complessi, Firenze, Italy)
Optimal dynamics for quantum-state and entanglement transfer through homogeneous quantum wires

22 July 2010
Senthil Todadri (Massachusetts Institute of Technology, USA)
Quantum spin liquids and the Mott transition

22 July 2010
Jason Ho (Ohio State University, USA)
Quantum simulation with cold atoms: challenges and opportunities

30 July 2010
Alexei Tsvelik (Brookhaven National Laboratory, USA)
Visual demonstration of spinon confinement

10 August 2010
Crispin Barnes (Cambridge University)
Experimental and theoretical analysis of magnetic moment enhancement in oxygen-deficient EuO

14 September 2010
Shinji Kohara (Japan Synchrotron Radiation Research Institute)
High-energy X-ray diffraction studies of disordered materials at SPring8

7 October 2010
Eberhard Engel (J.W.Goethe-Universitaet, Frankfurt, Germany)
Insulating ground states of transition-metal monoxides from exact exchange

14 October 2010
Professor Michel Gingras (University of Waterloo and Canadian Institute for Advanced Research, Canada)
Open problems in the physics of rare earth magnetic pyrochlore oxides

2-9 November 2010
Pierre Toledano (Univ. de Picardie, Amiens, France)
Theory of the amorphous solid state
Symmetry replication in liquid crystals, superconductors and multiferroics

18 January 2011
Natalie Malikova (Laboratoire Leon Brillouin, France)
Hydrophobic ions and polyelectrolytes in aqueous solution

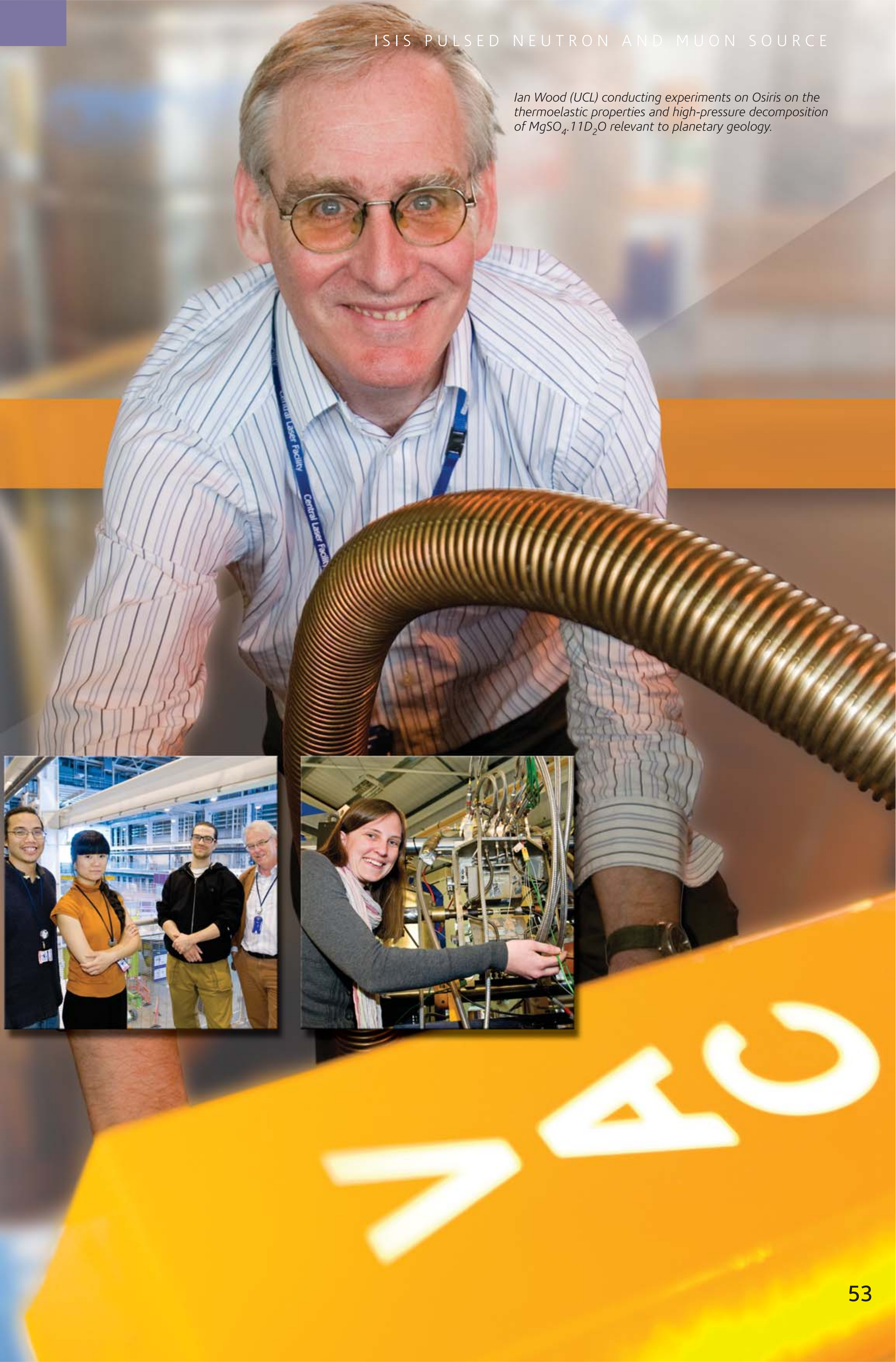
15 February 2011
Enrique Sanchez Marcos (Universidad de Sevilla, Spain)
Proving the synergy of MD-XAS for solving the structure of metal ion solutions: the actinide aqua ion contraction and the Pt environment in an anticancer drug

22 February 2011
Oleg Kirichek (ISIS)
New sample environment at ISIS

1 March 2011
Rahul Roy (Oxford University)
Topological invariants and topological insulators

22 March 2011
Peter Weightman (Liverpool University)
The physics of life: does quantum mechanics play a non trivial role?

29 March 2011
Bill David (ISIS)
Neutron, X-ray and computational studies of novel hydrogen storage materials



Ian Wood (UCL) conducting experiments on Osiris on the thermoelastic properties and high-pressure decomposition of $MgSO_4.11D_2O$ relevant to planetary geology.

Right: Greg Chasse (University of Wales, Bangor), Tian Kun (Semmelweiss University), Neville Greaves (Aberystwyth University) and David Setiad (University of Nottingham) exploring the structure and dynamics of biocompatible dental glass cements on Nimrod.

Far right: Nichola Middleton-Stewart (University of Manchester) using Engin-X to study temperature dependence of the coerciver stress in rhombohedral lead zirconate ceramics.

ISIS panels

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*	D McMorrow *Chair*	N Skipper *Chair*	D Paul *Chair*	J Bouchard *Chair*
D Allan	C Cabrillo	D Barlow	A Boothroyd	D Book	H Dilger	M Hutchings
A Bombardi	F Meersman	W Bouman	P Dai	F Bresme	A Drew	N O'Dowd
J Claridge	G Monaco	S Clarke	R De Renzi	S Golunski	R Osborn	J Quinta da Fonseca
A Florence	G Mountjoy	T Hase	B Gaulin	M Jones	I Terry	D Rugg
A Goodwin	J Tse	J Lakey	B Lake	M Krystyniak	J Titman	A Steuwer
M Hofmann	R Winter	T Nylander	O Petrenko	MP Marques	T Veal	H Stone
B Kennedy		E Sivaniah	S Raymond	A Nogales Ruiz	I Watanabe	J Yates
P Slater		P Steadman	D Reznik	R Senesi		
R Walton		I Tucker	N Shannon			
A Wills						
I Wood						
		C Neylon				
M Tucker	D Bowron	J Webster	J Taylor	J Mayers	S Cottrell	SY Zhang
S Hull	A Hannon	S Langridge	T Perring	F Demmel	A Hillier	J Kelleher

ISIS Facility Access Panel membership for the June 2011 meetings. The FAPs meet 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**	D Gregory A Powell	*University of Glasgow* *Heriot-Watt University*
IUG2	**Liquids & Amorphous**	J Holbrey B Webber	*Queen's University Belfast* *University of Kent*
IUG3	**Large Scale Structures**	A Zarbaksh J Lakey	*Queen Mary College, London* *University of Newcastle*
IUG4	**Excitations**	J Goff P Salmon	*Royal Holloway University London* *Bath University*
IUG5	**Molecular Spectroscopy**	F Kargl D Lennon	*University of Aberdeen* *University of Glasgow*
IUG6	**Muons**	S Kilcoyne T Lancaster A Drew	*University of Salford* *University of Oxford* *Queen Mary University of London*
IUG7	**Engineering**	M Fitzpatrick M Preuss D Dye	*The Open University* *University of Manchester* *Imperial College London*

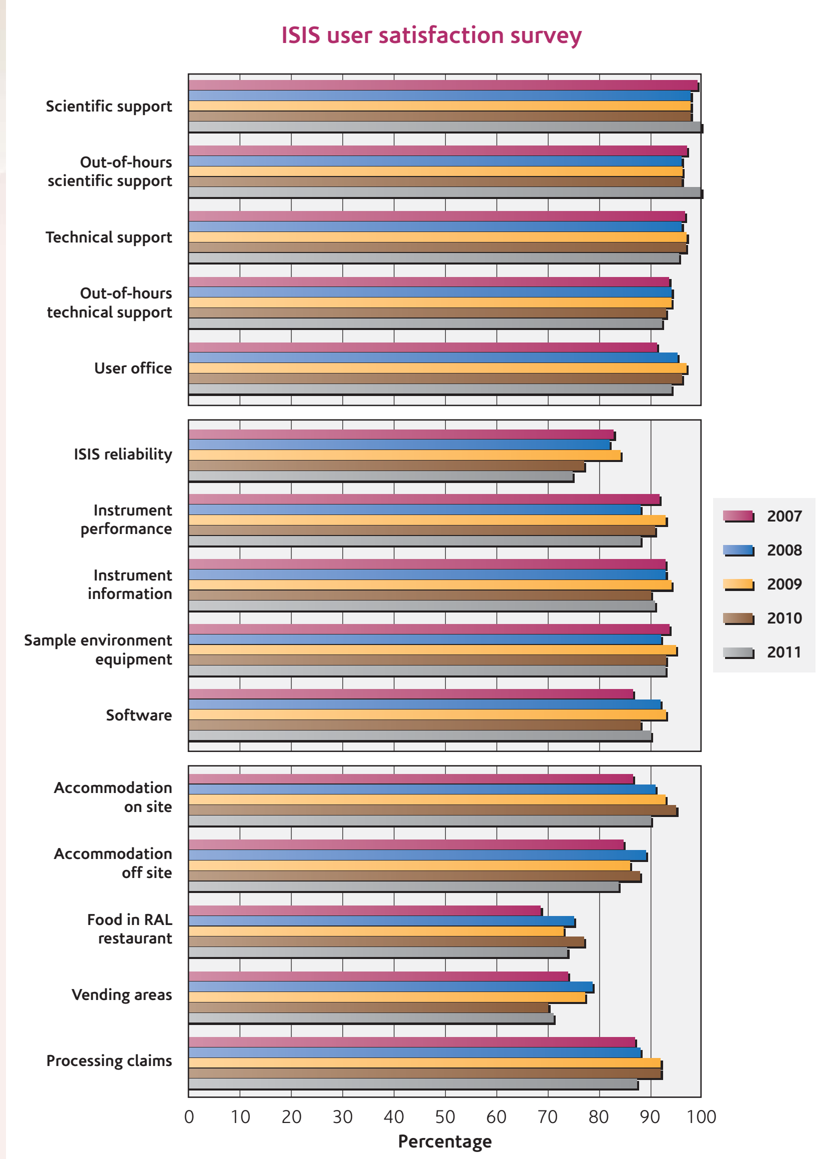
	Director ISIS	A D Taylor
	ISS Division Head	U Steigenberger
	IEO Division Head	Z A Bowden
	II Division Head	D Greenfield
	IDM Division Head	R L McGreevy
	ISS Deputy Division Head	P J C King
	A D Kaye	ISIS User Programme Manager

ISIS User Committee Membership for June 2011. The IUC exists to represent the user community on all aspects of facility operation.

Ricardo Fernandez-Perea (IEM, Spain), Febienne Barroso-Bujans and Carlos Cabrill (CSIC, Spain) during their studies of the kinetics of molecular intercalation into graphite oxide on Nimrod

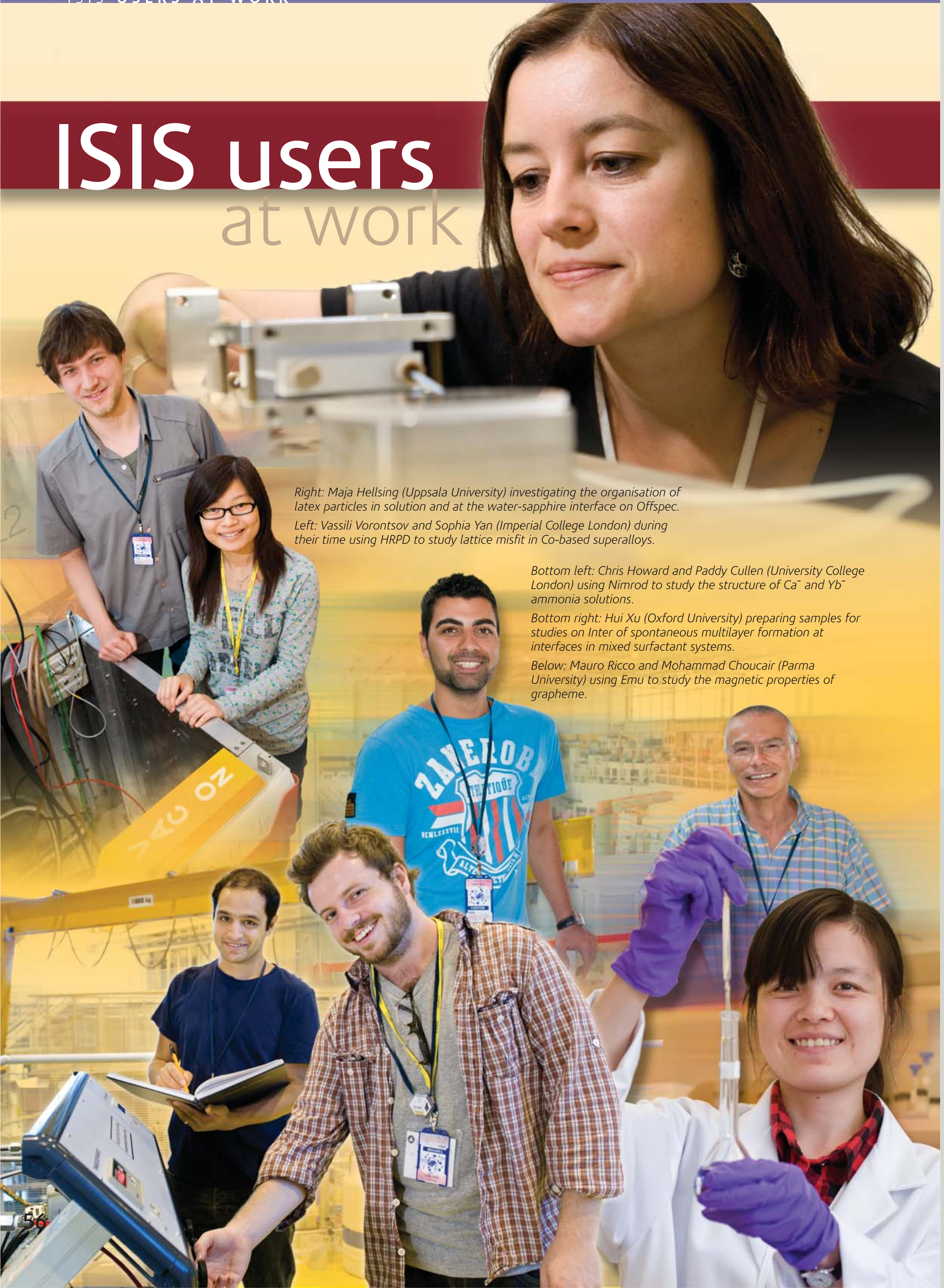
User Satisfaction

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 2007 to 2011.

ISIS users at work



Right: Maja Hellsing (Uppsala University) investigating the organisation of latex particles in solution and at the water-sapphire interface on Offspec.

Left: Vassili Vorontsov and Sophia Yan (Imperial College London) during their time using HRPD to study lattice misfit in Co-based superalloys.

Bottom left: Chris Howard and Paddy Cullen (University College London) using Nimrod to study the structure of Ca^- and Yb^- ammonia solutions.

Bottom right: Hui Xu (Oxford University) preparing samples for studies on Inter of spontaneous multilayer formation at interfaces in mixed surfactant systems.

Below: Mauro Ricco and Mohammad Choucair (Parma University) using Emu to study the magnetic properties of graphene.

ISIS

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