



The ISIS Neutron and Muon Source

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ISIS Neutron and Muon Source Annual Review 2017

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



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

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

Foreword

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

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

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

Robert McGreevy, ISIS Director



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

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



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



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

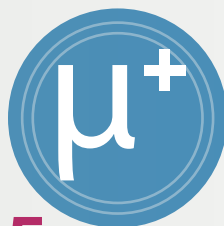
The ISIS Neutron and Muon Source

The ISIS neutron and muon source is a world-leading centre for research at the STFC Rutherford Appleton Laboratory near Oxford. Our suite of neutron and muon instruments give unique insights into the properties of materials on the atomic scale.

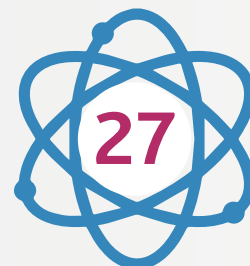
We are part of the global research structure, providing tools for over 2,000 scientists a year to use our suite of 32 instruments.

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

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



5 Muon instruments



27 Neutron instruments



including 1907 school pupils and public



607 PhD students visited as users



1156 proposals received from 35 countries

2278 user visits



56 Companies

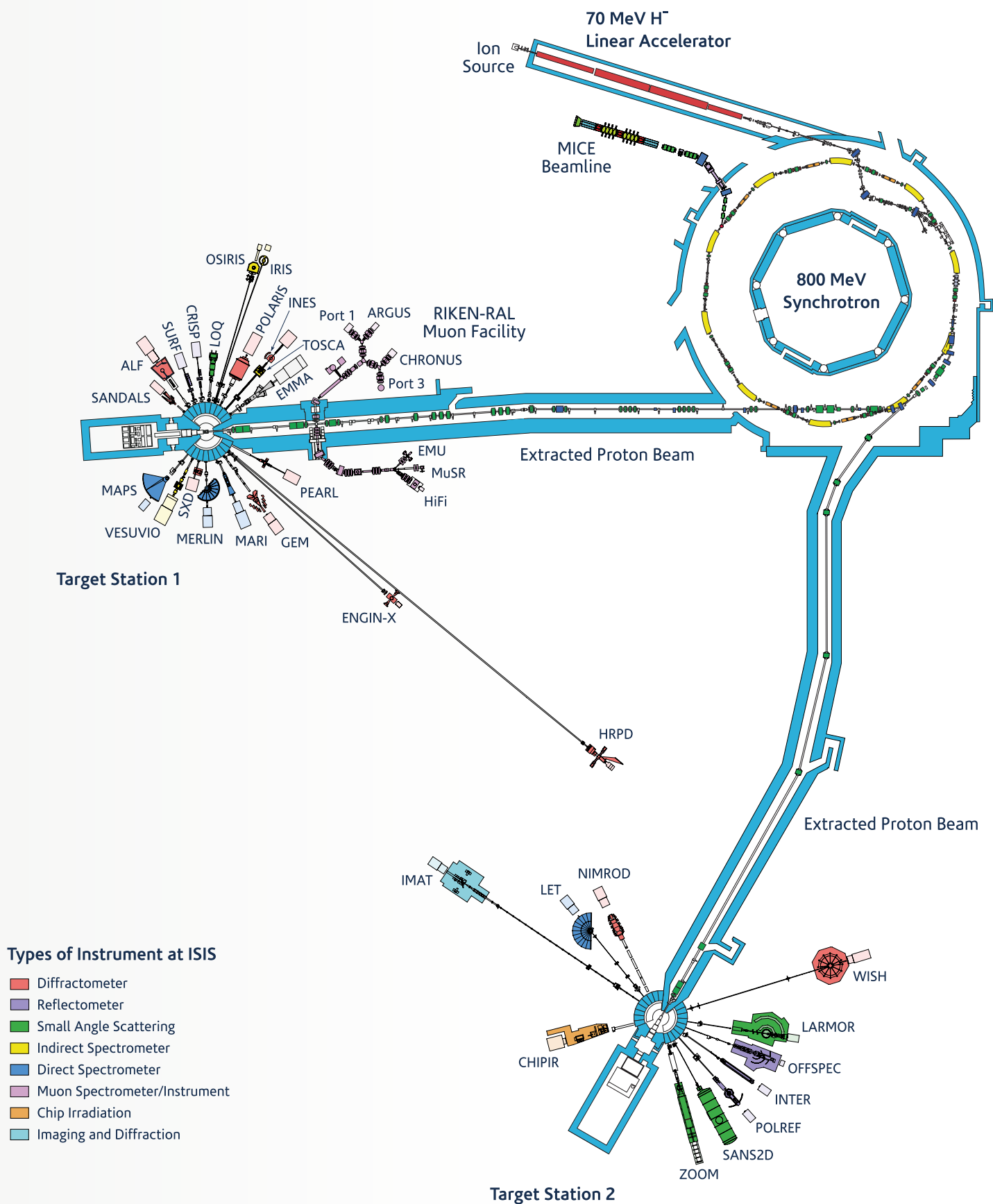
involved in experiments including healthcare, energy, automotive and chemical engineering



486 Journal publications



284 Xpress proposals

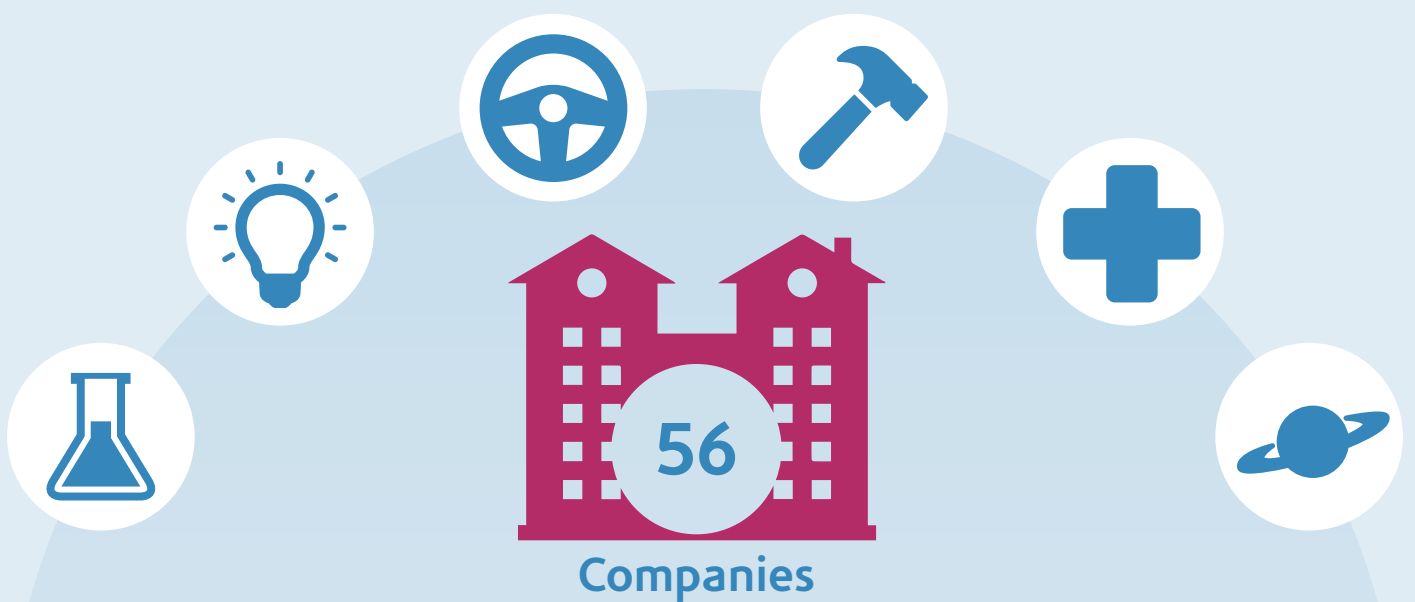
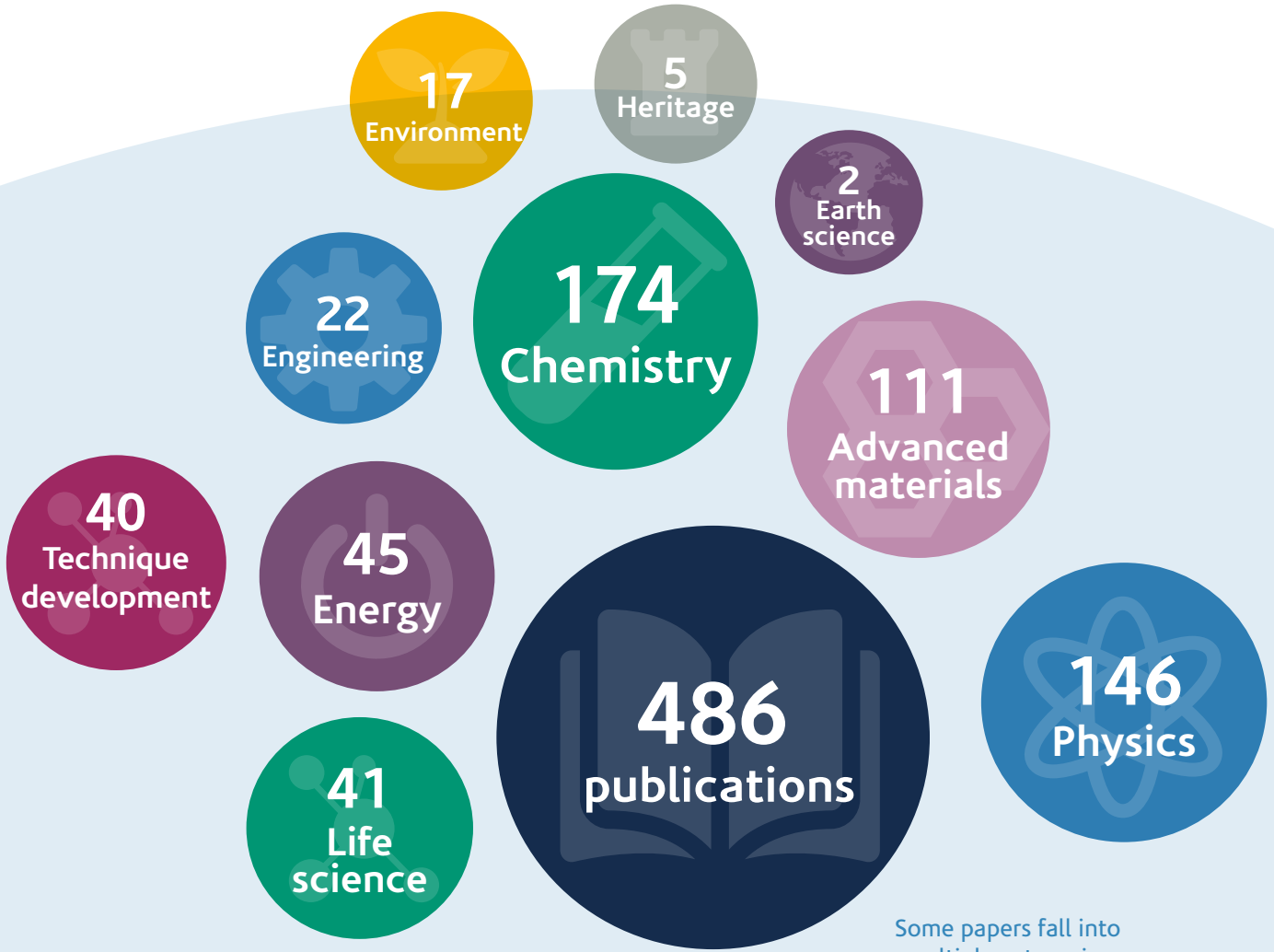


Science at ISIS



Science at ISIS

Science at ISIS spans a wide range of scientific disciplines, from pharmacology, cultural heritage, engineering, chemistry and fundamental research. The facility is used by over 2,000 scientists every year from both academia and industry. This section gives a snapshot of ISIS research over the past year.





Industrial Science

Industrial science

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

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

Rolls Royce

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

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

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

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

Neil D’Souza, Rolls Royce.

Infineum - Using neutron scattering to address complex additive challenges

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

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

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

Pete Dowding, Infineum

Pharmacology and Biology

Optimising the formulation of monoclonal antibodies

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

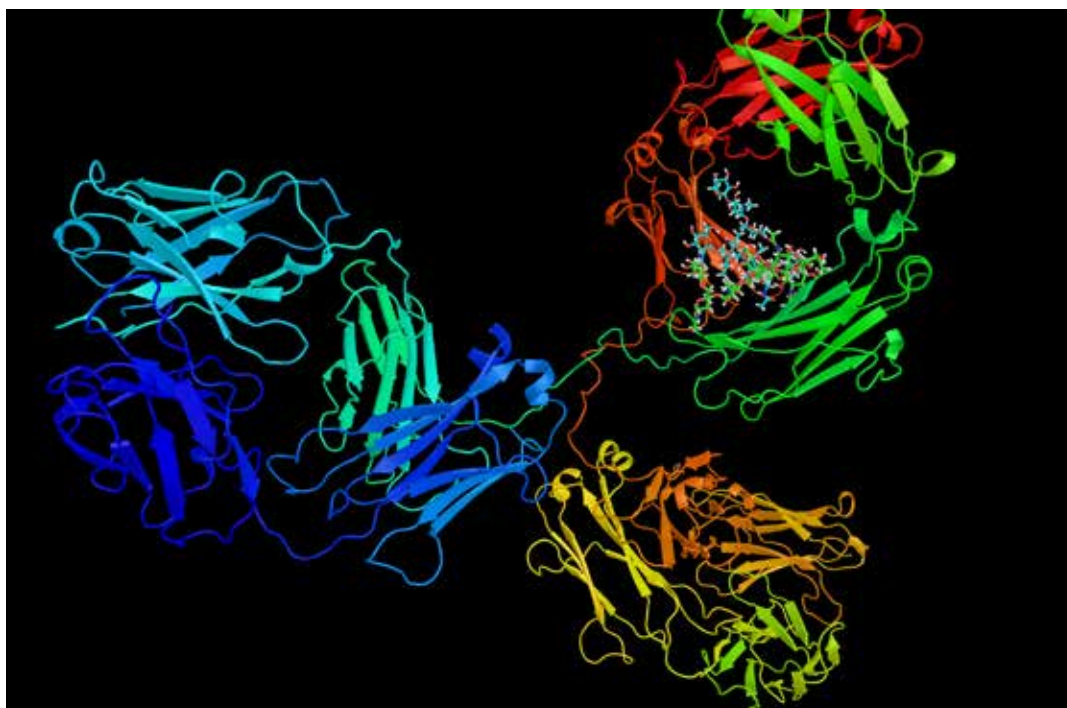
DOI: 10.1080/19420862.2016.1276141

Instrument: SURF

Funding: EPSRC

 Jian Lu (University of Manchester).

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



Monoclonal antibody © ibreakstock | Dreamstime.com


Intracellular water: a new target for breast cancer drugs

Related publication: M. P. M. Marques et al. "Intracellular water – an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons" *Phys. Chem. Chem. Phys.* 19 (2017), 2702-2713

DOI: 10.1039/C6CP05198G

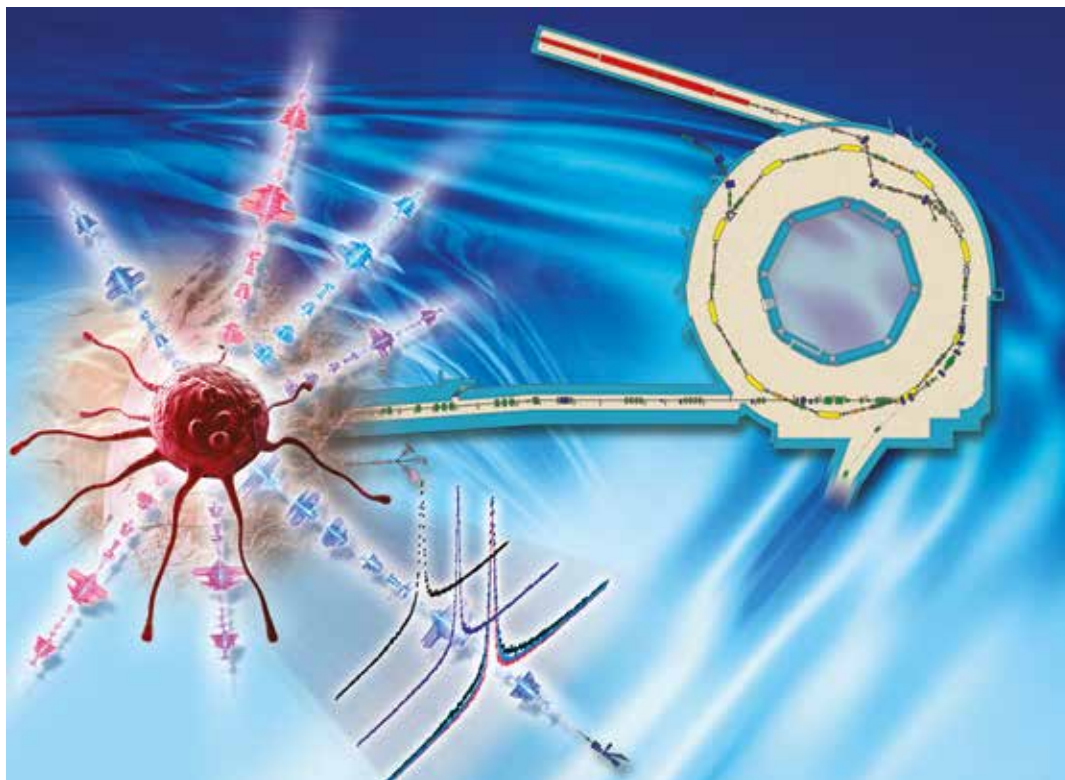
Instrument: OSIRIS and TOSCA

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

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

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

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



Reproduced from M. P. M. Marques et al. "Intracellular water – an overlooked drug target? Cisplatin impact in cancer cells probed by neutrons" *Phys. Chem. Chem. Phys.* 19 (2017), 2702-2713 DOI: 10.1039/C6CP05198G with permission from the PCCP Owner Societies.

Natural World

Meridianiite and planetary modelling


Related publication: D. Fortes et al. "Isothermal equation of state and high-pressure phase transitions of synthetic meridianiite ($\text{MgSO}_4 \cdot 11\text{D}_2\text{O}$) determined by neutron powder diffraction and quasielastic neutron spectroscopy", *Acta Cryst. B73* (2017): 33-46.

DOI: 10.1107/S2052520616018254

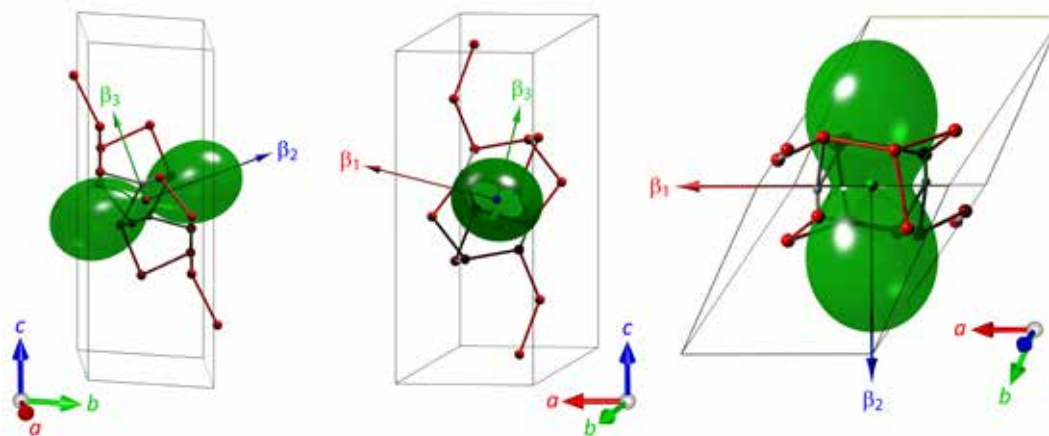
Additional reference D. Fortes et al. "Structure, thermal expansion and incompressibility of $\text{MgSO}_4 \cdot 9\text{H}_2\text{O}$, its relationship to meridianiite ($\text{MgSO}_4 \cdot 11\text{H}_2\text{O}$) and possible natural occurrences" *Acta Cryst. B. 73*(2017), 47-64 (DOI:10.1107/S2052520616018266)

Instrument: PEARL/HiPr and OSIRIS

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

 Dominic Fortes (ISIS Neutron and Muon Source).

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



*Image reproduced from A. D. Fortes et al. "Isothermal equation of state and high-pressure phase transitions of synthetic meridianiite ($\text{MgSO}_4 \cdot 11\text{D}_2\text{O}$) determined by neutron powder diffraction and quasielastic neutron spectroscopy", *Acta Cryst. B73* (2017): 33-46. DOI: 10.1107/S2052520616018254*

Energy


Detection of lithium diffusion using muon spin relaxation

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

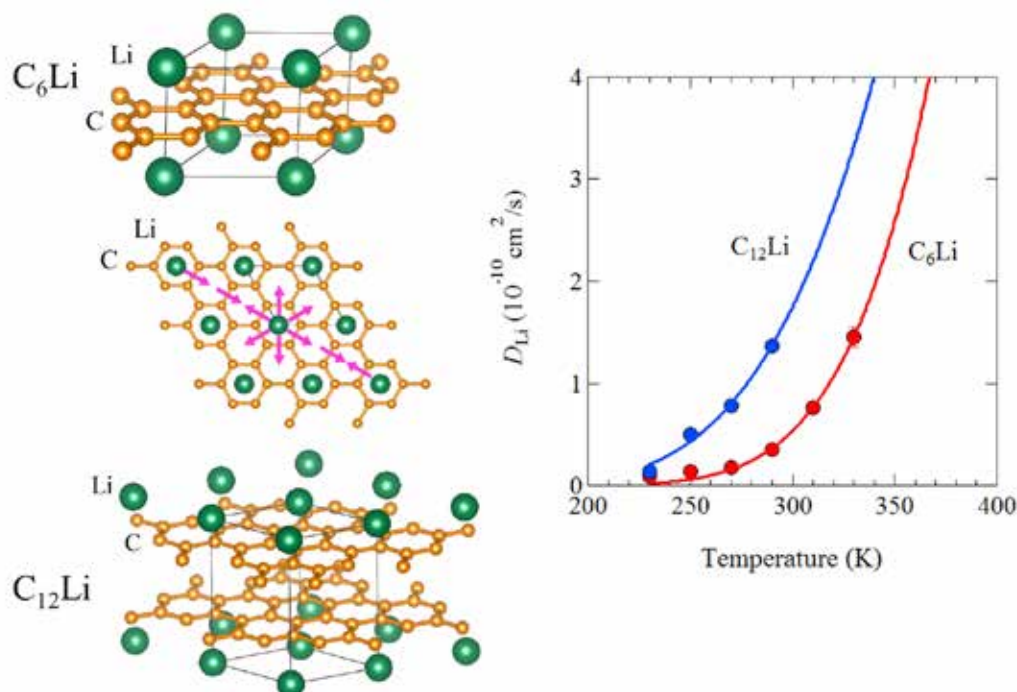
DOI: 10.1039/C7CP02047C

Instrument: EMU

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

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

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



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

Doping: a better approach to producing thermoelectric materials?

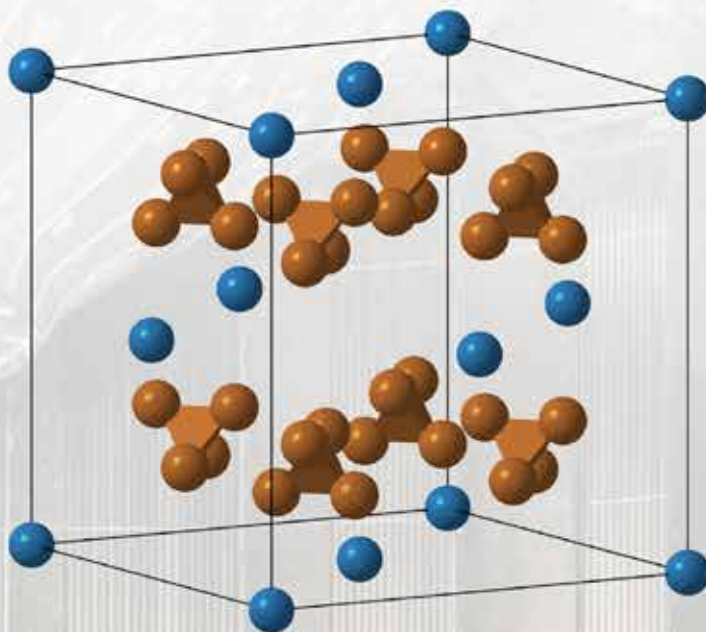
Related publication: D. J. Voneshen, et. al. "Hopping Time Scales and the Phonon-Liquid Electron-Crystal Picture in Thermoelectric Copper Selenide" *Phys. Rev. Lett.* 118 (2017) 145901-145905

DOI: 10.1103/PhysRevLett.118.145901

Instruments: LET and Merlin

 David Voneshen (ISIS Neutron and Muon Source)

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



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


Investigating the effect of counterions on selective catalytic reduction

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

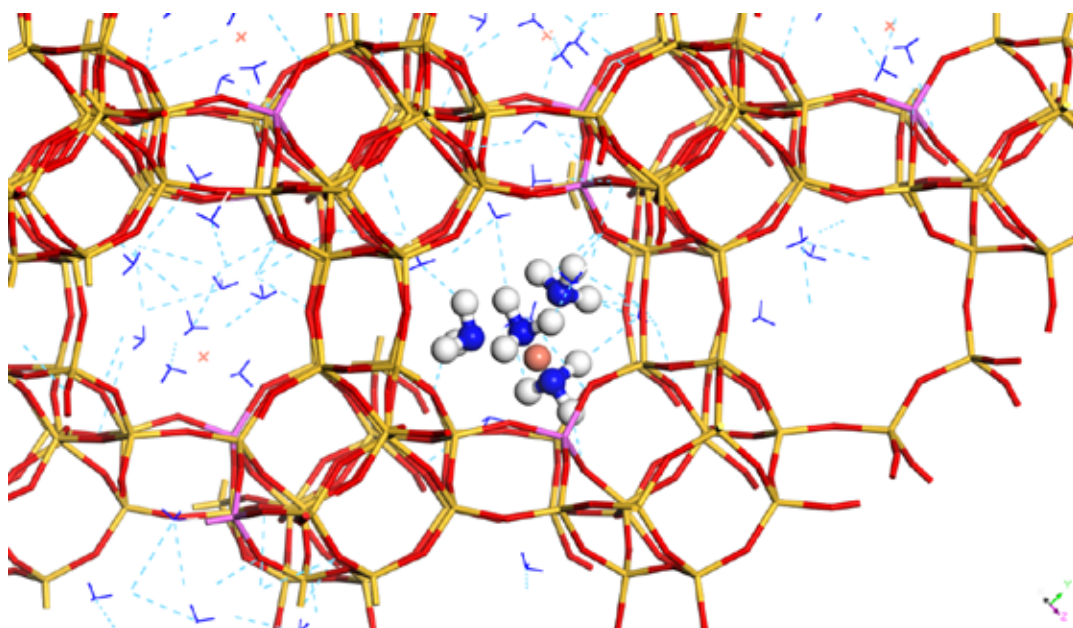
DOI: 10.1039/C6CP01160H

Instrument: OSIRIS

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

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

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



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

Advanced Materials

The magnetic phases of thin-film erbium

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

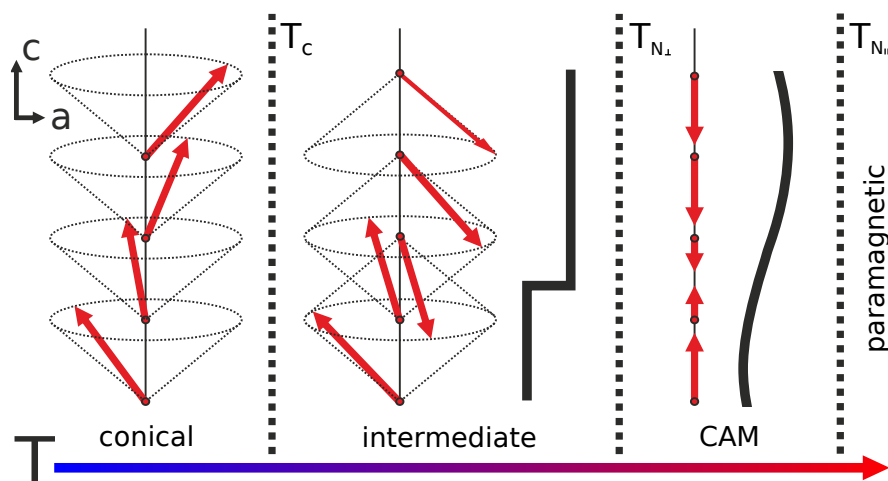
DOI: 10.1038/srep39021

Instrument: POLREF

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

 Gavin Burnell (University of Leeds).

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



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

Credit: STFC/John Willoughby


A magnetoelectric design strategy

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

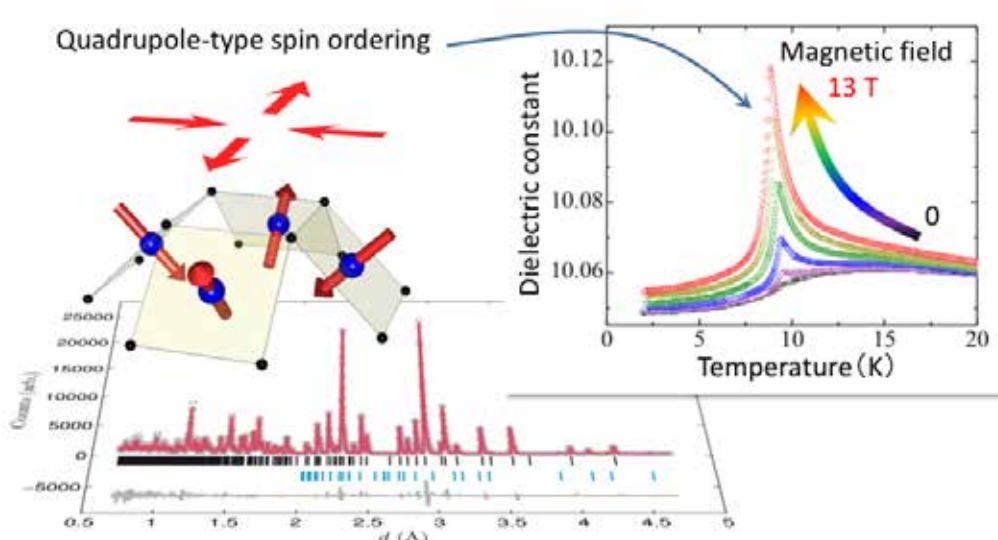
DOI: 10.1038/ncomms13039

Instrument: WISH

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

 Kenta Kimura (Osaka University)

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



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


A promising candidate for a quantum spin liquid

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

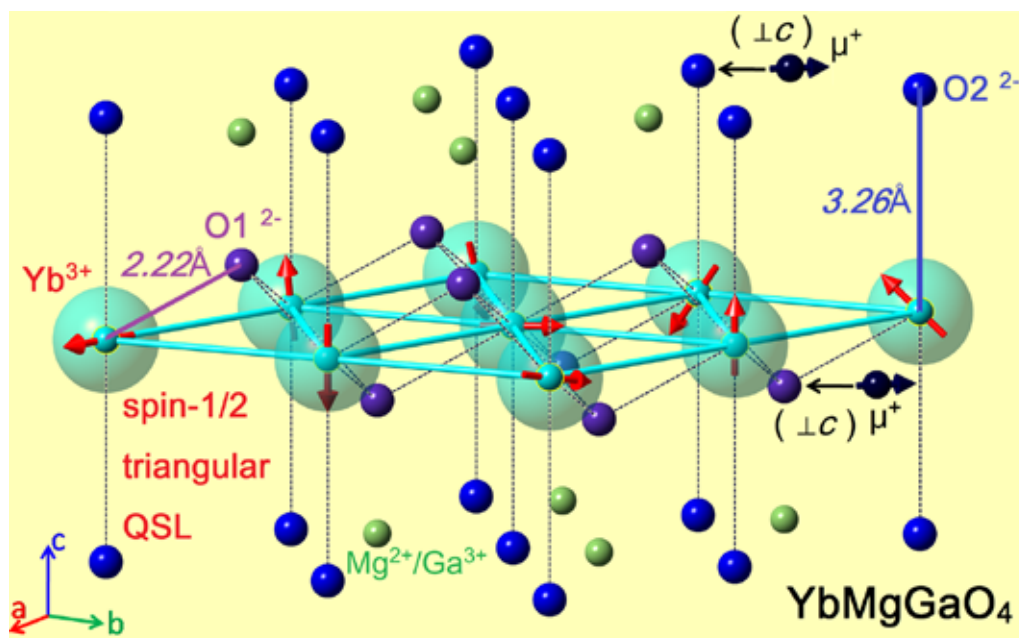
DOI: 10.1103/PhysRevLett.117.097201

Instrument: MuSR

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

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

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



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


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

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

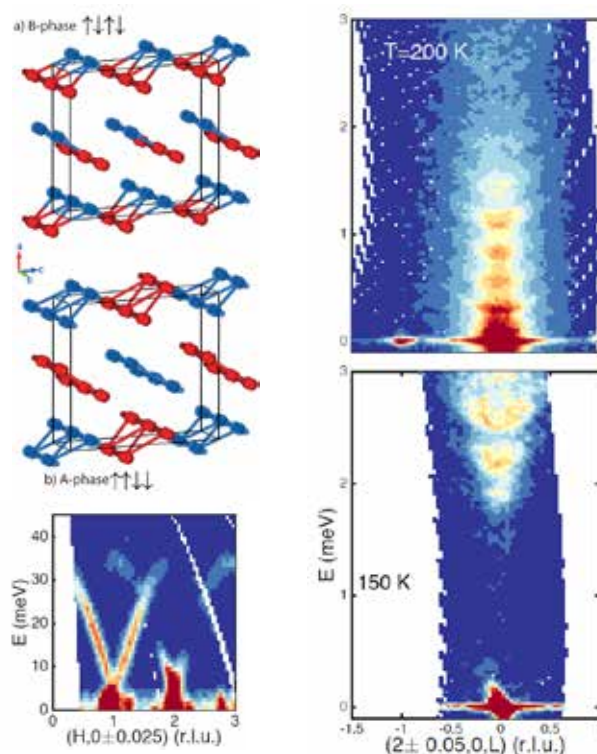
DOI: 10.1103/PhysRevLett.117.017201

Instrument: MAPS and OSIRIS

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

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

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



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

Finding the elusive Majorana fermion

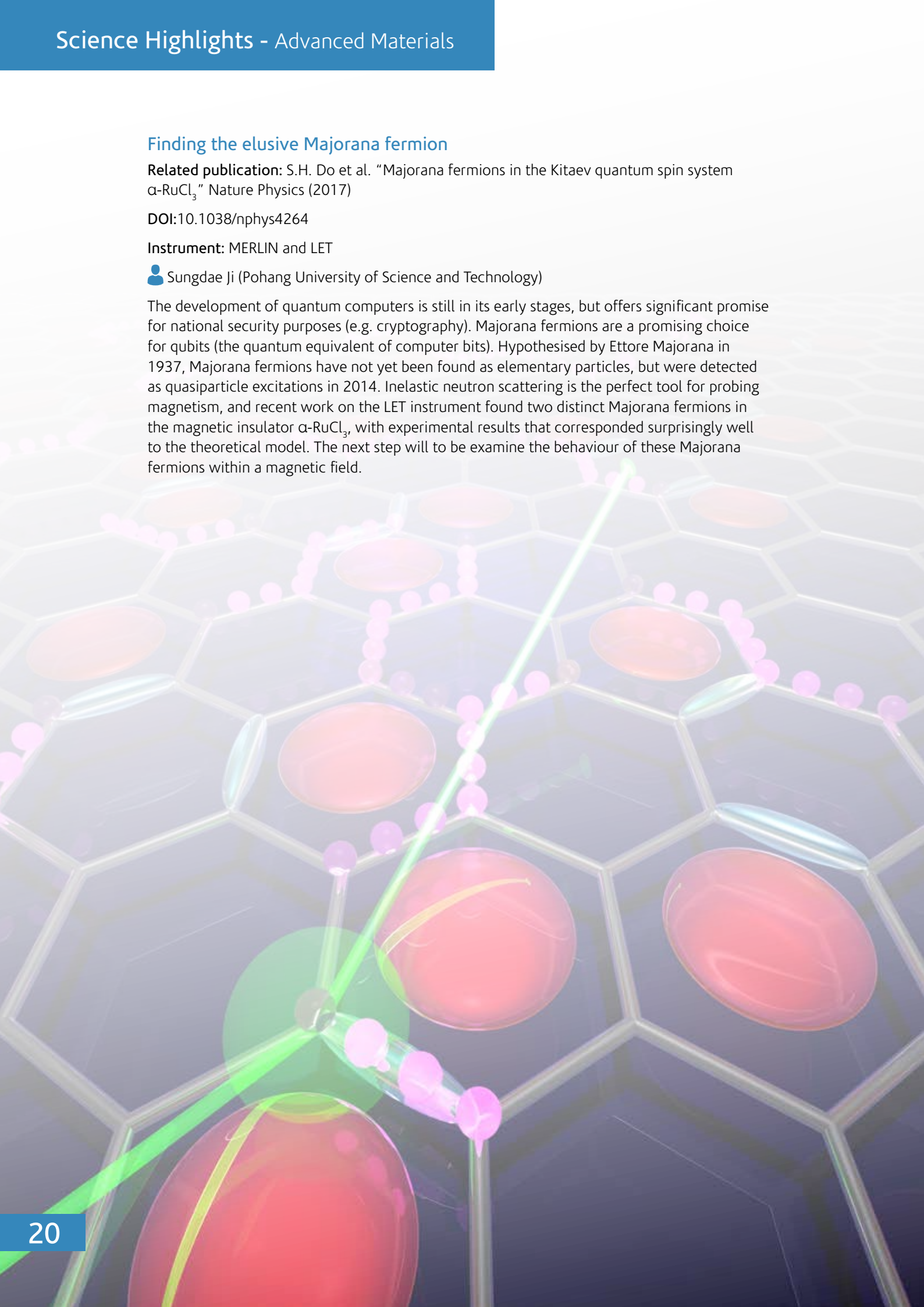
Related publication: S.H. Do et al. "Majorana fermions in the Kitaev quantum spin system α -RuCl₃" Nature Physics (2017)

DOI:10.1038/nphys4264

Instrument: MERLIN and LET

 Sungdae Ji (Pohang University of Science and Technology)

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




Realising 3D data transfer in nanomagnetic logic

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

DOI: 10.1002/admi.201600097

Instruments: OFFSPEC

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

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

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

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

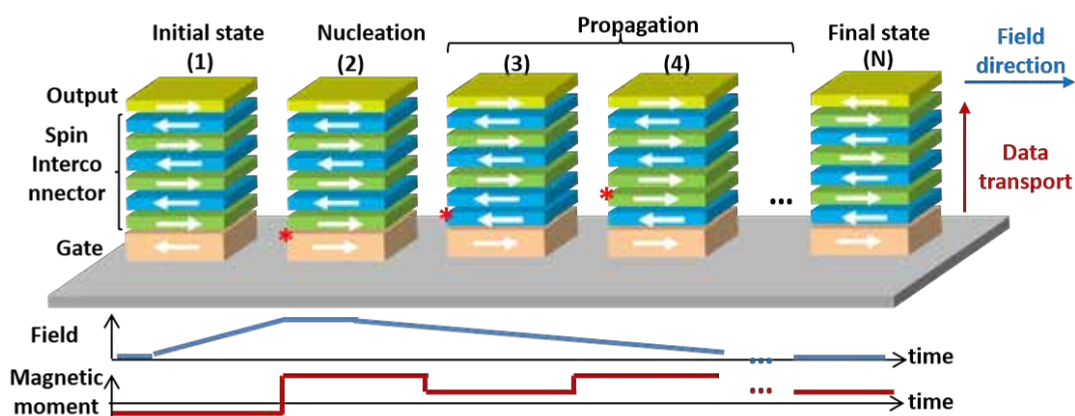


Image reproduced from Fernández-Pacheco A., Steinke Nina-Juliane, Mahendru D., Welbourne A., Mansell R., Chin S. L., Petit D., Lee J., Dalgliesh R., Langridge S., Cowburn R. P. (2016). Magnetic State of Multilayered Synthetic Antiferromagnets during Soliton Nucleation and Propagation for Vertical Data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


Topological numbers could be the key to novel materials

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

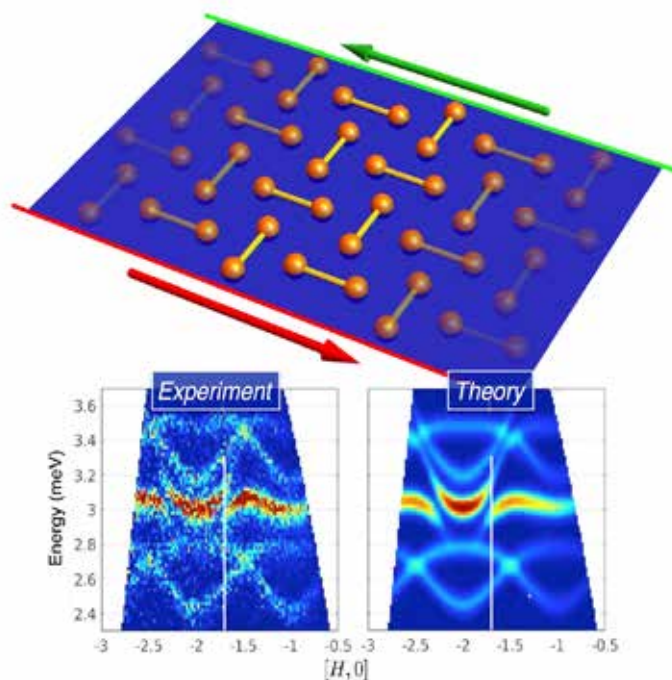
DOI:10.1038/nphys4117

Instruments: ALF and LET

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

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

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



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

Catalysis and Chemistry

A new class of economic, eco-friendly solvents

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

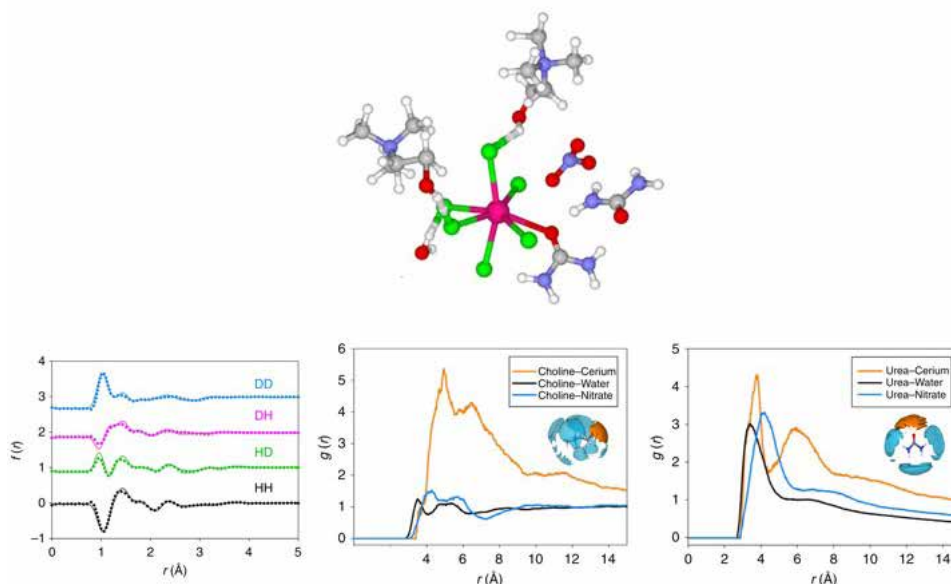
DOI: 10.1038/ncomms14150

Instruments: SANDALS

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

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

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



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

Using muonium radicals as surrogates for hydrogen radicals

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

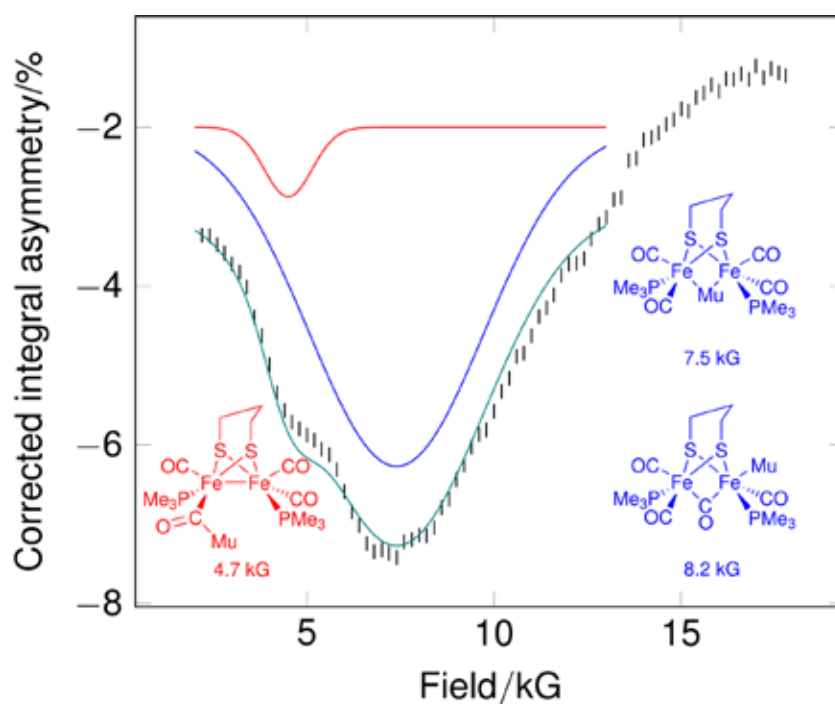
DOI: 10.1002/anie.201607109.

Instruments: MuSR

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

 Joseph Wright (University of East Anglia)

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



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

Probing the mysteries of molecular self-assembly

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

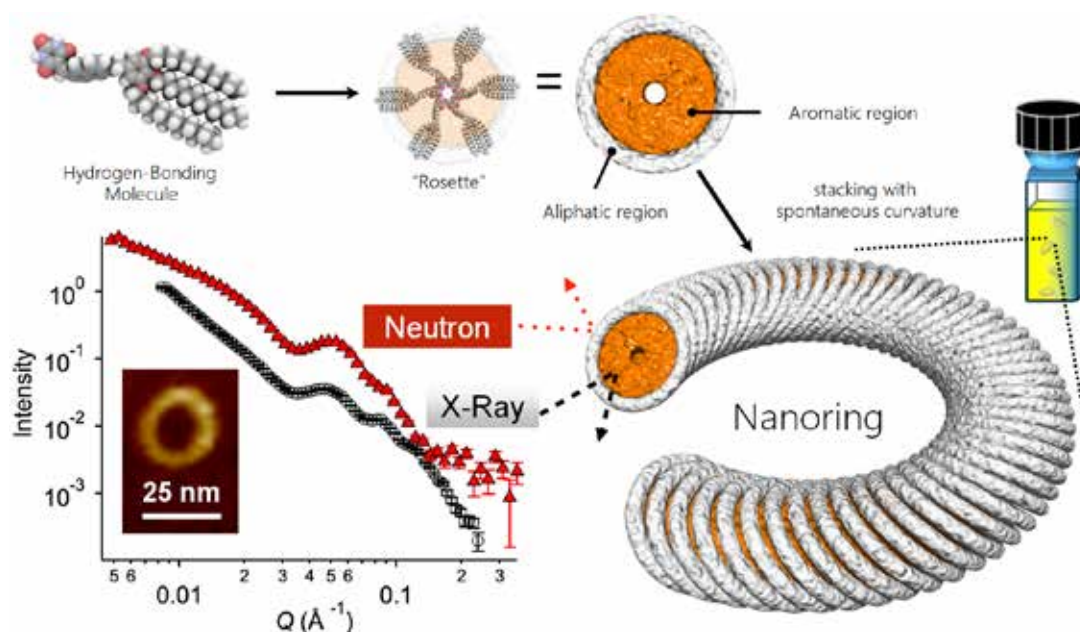
DOI: 10.1002/anie.201603370

Instruments: SANS2D

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

 Martin J. Hollamby (Keele University)

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



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

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

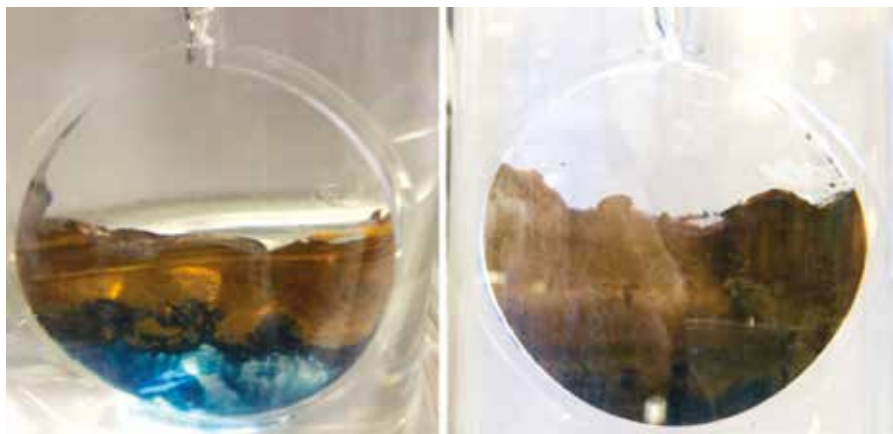
Related publication: A. G. Seel et al. "Electron Solvation and the Unique Liquid Structure of a Mixed-Amine Expanded Metal: The Saturated Li-NH₃-MeNH₂ System" *Angew. Chem. Int. Ed.* 56 (2017): 1561.

DOI: 10.1002/anie.201609192

Instruments: SANDALS

 Neal Skipper (University College London)

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



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

The kinetics of oil exchange in nanoemulsions

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

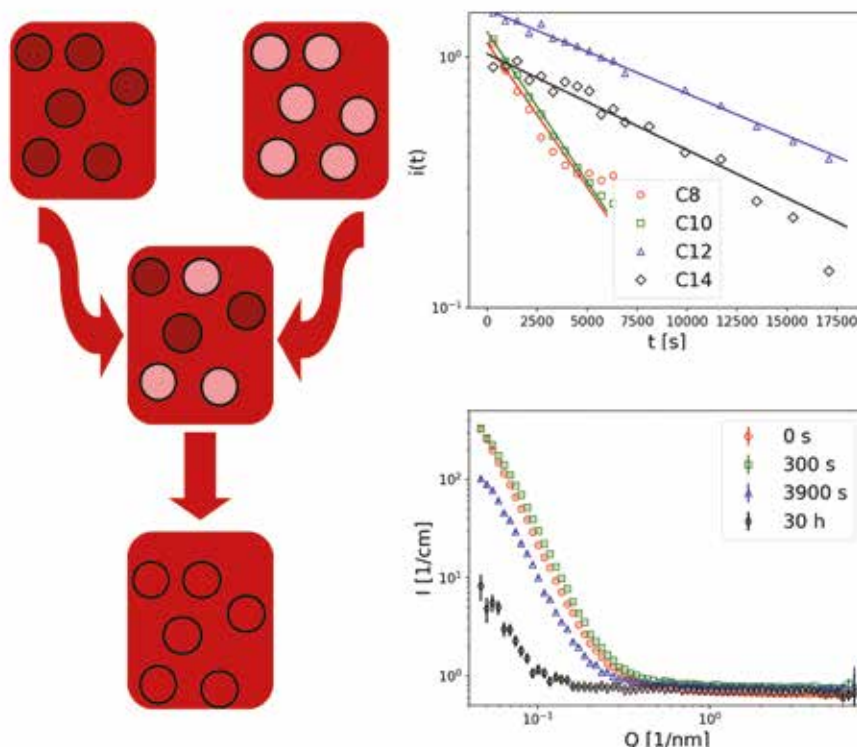
DOI: 10.1021/acs.langmuir.6b03009

Instrument: SANS2D

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

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

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



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

Improving our understanding of metal-organic frameworks

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

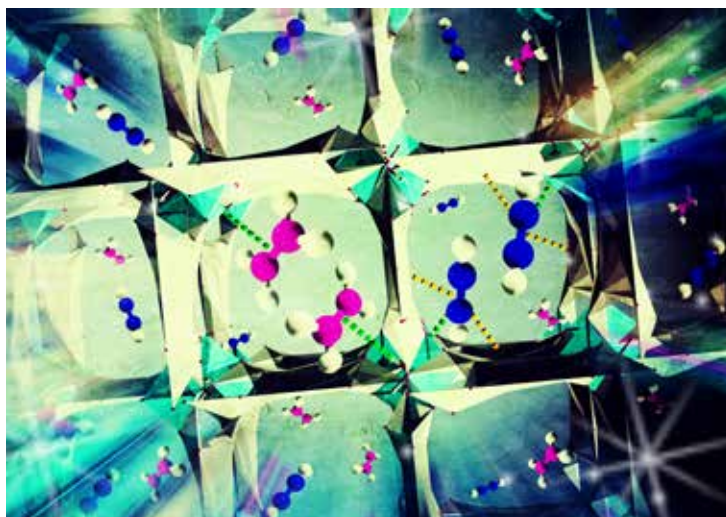
DOI: 10.1039/C6CS00603E

Instrument: TOSCA

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

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

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



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

Engineering

Looking for strain in high-entropy alloys

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

DOI: 10.1016/j.actamat.2016.09.032

Instrument: Polaris

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

 Nick Jones (University of Cambridge)

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

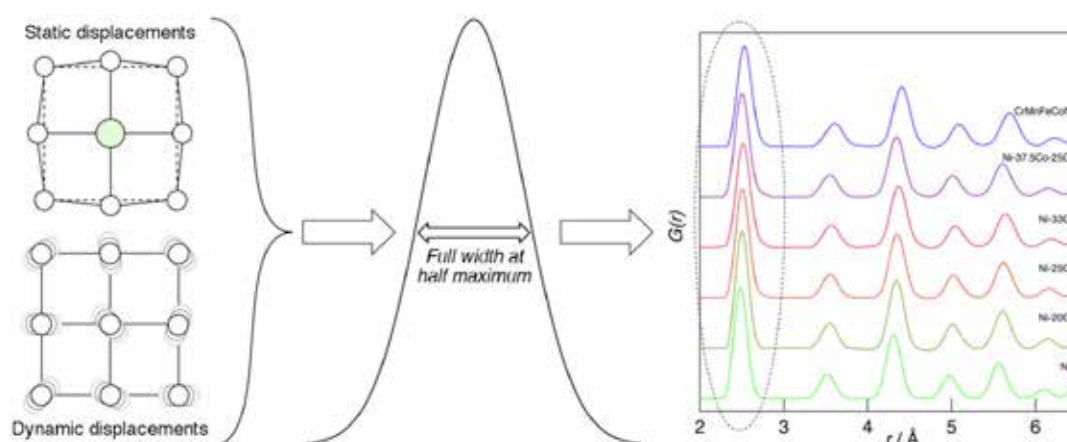



Image reproduced from L.R. Owen, E.J. Pickering, H.Y. Playford, H.J. Stone, M.G. Tucker, N.G. Jones, An assessment of the lattice strain in the CrMnFeCoNi high-entropy alloy, Acta Materialia, Volume 122, 2017, Pages 11-18, ISSN 1359-6454, <http://dx.doi.org/10.1016/j.actamat.2016.09.032>.

Neutrons illuminate stress/strain in high-temperature superalloys

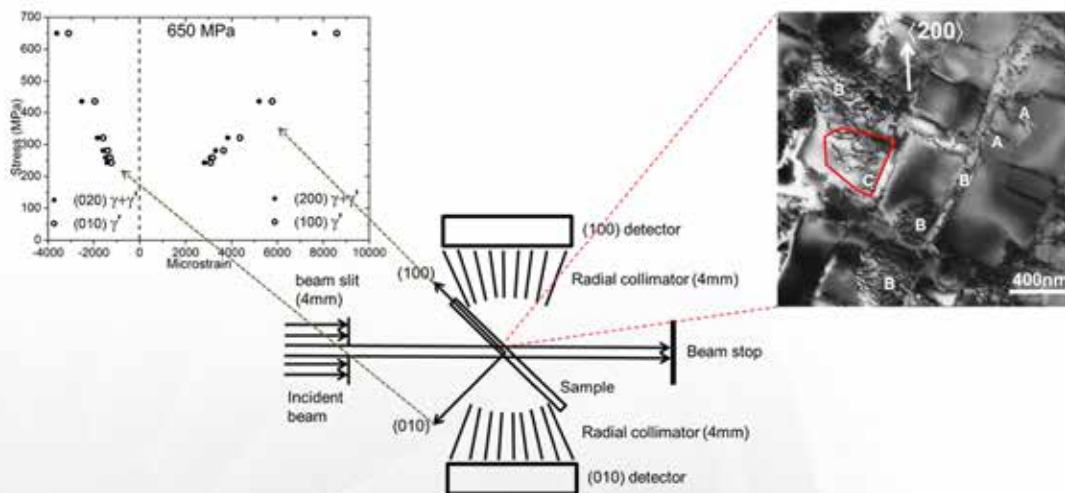
Related publication: Neil D'Souza et al. " The role of stress relaxation and creep during high temperature deformation in Ni-base single crystal superalloys – Implications to strain build-up during directional solidification" *Acta Materialia*, 106 (2016) 322-332.

DOI: 10.1016/j.actamat.2016.01.032.

Instrument: ENGIN-X

 Chinnapat Panwisawas (University of Birmingham)

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



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

Heritage Science

Examining Iron Age coins sheds light on our past

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

DOI:10.1016/j.microc.2016.01.006 .

Instrument: INES

Funding: Regione Piemonte (Italy); INFN-CHNET

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

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



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

International Collaborations

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

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

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



Sweden

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



India

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

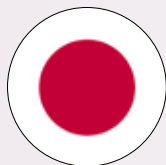


Italy

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



USA



Japan



China



Spain



The Netherlands



Newton Funding

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

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

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

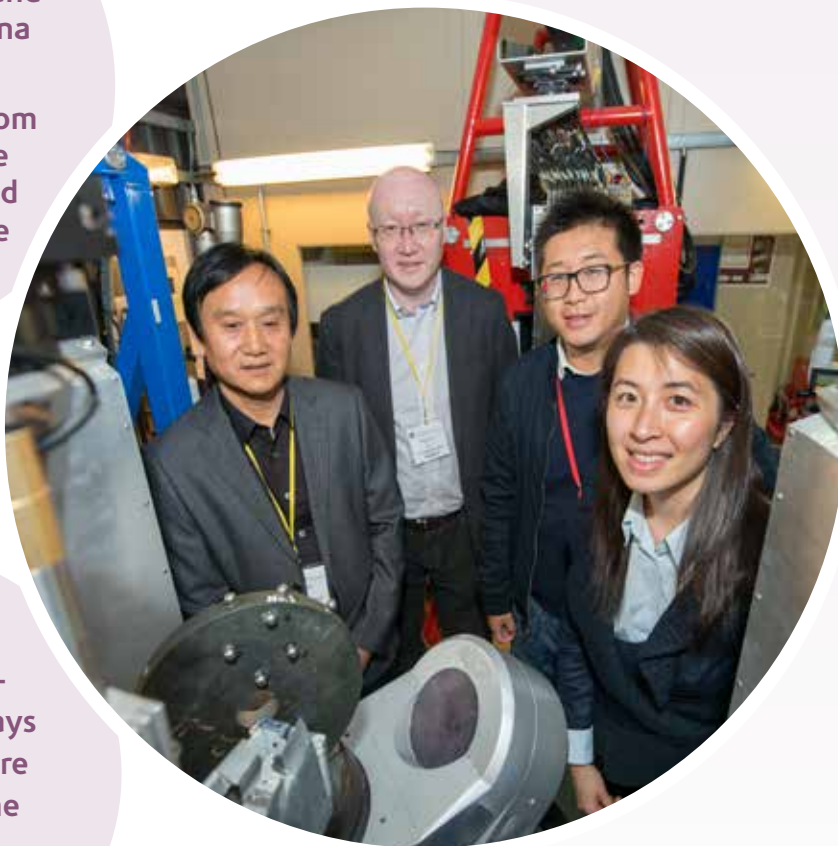
“Newton funds offer opportunity not only to perform state-of-art research but it opens a platform to train manpower”

Comments from a Newton Funded supported researcher

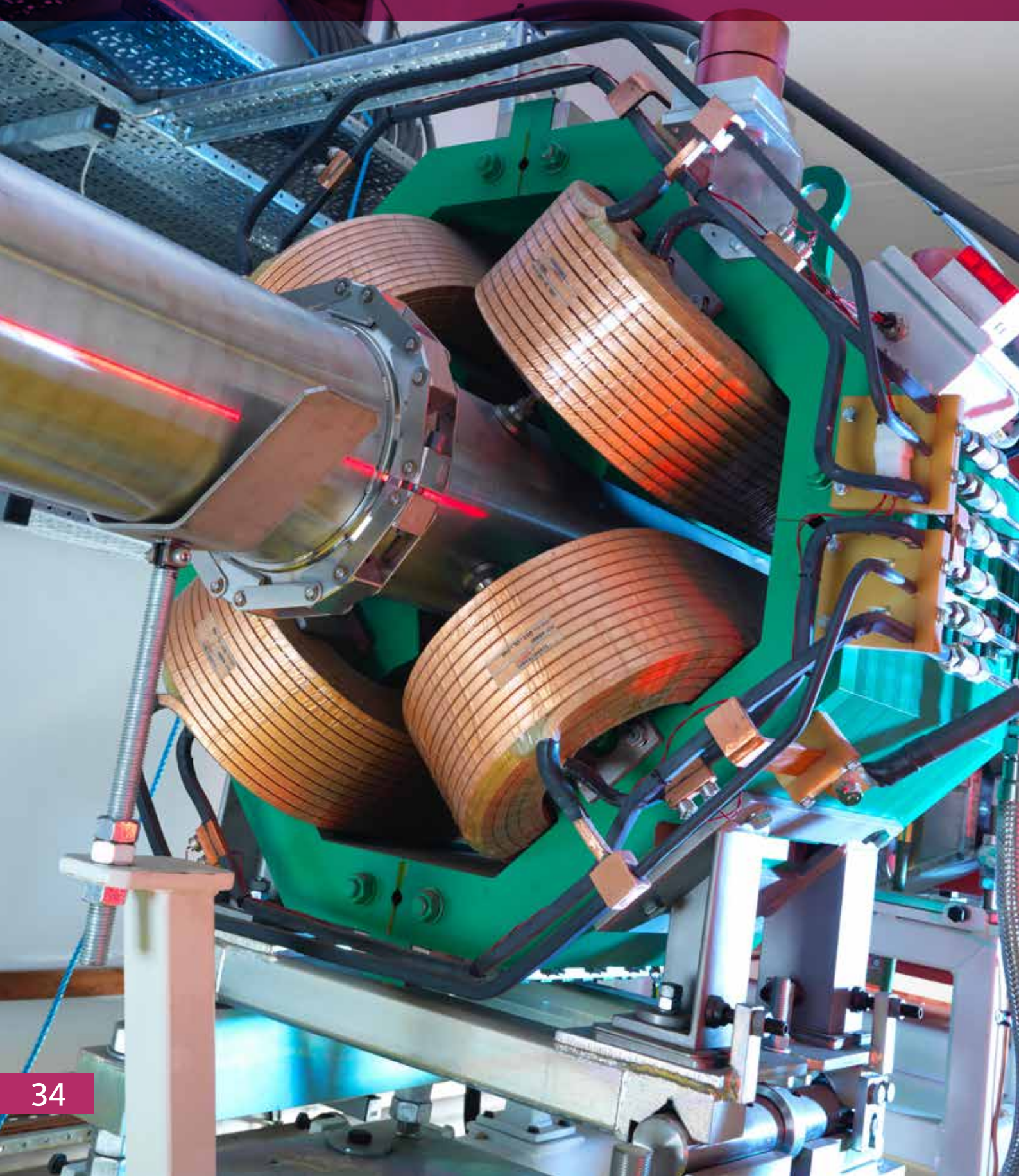
The Newton fund has led to 2 new agreements and partnerships with China and India.

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

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

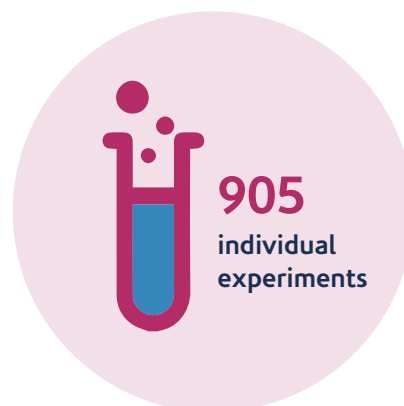
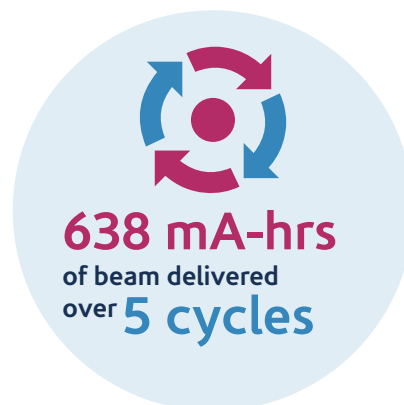
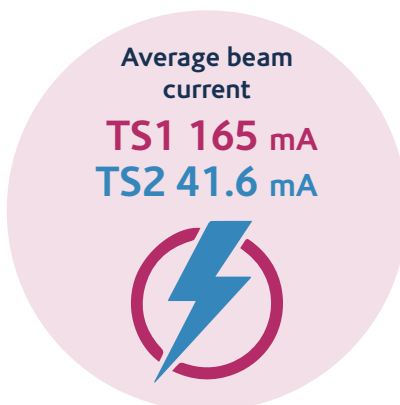


Technology



Technology

Cutting edge science at ISIS must be underpinned by cutting edge technology. ISIS has an ongoing programme of developments on its accelerator complex and instruments, extending capabilities and improving performance.



*Taking into account instrument down-time, plus calibration and commissioning time.

Table 1.1: Performance in 2016/2017 Cycle by Cycle

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

Major Projects

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

Target Station 1

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

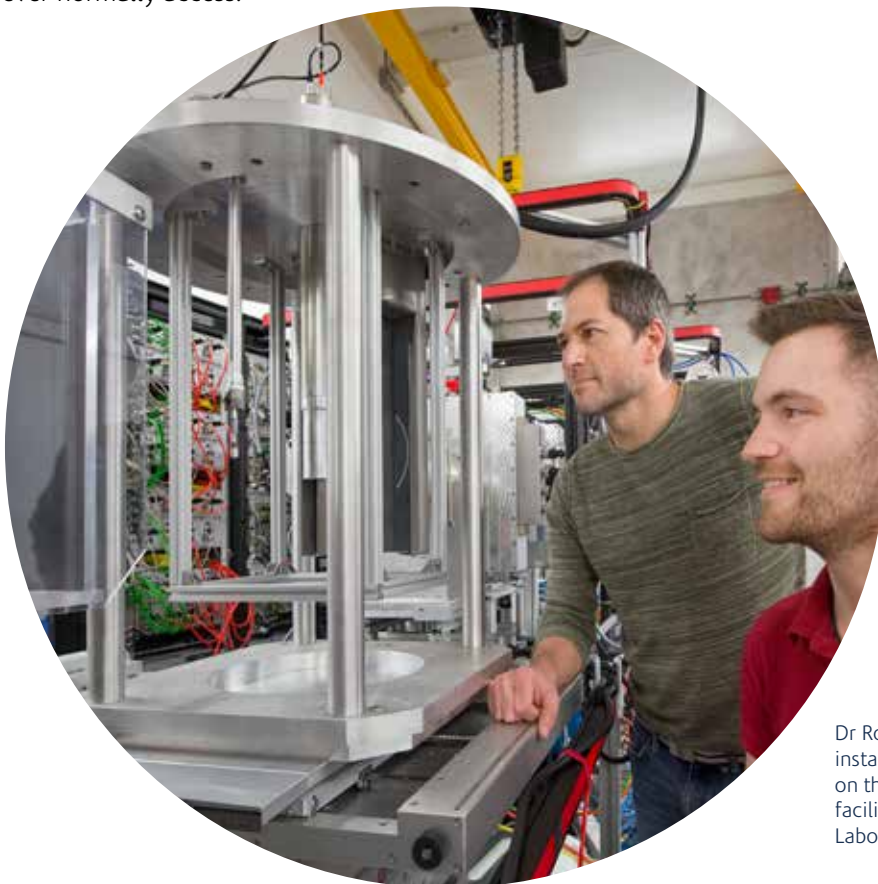
Preparation is already well underway with over 20,000 people hours already invested in the project. Highlights last year include: the creation of a characterisation rig that can take absolute flux and time of flight data, ortho/para ratio measurements for liquid hydrogen in both the target stations,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

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

Target Station 2 Phase II Instruments

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

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

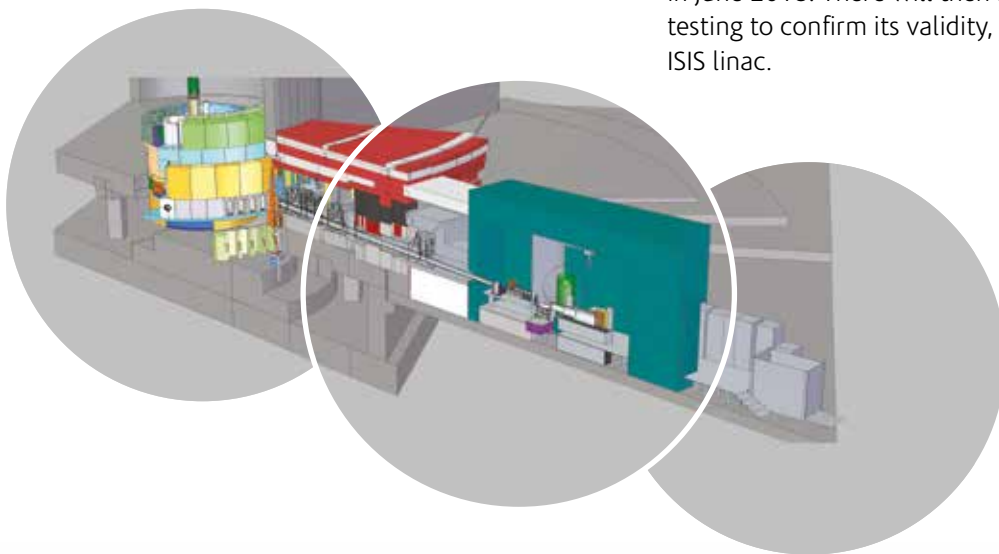


Dr Robert Bewley and Dr Daniel Pooley installing the TS1 Characterisation rig on the LARMOR instrument at ISIS's TS2 facility at STFC's Rutherford Appleton Laboratory

ISIS Supporting the European Spallation Source

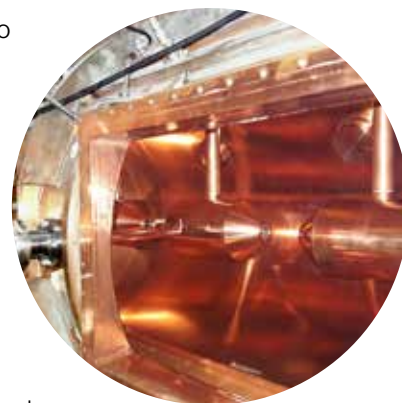
Staff at ISIS Neutron and Muon Source have been busy continuing their important contributions to several areas of the €1.8Bn European Spallation Source (ESS), currently being built near Lund in southern Sweden.

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



Linac tank 4

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



The Helium Recovery Project

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

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

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

Instrument Updates

A blue circular icon with a white border and the word "TOSCA" in white capital letters.

TOSCA

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

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

A maroon circular icon with a white border and the word "ENGIN-X" in white capital letters.

ENGIN-X

A blue circular icon with a white border and the word "LARMOR" in white capital letters.

LARMOR

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

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

A maroon circular icon with a white border and the word "ZOOM" in white capital letters.

ZOOM

A blue circular icon with a white border and the word "ChipIR" in white capital letters.

ChipIR

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

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



MARI

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

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

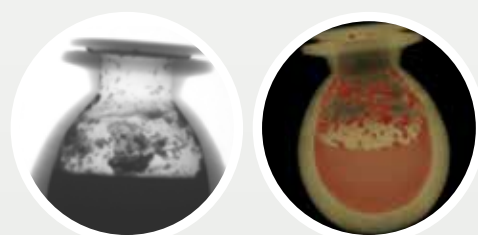
MAPS

IMAT

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

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

Users setting up samples on IMAT

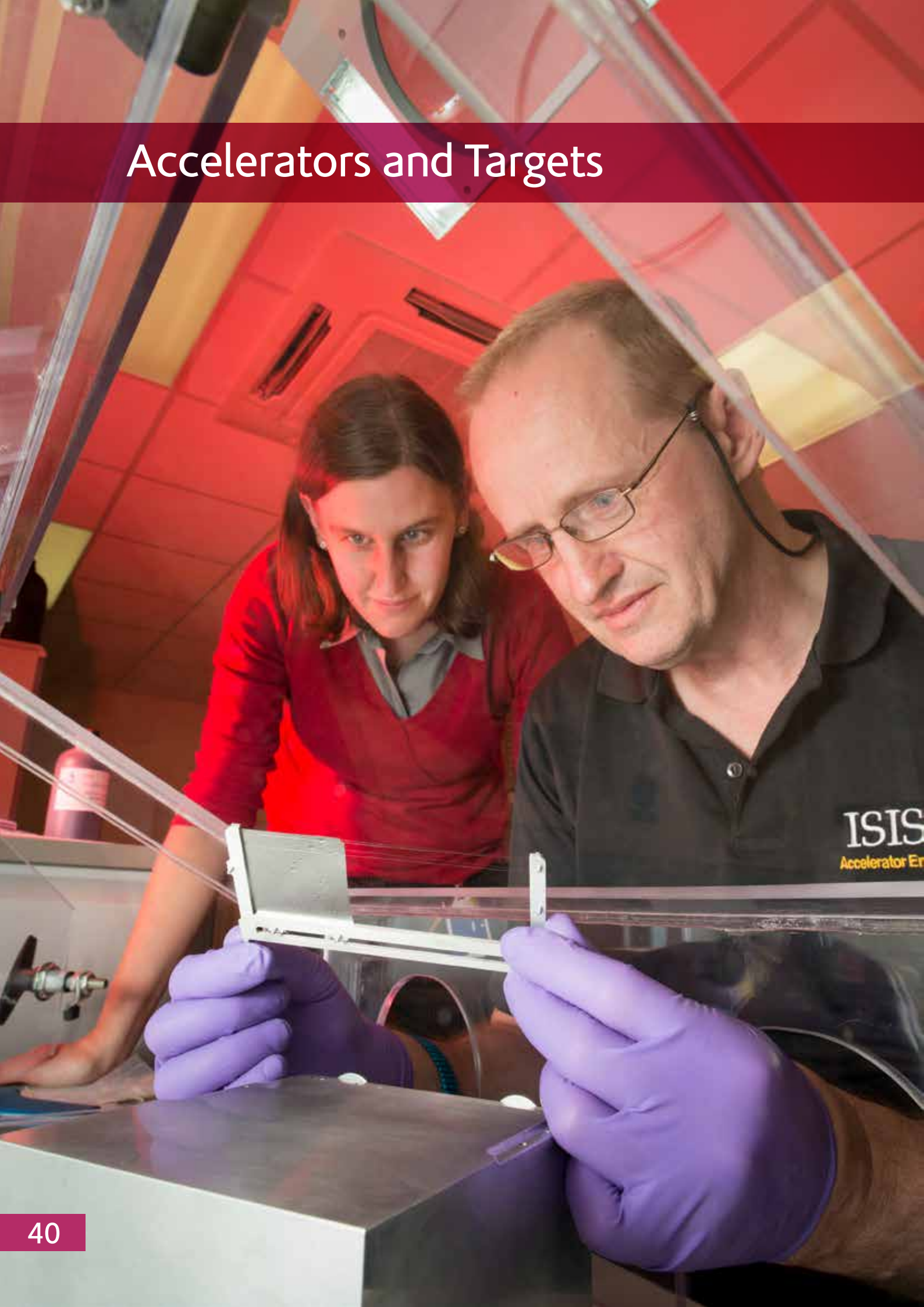


Neutron radiographies and tomographies of the vases and ceramic vessels were collected.



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

Accelerators and Targets



Accelerators and Targets

The Accelerators and Experimental Operations divisions are responsible for developing and operating the ISIS machine. Over the past 12 months the divisions have been involved in a range of activities including new power drives for the RF cavities and new beam chopper prototypes as well as organising international conferences and a Particle Accelerator Careers Open Day. Here are some of the highlights.

New Ionisation Profile Monitor

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

Linac Tank 4

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

Carbon Stripping Foil Tests with the ISIS Diagnostic Test Vessel

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

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

Collaboration with Hiroshima University

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

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



Computing




Computing

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

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

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



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

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

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

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





Skills

Developing the skills of our staff and wider scientific community is vital to maintaining our status as a world-leading research facility. We also have a key role to play in inspiring the scientists and engineers of the future. We offer a wide range of hands-on training, offer around 150 placement opportunities and have an active public engagement programme.

Placements



18
Graduate
Students



49
co-sponsored
PhD students



25
vacation
students



20
work experience
placements



26
Apprentice
placements



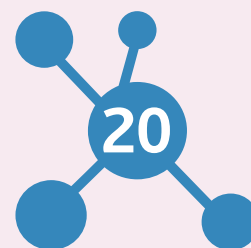
22
undergraduate
sandwich
students



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



17
days of teacher
training



20
scientific
seminars



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



22
events
organised by
the community



250
staff
talks
at meetings,
conferences and
workshops

Inspiring the next generation



Inspiring the next generation

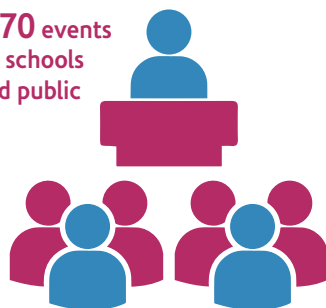
2017 has been a busy year in public engagement with over 2000 school pupils, teachers and members of the general public pouring into the facility for ISIS talks and tours of the experimental halls, hearing about the amazing science and engineering we undertake.

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

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



Over 70 events
for schools
and public



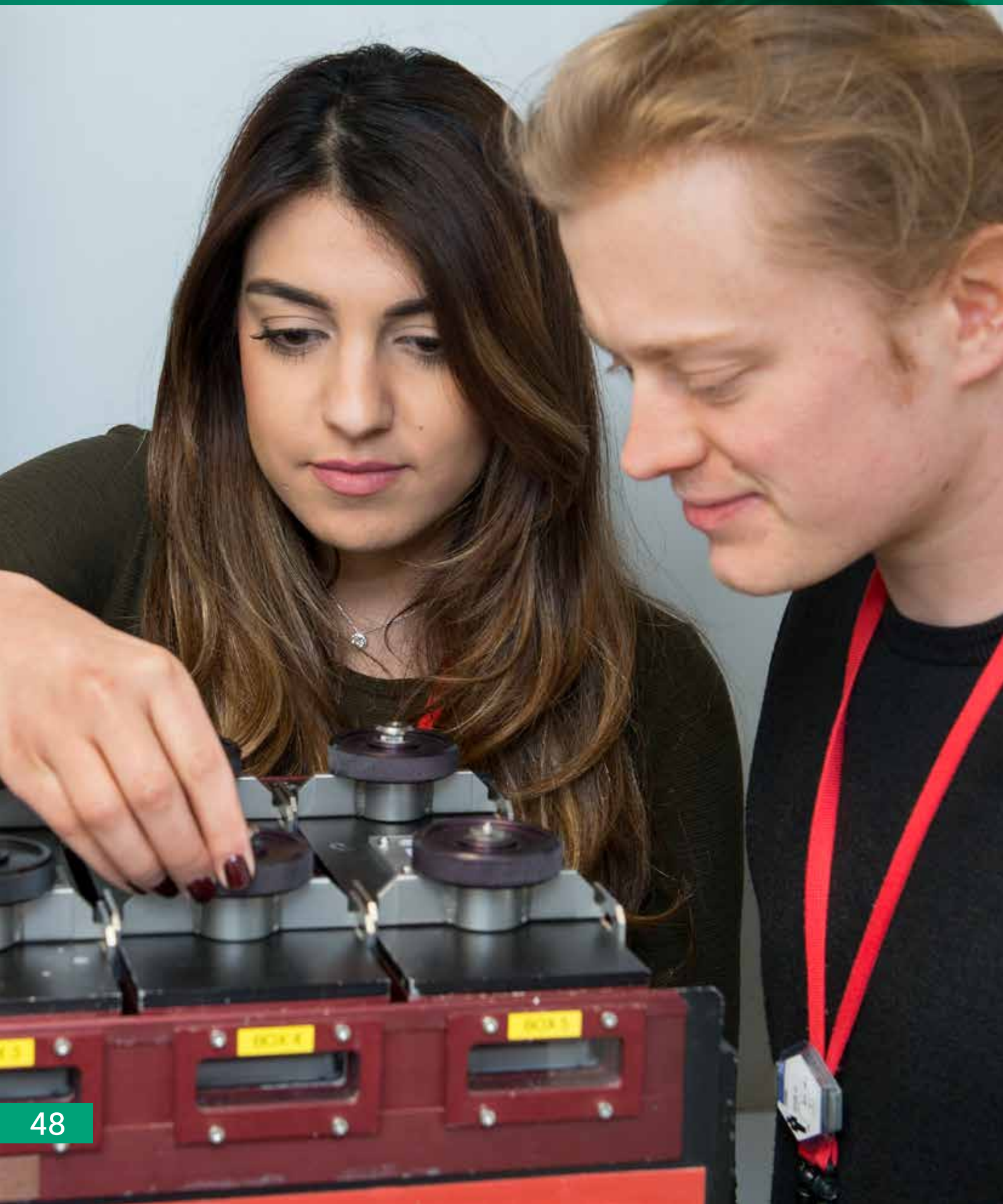
Chris Frost's liquid nitrogen show during Ashcroft Academy's visit to RAL on 3rd May

Case study: Chemistry at Work

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



Developing the student community



Developing the student community

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

Training Events

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

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

Supervision

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

On the job training

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

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



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



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



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

Events for the neutron community



Developing the wider neutron community

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

NIBS'16

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

Mantid Developer Workshop

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

Faraday Conference 2017

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

ICANS XXII

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

UK Neutron and Muon Science and User Meeting

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

The Oxford School of Neutron Scattering

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



Attendees at the Oxford School of Neutron Scattering 2017



Attendees at Mantid's 10th developer workshop

Developing our people



Developing our people

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

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

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

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

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

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

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

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



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



Publications 2016

P Aba-Perea et al. "Determination of the high temperature elastic properties and diffraction elastic constants of Ni-base superalloys". *Mater Des* **89** (2016): 856-863. doi:10.1016/j.matdes.2015.09.152.

SB Abbott et al. "Switching the Interpenetration of Confined Asymmetric Polymer Brushes". *Macromolecules* **49**, no. 11 (2016): 4349-4357. doi:10.1021/acs.macromol.6b00310.

F Abou-Chahine et al. "Proceedings of the Molecular Spectroscopy Science Meeting 2016". RAL Technical Reports RAL-TR-2016-020. 2016. Is in proceedings of: *Molecular Spectroscopy Science Meeting 2016*, Cosener's House, Abingdon, UK, 9-10th November 2016. <http://purl.org/net/epubs/manifestation/30996521>.

AA Aczel et al. "Structural and magnetic properties of the 5d2 double perovskites Sr_2BReO_6 (B=Y, In)". *Phys Rev B* **93**, no. 21 (2016): 214407. doi:10.1103/PhysRevB.93.214407.

DJ Adams et al. "Operational Experience and Future Plans at ISIS". In *57th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams* (HB2016), Malmo, Sweden, 3-8 Jul 2016, (2016): TUPM3Y01. <https://hb2016.esss.se/prepress/papers/tupm3y01.pdf>.

DT Adroja et al. "Inelastic Neutron Scattering Investigations of an Anisotropic Hybridization Gap in the Kondo Insulators: CeT_2Al_{10} (T=Fe, Ru and Os)". *Solid State Phenomena* **257** (2016): 11-25. doi:10.4028/www.scientific.net/SSP.257.11.

A Agbelele et al. "Strain and magnetic field induced spin-structure transitions in Multiferroic $BiFeO_3$ ". *Adv Mater* **29**, no. 9 (2016): 1602327. doi:10.1002/adma.201602327.

K Ahn et al. "Pressure-structure relationships in the 10 K layered carbide halide superconductor $Y_2C_2I_2$ ". *J Phys-Condens Mat* **28**, no. 37 (2016): 375703. doi:10.1088/0953-8984/28/37/375703.

D Alba Venero et al. "Magnetic nanoscopic correlations in the crossover between a superspin glass and a superferromagnet". *J Appl Phys* **119**, no. 14 (2016): 143902. doi:10.1063/1.4945427.

G Albani et al. "Evolution in boron-based GEM detectors for diffraction measurements : from planar to 3D converters". *Measurement Sci Technol* **27**, no. 11 (2016): 115902. doi:10.1088/0957-0233/27/11/115902.

P Albers et al. "Neutron scattering study of the terminating protons in the basic structural units of non-graphitising and graphitising carbons". *Carbon* **109** (2016): 239-245. doi:10.1016/j.carbon.2016.08.007.

RS Alvim et al. "Adsorption of asphaltenes on the calcite (10.4) surface by first-principles calculations". *RSC Adv* **6**, no. 97 (2016): 95328-95336. doi:10.1039/c6ra19307b.

M Amores et al. "Fast microwave-assisted synthesis of Li-stuffed garnets and insights into Li diffusion from muon spin spectroscopy". *J Mater Chem A* **4**, no. 5 (2016): 1729-1736. doi:10.1039/c5ta08107f.

VK Anand et al. "Physical properties of the candidate quantum spin-ice system $Pr_2Hf_2O_7$ ". *Phys Rev B* **94**, no. 14 (2016): 144415. doi:10.1103/PhysRevB.94.144415.

VK Anand et al. "Crystal-field states of Kondo lattice heavy fermions $CeRuSn_3$ and $CeRhSn_3$ ". *Phys Rev B* **94**, no. 1 (2016): 014440. doi:10.1103/PhysRevB.94.014440.

JM Andersson et al. "Multilayers of Lung Surfactant at the Air/Water Interface Observed by Neutron Reflectometry under Compression-Expansion Cycles". *Biophys J* **110**, no. 3 (2016): 82a. Is in proceedings of: 60th Annual Meeting of the Biophysical-Society, Los Angeles, CA, 27 Feb - 2 Mar 2016. doi:10.1016/j.bpj.2015.11.502.

C Andreani, G Romanelli and R Senesi. "Direct measurements of quantum kinetic energy tensor in stable and metastable water near the triple point: an experimental benchmark". *J Phys Chem Lett* **7**, no. 12 (2016): 2216-2220. doi:10.1021/acs.jpclett.6b00926.

J Armstrong et al. "Heads or tails: How do chemically substituted fullerenes melt?". *Phys Chem Chem Phys* **18**, no. 26 (2016): 17202-17209. doi:10.1039/C6CP01333C.

SW Arulnesan et al. "The impact of room temperature polymorphism in K doped $NaTaO_3$ on structural phase transition behaviour". *J Solid State Chem* **238** (2016): 109-112. doi:10.1016/j.jssc.2016.03.008.

SW Arulnesan et al. "Phase separation in $NaTaO_3$. Impact of temperature and doping". *Solid State Sci* **52** (2016): 149-153. doi:10.1016/j.solidstatesciences.2016.01.001.

M Asaad et al. "Thermoelectric properties and high-temperature stability of the $Ti_{1-x}V_xCoSb_{1-x}Sn_x$ half-Heusler alloys". *RSC Adv* **6**, no. 61 (2016): 56511-56517. doi:10.1039/C6RA09549F.

KR Asiani et al. "SiE is an intrinsically disordered periplasmic "molecular sponge" involved in bacterial silver resistance". *Mol Microbiol* **101**, no. 5 (2016): 731-742. doi:10.1111/mmi.13399.

M Bagatin et al. "Muon-induced soft errors in 16-nm NAND flash memories". In *2016 IEEE International Reliability Physics Symposium (IRPS 2016)*, Pasadena, California, USA, 17-21 May 2016, (2016): 5C-1-1-5C-1-5. doi:10.1109/IRPS.2016.7574552.

E Bahn et al. "Diffusion of molecular hydrogen in carbon aerogel". *Carbon* **98** (2016): 572-581. doi:10.1016/j.carbon.2015.11.034.

- ML Baker et al. "Studies of a Large Odd-Numbered Odd-Electron Metal Ring: Inelastic Neutron Scattering and Muon Spin Relaxation Spectroscopy of CrMn". *Chem Eur J* **22**, no. 5 (2016): 1779-1788. doi:10.1002/chem.201503431.
- C Balz et al. "Physical realization of a quantum spin liquid based on a complex frustration mechanism". *Nat Phys* **12** (2016): 942-949. doi:10.1038/nphys3826.
- A Banerjee et al. "Spin wave excitations in the pyrovanadate alpha - $\text{Cu}_2\text{V}_2\text{O}_7$ ". *Phys Rev B* **94**, no. 14 (2016): 144426. doi:10.1103/PhysRevB.94.144426.
- LJ Bannenberg et al. "Impact of Nanostructuring on the Phase Behavior of Insertion Materials: The Hydrogenation Kinetics of a Magnesium Thin Film". *J Phys Chem C* **120**, no. 19 (2016): 10185-10191. doi:10.1021/acs.jpcc.6b02302.
- F Barroso-Bujans et al. "Dynamics and structure of Poly(ethylene oxide) intercalated in the nanopores of Resorcinol-Formaldehyde resin nanoparticles". *Macromolecules* **49**, no. 15 (2016): 5704-5713. doi:10.1021/acs.macromol.6b01285.
- MT Batchelor and A Foerster. "Yang-Baxter integrable models in experiments: from condensed matter to ultracold atoms". *J Phys A-Math Theor* **49**, no. 17 (2016): 173001. doi:10.1088/1751-8113/49/17/173001.
- EF Baxter et al. "A comparison of the amorphization of zeolitic imidazolate frameworks (ZIFs) and aluminosilicate zeolites by ball-milling". *Dalton Trans* **45**, no. 10 (2016): 4258-4268. doi:10.1039/c5dt03477a.
- RD Bayliss et al. "Synthetic versiliaite and apuanite: investigation by ^{57}Fe Mössbauer spectroscopy". *Hyperfine Interact* **237**, no. 1 (2016): 98. doi:10.1007/s10751-016-1308-3.
- E Beake et al. "Orientational disorder in adamantane and adamantanecarboxylic acid". *ChemPhysChem* **18**, no. 5 (2016): 459-464. doi:10.1002/cphc.201601219.
- CM Beddoes et al. "Hydrophilic nanoparticles stabilising mesophase curvature at low concentration but disrupting mesophase order at higher concentrations". *Soft Matter* **12**, no. 28 (2016): 6049-6057. doi:10.1039/c6sm00393a.
- SL Benjamin et al. "Niobium tetrahalide complexes with neutral diphosphine ligands". *Dalton Trans* **45**, no. 19 (2016): 8192-8200. doi:10.1039/C6DT01099G.
- N Bennett et al. "Mesoporous tertiary oxides via a novel amphiphilic approach". *APL Materials* **4**, no. 1 (2016): 015701. doi:10.1063/1.4930808.
- TD Bennett et al. "Melt-Quenched Glasses of Metal-Organic Frameworks". *J Am Chem Soc* **138**, no. 10 (2016): 3484-3492. doi:10.1021/jacs.5b13220.
- TD Bennett et al. "Connecting defects and amorphization in UiO-66 and MIL-140 metal-organic frameworks: a combined experimental and computational study". *Phys Chem Chem Phys* **18**, no. 3 (2016): 2192-2201. doi:10.1039/c5cp06798g.
- O Benson et al. "Amides do not always work : observation of guest binding in an amide-functionalised porous host". *J Am Chem Soc* **138**, no. 45 (2016): 14828-14831. doi:10.1021/jacs.6b08059.
- A Bento et al. "Catalytic application of Fe-doped MoO_2 tremella-like nanosheets". *Top Catal* **59**, no. 13 (2016): 1123-1131. doi:10.1007/s11244-016-0631-x.
- A Berenov, F Le Goupil and N Alford. "Effect of ionic radii on the Curie temperature in $\text{Ba}_{1-x}\text{Sr}_x\text{Ca}_y\text{TiO}_3$ compounds". *Sci Rep* **6** (2016): 28055. doi:10.1038/srep28055.
- M Berg et al. "Water dynamics in glass ionomer cements". *EPJ ST* **225**, no. 4 (2016): 773-777. doi:10.1140/epjst/e2015-50287-3.
- A Berlie et al. "Tuneability and criticality in a three-dimensional stacked molecular system". *Phys Rev B* **93**, no. 5 (2016): 054422. doi:10.1103/PhysRevB.93.054422.
- A Berlie et al. "Dipolar glass and magneto-electric coupling within a pi-stacked organic system". *J Mater Chem C* **4**, no. 25 (2016): 6090-6095. doi:10.1039/C6TC01538G.
- G Bernardo et al. "Phase behavior of blends of PCBM with amorphous polymers with different aromaticity". *J Polym Sci Part B* **54**, no. 10 (2016): 994-1001. doi:10.1002/polb.24002.
- A Bernasconi et al. "Modeling the structure of complex aluminosilicate glasses: the effect of zinc addition". *J Phys Chem B* **120**, no. 9 (2016): 2526-2537. doi:10.1021/acs.jpcc.5b10886.
- A Bernasconi et al. "Aluminosilicate-based glasses structural investigation by high-energy X-ray diffraction". *J Mater Sci* **51**, no. 19 (2016): 8845-8860. doi:10.1007/s10853-016-0132-0.
- G Berti et al. "Observation of Mixed Valence Ru Components in Zn Doped $\text{Y}_2\text{Ru}_2\text{O}_7$ Pyrochlores". *J Phys Chem C* (2016). doi:10.1021/acs.jpcc.5b12411.
- A Bhattacharyya et al. "Incommensurate spin-density-wave antiferromagnetism in $\text{CeRu}_2\text{Al}_2\text{B}$ ". *Phys Rev B* **93**, no. 6 (2016): 060410. doi:10.1103/PhysRevB.93.060410.
- A Bhattacharyya et al. "Exploring the complex magnetic phase diagram of Ce_2PdGe_3 : A neutron powder diffraction and μ SR study". *Phys Rev B* **94**, no. 1 (2016): 014418. doi:10.1103/PhysRevB.94.014418.

T Bian et al. "Hybrid silicon nanostructures with conductive ligands and their microscopic conductivity". *Journal of Electronic Materials* **46**, no. 5 (2016): 3221-3226. doi:10.1007/s11664-016-4954-y.

J Bielecki et al. "Structure and dehydration mechanism of the proton conducting oxide $\text{Ba}_2\text{In}_2\text{O}_5(\text{H}_2\text{O})_x$ ". *J Mater Chem A* (2016): 1224-1232.

J Binns et al. "Use of a miniature diamond-anvil cell in high-pressure single-crystal neutron Laue diffraction". *IUCr* **3**, no. 3 (2016): 168-179. doi:10.1107/S2052252516000725.

PK Biswas et al. "Fully gapped superconductivity in the topological superconductor Beta-PdBi_2 ". *Phys Rev B* **93**, no. 22 (2016): 220504. doi:10.1103/PhysRevB.93.220504.

VI Bodnarchuk et al. "Geometric factor in the spin-echo small-angle neutron scattering technique based on magnetic fields that increase linearly with time". *Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques* **10**, no. 6 (2016): 1129-1132. doi:10.1134/S1027451016050475.

D Boldrin, K Knight and AS Wills. "Orbital frustration in the $S = 1/2$ kagome magnet vesignieite, $\text{BaCu}_3\text{V}_2\text{O}_8(\text{OH})_2$ ". *J Mater Chem C* **4**, no. 43 (2016): 10315-10322. doi:10.1039/c6tc02935c.

GE Boorman et al. "Characterising the Signal Processing System for Beam Position Monitors at the Front End Test Stand". In Proceedings of the *4th International Beam Instrumentation Conference (IBIC2015)*, Melbourne, Australia, 13-17 September, 2015, (2016): TUPB073. doi:10.18429/JACoW-IBIC2015-TUPB071.

AL Bosser et al. "Methodologies for the statistical analysis of memory response to radiation". IEEE Trans Nucl Sci **63**, no. 4 (2016): 2122-2128. Is in proceedings of: *15th European Conference on Radiation and Its Effects on Components and Systems (RADECS 2015)*, Moscow, Russia, 14-18 Sep 2015. doi:10.1109/TNS.2016.2527781.

CJ Bosson et al. "Crystal Structure and Cation Disorder in Bulk $\text{Cu}_2\text{ZnSnS}_4$ Using Neutron Diffraction and X-Ray Anomalous Scattering". In *43rd Photovoltaic Specialists Conference (PVSC)*, Portland, Oregon, USA, 5-10 Jun 2016, (2016): 0405-0410. doi:10.1109/PVSC.2016.7749621.

A Bouzid et al. "Pressure-induced structural changes in the network-forming isostatic glass GeSe_4 : An investigation by neutron diffraction and first-principles molecular dynamics". *Phys Rev B* **93**, no. 1 (2016): 014202. doi:10.1103/PhysRevB.93.014202.

G Bowden, G Stenning and G van der Laan. "Asymptotic behavior of local dipolar fields in thin films". *J Magnetism Magnetic Mater* **416** (2016): 449-456. doi:10.1016/j.jmmm.2016.04.063.

GJ Bowden, GBG Stenning and G van der Laan. "Inter and intra macro-cell model for point dipole-dipole energy calculations". *J Phys-Condens Mat* **28**, no. 6 (2016): 066001. doi:10.1088/0953-8984/28/6/066001.

M Bowker et al. "Methanol oxidation on Fe_2O_3 catalysts and the effects of surface Mo". *Faraday Discuss* **188** (2016): 387-398. doi:10.1039/c5fd00225g.

DT Bowron and KJ Edler. "Decyltrimethylammonium bromide micelles in acidic solutions: counterion binding, water structuring and micelle shape". *Langmuir* **33**, no. 1 (2016): 262-271. doi:10.1021/acs.langmuir.6b03880.

R Brabury et al. "Enhanced perfume surface delivery to interfaces using surfactant surface multilayer structures". *J Coll Int Sci* **461** (2016): 352-358. doi:10.1016/j.jcis.2015.09.045.

R Bradbury et al. "Manipulating perfume delivery to the interface using polymer-surfactant interactions". *J Coll Int Sci* **466** (2016): 220-226. doi:10.1016/j.jcis.2015.12.041.

WR Brant et al. "A large format in operando wound cell for analysing the structural dynamics of lithium insertion materials". *J Power Sources* **336** (2016): 279-285. doi:10.1016/j.jpowsour.2016.10.071.

F Bresme, A Lervik and J Armstrong. "Non-equilibrium Molecular Dynamics. in *Experimental Thermodynamics Volume X: Non-equilibrium Thermodynamics with Applications*. Edited by D Bedeaux, S Kjelstrup, J Sengers, 105-133. Cambridge: Royal Society of Chemistry, 2016. doi:10.1039/9781782622543-00105.

A Briddick et al. "Surfactant and Plasticiser Segregation in Thin Polyvinyl Alcohol Films". *Langmuir* **32**, no. 3 (2016): 864-872. doi:10.1021/acs.langmuir.5b03758.

J Brower et al. "The performance improvement initiative at ISIS". Presented at *Workshop on Accelerator Operations 2016 (WAO2016)*, Shanghai, China, 18-23 Sep 2016. <http://purl.org/net/epubs/manifestation/30850161>.

P Brown et al. "Magnetic surfactants as molecular based-magnets with spin glass-like properties". *J Phys-Condens Mat* **28**, no. 17 (2016): 176002. doi:10.1088/0953-8984/28/17/176002.

C Bull et al. "PEARL: the high pressure neutron powder diffractometer at ISIS". *Int J High Pressure Res* **36**, no. 4 (2016): 493-511. doi:10.1080/08957959.2016.1214730.

CL Bull et al. "Magnetic and structural phase diagram of the solid solution $\text{LaCo}_x\text{Mn}_{1-x}\text{O}_3$ ". *Phys Rev B* **94**, no. 1 (2016): 014102. doi:10.1103/PhysRevB.94.014102.

CL Bull and KS Knight. "Low-temperature structural behaviour of LaCoO₃ – a high-resolution neutron study". *Solid State Sci* **57** (2016): 38-43. doi:10.1016/j.solidstatesciences.2016.04.012.

CJ Burnham and NJ English. "Communication: Librational dynamics in water, sl and sll clathrate hydrates, and ice Ih: Molecular-dynamics insights". *J Chem Phys* **144**, no. 5 (2016): 051101. doi:10.1063/1.4941330.

C Cabrillo et al. "Absorbate-induced ordering and bilayer formation in propanol-graphite-oxide intercalates". *Carbon* **100** (2016): 546-555. doi:10.1016/j.carbon.2016.01.062.

AB Cairns et al. "Encoding complexity within supramolecular analogues of frustrated magnets". *Nat Chem* **8**, no. 5 (2016): 442-447. doi:10.1038/NCHEM.2462.

I Calabrese et al. "Porous materials as delivery and protective agents for Vitamin A". *RSC Adv* **6**, no. 71 (2016): 66495-66504. doi:10.1039/C6RA12026A.

SK Callear et al. "The reaction of formic acid with Raney (TM) copper". *Proc Math Phys Eng Sci* **472** (2016): 20160126. http://purl.org/net/epubs/manifestation/32679554.

SK Callear et al. "The reaction of formic acid with Raney (TM) copper". *Proc Math Phys Eng Sci* **472**, no. 2188 (2016): 20160126. doi:10.1098/rspa.2016.0126.

M Cao et al. "Direct exfoliation of graphite into graphene in aqueous solutions of amphiphilic peptides". *J Mater Chem B* **4**, no. 1 (2016): 152-161. doi:10.1039/c5tb02065d.

SV Carr et al. "Electron doping evolution of the magnetic excitations in NaFe_{1-x}Co_xAs". *Phys Rev B* **93**, no. 21 (2016): 214506. doi:10.1103/PhysRevB.93.214506.

ME Casco et al. "Paving the way for methane hydrate formation on metal-organic frameworks (MOFs)". *Chem Sci* **7**, no. 6 (2016): 3658-3666. doi:10.1039/C6SC00272B.

SJ Cassidy et al. "Complex Microstructure and Magnetism in Polymorphic CaFeSeO". *Inorg Chem* **55**, no. 20 (2016): 10714-10726. doi:10.1021/acs.inorgchem.6b01951.

AM Castilla et al. "On the syneresis of an OPV functionalised dipeptide hydrogel". *Soft Matter* **12**, no. 37 (2016): 7848-7854. doi:10.1039/c6sm01194b.

C Cavallari et al. "Hydrogen motions in defective graphene: the role of surface defects". *Phys Chem Chem Phys* **18**, no. 36 (2016): 24820-24824. doi:10.1039/C6CP04727K.

C Cazzaniga et al. "Light response of YAP:Ce and LaBr₃:Ce scintillators to 4–30MeV protons for applications to Telescope Proton Recoil neutron spectrometers". *Nucl Instrum Meth A* **820** (2016): 85-88. doi:10.1016/j.nima.2016.03.026.

C Cazzaniga et al. "Characterization of the high-energy neutron beam of the PRISMA beamline using a diamond detector". *JINST* **11**, no. 07 (2016): P07012. doi:10.1088/1748-0221/11/07/P07012.

M Ceriotti et al. "Nuclear quantum effects in water and aqueous systems: experiment, theory, and current challenges". *Chem Rev* **116**, no. 13 (2016): 7529-7550. doi:10.1021/acs.chemrev.5b00674.

CA Chatzidimitriou-Dreismann. "Weak measurement and two-state-vector formalism : deficit of momentum transfer in scattering processes". *Quanta* **5**, no. 1 (2016): 61. doi:10.12743/quanta.v5i1.48.

AK Chaudhari, MR Ryder and J Tan. "Photonic hybrid crystals constructed from *in situ* host-guest nanoconfinement of a light-emitting complex in metal-organic framework pores". *Nanoscale* **8**, no. 12 (2016): 6851-6859. doi:10.1039/C6NR01122E.

T Chen et al. "A potential wasteform for Cs immobilization : synthesis, structure determination, and aqueous durability of Cs₂TiNb₆O₁₈". *Inorg Chem* **55**, no. 24 (2016): 12686-12695. doi:10.1021/acs.inorgchem.6b01826.

B Cheng, J Behler and M Ceriotti. "Nuclear quantum effects in water at the triple point: using theory as a link between experiments". *J Phys Chem Lett* **7**, no. 12 (2016): 2210-2215. doi:10.1021/acs.jpcllett.6b00729.

R Chisnell et al. "Magnetic transitions in the topological magnon insulator Cu(1,3-bdc)". *Phys Rev B* **93**, no. 21 (2016): 214403. doi:10.1103/PhysRevB.93.214403.

E Choi et al. "Interface-coupled BiFeO₃/BiMnO₃ superlattices with magnetic transition temperature up to 410 K". *Adv Mater Inter* **3**, no. 5 (2016): 1500597. doi:10.1002/admi.201500597.

A Chutia et al. "Adsorption of formate species on Cu(h,k,l) low index surfaces". *Surf Sci* **653** (2016): 45-54. doi:10.1016/j.susc.2016.05.002.

D Ciunac et al. "Implications of lipid monolayer charge characteristics on their selective interactions with a short antimicrobial peptide". *Colloids and Surfaces B: Biointerfaces* **150** (2016): 308-316. doi:10.1016/j.colsurfb.2016.10.043.

SJ Clark et al. "Li(V_{0.5}Ti_{0.5})S₂ as a 1 V lithium intercalation electrode". *Nat Commun* **7** (2016): 10898. doi:10.1038/ncomms10898.

O Clemens et al. "Anion ordering, magnetic structure and properties of the vacancy ordered perovskite Ba₃Fe₃O₇F". *J Solid State Chem* **243** (2016): 31-37. doi:10.1016/j.jssc.2016.07.033.

LA Clifton et al. "The Effect of Lipopolysaccharide Core Oligosaccharide Size on the Electrostatic Binding of Antimicrobial Proteins to Models of the Gram Negative Bacterial Outer Membrane". *Langmuir* **32**, no. 14 (2016): 3485-3494. doi:10.1021/acs.langmuir.6b00240.

LA Clifton et al. "The Complex, Asymmetric, Escherichia Coli Envelope Studied by Neutron Scattering". *Biophys J* **110**, no. 3 (2016): 35a. doi:10.1016/j.bpj.2015.11.256.

JM Cole, X Cheng and MC Payne. "Modeling pair distribution functions of rare-Earth Phosphate glasses using principal component analysis". *Inorg Chem* **55**, no. 21 (2016): 10870-10880. doi:10.1021/acs.inorgchem.6b00907.

JM Cole et al. "Relating the structure of geminal amido esters to their molecular hyperpolarizability". *J Phys Chem C* **120**, no. 51 (2016): 29439-29448. doi:10.1021/acs.jpcc.6b10724.

JM Cole and M Irie. "Solid-state photochemistry". *CrystEngComm* **18**, no. 38 (2016): 7175-7179. doi:10.1039/c6ce90146h.

IE Collings et al. "Structural distortions in the high-pressure polar phases of ammonium metal formates". *CrystEngComm* **18**, no. 46 (2016): 8849-8857. doi:10.1039/C6CE01891B.

LJ Collins-McIntyre et al. "Structural, electronic, and magnetic investigation of magnetic ordering in MBE-grown $\text{Cr}_x\text{Sb}_{2-x}\text{Te}_3$ thin films". *Europhys Lett* **115**, no. 2 (2016): 27006. doi:10.1209/0295-5075/115/27006.

BJ Corrie et al. "Neutron diffraction and multinuclear solid state NMR investigation into the structures of oxide ion conducting $\text{La}_{9.6}\text{Si}_6\text{O}_{26.4}$ and $\text{La}_8\text{Sr}_2\text{Si}_6\text{O}_{26}$, and their hydrated phases". *Dalton Trans* **45**, no. 1 (2016): 121-133. doi:10.1039/c5dt03190g.

J Corsi et al. "Compositional and microstructural characterization of Celtic silver coins from northern Italy using neutron diffraction analysis". *Microchemical Journal* **126** (2016): 501-508. doi:10.1016/j.microc.2016.01.006.

D Coutandin et al. "Quality control in oocytes by p63 is based on a spring-loaded activation mechanism on the molecular and cellular level". *eLife* **5** (2016): e13909. doi:10.7554/eLife.13909.

AJ Cramer and JM Cole. "Topological Analysis of Void Space in Phosphate Frameworks: Assessing Storage Properties for the Environmentally Important Guest Molecules and Ions: CO_2 , H_2O , UO_2 , PuO_2 , U, Pu, Sr_{2+} , Cs^+ , CH_4 , and H_2 ". *ACS Sustainable Chemistry & Engineering* **4**, no. 8 (2016): 4094-4112. doi:10.1021/acssuschemeng.6b00316.

J Cumby et al. "Synthetic analogues of Fe(II)-Fe(III) minerals containing a pentagonal 'Cairo' magnetic lattice". *Dalton Trans* **45**, no. 29 (2016): 11801-11806. doi:10.1039/C6DT01672C.

R Cunningham et al. "Solubility study of tobramycin in room temperature ionic liquids: an experimental and computational based study". *RSC Adv* **6**, no. 109 (2016): 107214-107218. doi:10.1039/c6ra23078d.

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

D Das et al. "Neutron diffraction study on heavy-fermion compound". *Phys Rev B* **94**, no. 17 (2016): 174415. doi:10.1103/PhysRevB.94.174415.

K Datta et al. "Direct mapping of microscopic polarization in ferroelectric $x(\text{BiScO}_3)-(1-x)(\text{PbTiO}_3)$ throughout its morphotropic phase boundary". *Phys Rev B* **93**, no. 6 (2016): 064102. doi:10.1103/PhysRevB.93.064102.

NR Davies et al. "Spin resonance in the superconducting state of $\text{Li}_{1-x}\text{Fe}_x\text{ODFe}_{1-y}\text{Se}$ observed by neutron spectroscopy". *Phys Rev B* **94**, no. 14 (2016): 144503. doi:10.1103/PhysRevB.94.144503.

NR Davies et al. "Coupled commensurate charge density wave and lattice distortion in $\text{Na}(2)\text{Ti}(2)\text{Pn}(2)\text{O}$ (Pn = As, Sb) determined by x-ray diffraction and angle-resolved photoemission spectroscopy". *Phys Rev B* **94**, no. 10 (2016): 104515. doi:10.1103/PhysRevB.94.104515.

J Dawidowski et al. "Effective temperatures and scattering cross sections in water mixtures determined by Deep Inelastic Neutron Scattering". *Ann Nucl Energy* **90** (2016): 247-255. doi:10.1016/j.anucene.2015.11.023.

N Deb et al. "Harnessing Structure-Property Relationships for Poly(alkyl thiophene)-Fullerene Derivative Thin Films to Optimize Performance in Photovoltaic Devices". *Adv Funct Mater* **26**, no. 12 (2016): 1908-1920. doi:10.1002/adfm.201502653.

Y Delavoux et al. "Intermolecular structure and hydrogen-bonding in liquid 1,2-propylene carbonate and 1,2-glycerol carbonate determined from neutron scattering". *Phys Chem Chem Phys* **19** (2016): 2867-2876. doi:10.1039/C6CP07790K.

F Demmel, O Alcaraz and J Trullas. "Br diffusion in molten NaBr explored by coherent quasielastic neutron scattering". *Phys Rev E* **93**, no. 4 (2016): 042604. doi:10.1103/PhysRevE.93.042604.

F Demmel et al. "Nickel self-diffusion in a liquid and undercooled NiSi alloy". *Phys Rev B* **94**, no. 1 (2016): 014206. doi:10.1103/PhysRevB.94.014206.

F Demmel and S Mukhopadhyay. "Quasielastic neutron scattering measurements and ab initio MD-simulations on single ion motions in molten NaF". *J Chem Phys* **144**, no. 1 (2016): 014503, 014503. doi:10.1063/1.4939072.

D Di Martino et al. "Disclosing mineralogical phases in medioeval iron nails by non-destructive neutron techniques". *Archaeological and Anthropological Sciences* **9**, no. 4 (2016): 515-522. doi:10.1007/s12520-016-0384-2.

M Dodge et al. "Assessment of Residual Stress and Suitability for Subsea Service of a Welded Superduplex Stainless Steel Flange Joint". In *35th International Conference on Ocean, Offshore and Arctic Engineering*, Busan, South Korea, 19-24 Jun 2016, (2016): V004T03A027. doi:10.1115/OMAE2016-54004.

B Dong et al. "Synthesis, structure and electrical properties of N-doped Li_3VO_4 ". *J Mater Chem A* **4**, no. 4 (2016): 1408-1413. doi:10.1039/c5ta07823g.

LHR Dos Santos et al. "Experimental and Theoretical Electron Density Analysis of Copper Pyrazine Nitrate Quasi-Low-Dimensional Quantum Magnets". *J Am Chem Soc* **138**, no. 7 (2016): 2280-2291. doi:10.1021/jacs.5b12817.

K Druzicki et al. "Unexpected cation dynamics in the low-temperature phase of methylammonium lead iodide – the need for improved models". *J Phys Chem Lett* **7**, no. 22 (2016): 4701-4709. doi:10.1021/acs.jpcllett.6b01822.

HD Duncan et al. "Local structure of the metal-organic perovskite dimethylammonium manganese(II) formate". *Dalton Trans* **45**, no. 10 (2016): 4380-4391. doi:10.1039/c5dt03687a.

MT Dunstan et al. "In situ studies of materials for high temperature CO_2 capture and storage". *Faraday Discuss* **192** (2016): 217-240. doi:10.1039/C6FD00047A.

ZO Et-Tarhouni et al. "Quantifying the micellar structure formed from hydrocarbon-fluorocarbon surfactants". *Coll Surf A* **492** (2016): 255-262. doi:10.1016/j.colsurfa.2015.12.015.

R Ewings et al. "HORACE : software for the analysis of data from single crystal spectroscopy experiments at time-of-flight neutron instruments". *Nucl Instrum Meth A* **834** (2016): 132-142. doi:10.1016/j.nima.2016.07.036.

RA Ewings et al. "Spin excitations used to probe the nature of exchange coupling in the magnetically ordered ground state of $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ ". *Phys Rev B* **94**, no. 1 (2016): 014405. doi:10.1103/PhysRevB.94.014405.

H Fahlquist et al. "Stabilization of 3d transition metal hydrido complexes in $\text{SrH}_2\text{Mg}_2[\text{Co}(\text{I})\text{H}_5]$, $\text{BaH}_2\text{Mg}_5[\text{Co}(\text{I})\text{H}_4]_2$, and $\text{RbH}_2\text{Mg}_5[\text{Co}(\text{I})\text{H}_4\text{Ni}(\text{O})\text{H}_4]$ with a novel "back donation" mechanism". *Inorg Chem* **55** (2016): 3576-3582. <http://pubs.rsc.org/net/epubs/manifestation/32202055>.

D Faircloth et al. "Initial Commissioning of the Rutherford Appleton Laboratory (RAL) Scaled Negative Penning Ion Source". In *7th International Particle Accelerator Conference (IPAC'16)*, Busan, Korea, 8-13 May 2016, (2016): 1314-1316. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/tupmr032.pdf>.

J Fajoui et al. "Bauschinger Effect in an Austenitic Steel: Neutron Diffraction and a Multiscale Approach". *Metall Mater Trans A* **47**, no. 5 (2016): 1-13. doi:10.1007/s11661-016-3362-5.

M Falkowska et al. "Determination of toluene hydrogenation kinetics with neutron diffraction". *Phys Chem Chem Phys* **18**, no. 26 (2016): 17237-17243. doi:10.1039/C6CP01494A.

M Falkowska et al. "Neutron scattering of aromatic and aliphatic liquids". *ChemPhysChem* **17**, no. 13 (2016): 2043-2055. doi:10.1002/cphc.201600149.

K Fan et al. "Neutron diffraction residual stress analysis of $\text{Al}_2\text{O}_3/\text{Y-TZP}$ ceramic composites". *Boletín de la Sociedad Española de Cerámica y Vidrio* **55**, no. 1 (2016): 13-23. doi:10.1016/j.bsecv.2015.10.006.

C Fanelli et al. "Pion generalized parton distributions within a fully covariant constituent quark model". *Europ Phys J C* **76**, no. 5 (2016): 253. doi:10.1140/epjc/s10052-016-4101-1.

AH Farmahini and SK Bhatia. "Effect of structural anisotropy and pore-network accessibility on fluid transport in nanoporous Ti_3SiC_2 carbide-derived carbon". *Carbon* **103** (2016): 16-27. doi:10.1016/j.carbon.2016.02.093.

CI Fernandes et al. "Looking inside the pores of a MCM-41 based Mo heterogeneous styrene oxidation catalyst: an inelastic neutron scattering study". *Phys Chem Chem Phys* **18**, no. 26 (2016): 17272-17280. doi:10.1039/C6CP01243D.

A Fernández-Pacheco et al. "Magnetic state of multilayered synthetic antiferromagnets during soliton nucleation and propagation for vertical data transfer". *Adv Mater Inter* **3**, no. 15 (2016): 1600097. doi:10.1002/admi.201600097.

P Ferrer, I da Silva and I Puentes-Orench. "Solid acetone structure dependence on pressure: a new fibre textured thin film crystallographic structure studied by grazing-incidence X-ray diffraction". *CrystEngComm* **18**, no. 42 (2016): 8220-8228. doi:10.1039/c6ce01333c.

G Festa, N Kardjilov and C Andreani. "Probing our heritage with neutrons — one successful story. in Neutron Methods for Archaeology and Cultural Heritage". Neutron Scattering Applications and Techniques edited by N Kardjilov, G Festa, part 1, 3-18. Springer International Publishing, 2016. doi:10.1007/978-3-319-33163-8_1.

G Festa et al. "Isotope identification capabilities using time resolved prompt gamma emission from epithermal neutrons". *JINST* **11** (2016): C03060. Is in proceedings of: *International Workshop on Imaging*, Varenna, ITALY, 7-10 Sep 2015. doi:10.108

G Festa, D Mannes and A Scherillo. Neutrons unveil secrets of musical instruments. in **Neutron Methods for Archaeology and Cultural Heritage. Neutron Scattering Applications and Techniques** edited by N Kardjilov, G Festa, part 1, 53-66. Springer International Publishing, 2016. doi:10.1007/978-3-319-33163-8_4.

SK Filippov et al. Internal nanoparticle structure of temperature-responsive self-assembled PNIPAM-b-PEG-b-PNIPAM triblock copolymers in aqueous solutions: NMR, SANS and Light Scattering studies. **Langmuir** **32**, no. 21 (2016): 5314-5323. doi:10.1021/acs.langmuir.6b00284.

F Fillaux and A Cousson. Quantum interferences revealed by neutron diffraction accord with a macroscopic-scale quantum-theory of ferroelectrics $\text{KH}_{2(1-\theta)}\text{D}_\theta\text{PO}_4$. **Eur Phys J B** **89**, no. 3 (2016): 72. doi:10.1140/epjb/e2016-50749-0.

D Findlay. 'Universal' representation of HPGe detector efficiencies. **Radiat Meas** **94** (2016): 23-26. doi:10.1016/j.radmeas.2016.08.006.

Y Finkelstein and R Moreh. Proton dynamics in hydrogen-bonded systems. **Mol Phys** (2016): 1-7. doi:10.1080/00268976.2016.1184342.

Y Finkelstein et al. On the mean kinetic energy of the proton in strong hydrogen bonded systems. **J Chem Phys** **144**, no. 5 (2016): 054302. doi:10.1063/1.4940730.

A Fitzner et al. The effect of aluminium on twinning in binary alpha-titanium. **Acta Mater** **103** (2016): 341-351. doi:10.1016/j.actamat.2015.09.048.

S Fop et al. Oxide ion conductivity in the hexagonal perovskite derivative $\text{Ba}_3\text{MoNbO}_{8.5}$. **J Am Chem Soc** **138**, no. 51 (2016): 16764-16769. doi:10.1021/jacs.6b10730.

AD Fortes et al. Glycine zinc sulfate pentahydrate, redetermination at 10K from time-of-flight neutron Laue diffraction. **Acta Crystallogr E** **72**, no. 10 (2016): 1438-1445. doi:10.1107/S2056989016014304.

K Fujita et al. LiNbO_3 -Type InFeO_3 : room-temperature polar magnet without second-order Jahn-Teller active ions. **Chem Mater** **28**, no. 18 (2016): 6644-6655. doi:10.1021/acs.chemmater.6b02783.

S Furse and DJ Scott. Three-dimensional distribution of phospholipids in gram negative bacteria. **Biochemistry** **55**, no. 34 (2016): 4742-4747. doi:10.1021/acs.biochem.6b00541.

A Gagin and I Levin. Applications of Bayesian corrections for systematic errors in Rietveld refinements. **J Appl Crystallogr** **49**, no. 3 (2016): 814-822. doi:10.1107/S1600576716004209.

J Gardner et al. Relaxor-to-ferroelectric crossover and disruption of polar order in "empty" tetragonal tungsten bronzes. **Chem Mater** **28**, no. 13 (2016): 4616-4627. doi:10.1021/acs.chemmater.6b01306.

A Gauzzi et al. Bulk superconductivity at 84 K in the strongly overdoped regime of cuprates. **Phys Rev B** **94**, no. 18 (2016): 180509. doi:10.1103/PhysRevB.94.180509.

O Gerlits et al. Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. **Angew Chem Int Ed** **55**, no. 16 (2016): 4924-4927. doi:10.1002/anie.201509989.

O Gerlits et al. Long-Range Electrostatics-Induced Two-Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. **Angew Chem** **128**, no. 16 (2016): 5008-5011. doi:10.1002/ange.201509989.

EK Gibson et al. *In Situ* and *Operando* Measurement of Catalysts at Synchrotron X-ray and Neutron Sources. in **Modern Developments in Catalysis**. Edited by G Hutchings, M Davidson, R Catlow, C Hardacre, N Turner, P Collier, 41-88. World Scientific, 2016. doi:10.1142/9781786341228_0002.

PA Goddard et al. Control of the third dimension in copper-based square-lattice antiferromagnets. **Phys Rev B** **93**, no. 9 (2016): 094430. doi:10.1103/PhysRevB.93.094430.

M Gomilšek et al. Instabilities of spin-liquid states in a quantum kagome antiferromagnet. **Phys Rev B** **93**, no. 6 (2016): 060405. doi:10.1103/PhysRevB.93.060405.

G Gorini et al. Neutron Resonance Imaging. in **Neutron Methods for Archaeology and Cultural Heritage. Neutron Scattering Applications and Techniques** edited by N Kardjilov, G Festa, part 2, 285-301. Springer International Publishing, 2016. doi:10.1007/978-3-319-33163-8_13.

J Goura et al. Heterometallic trinuclear $\{\text{CoIII}2\text{Ln}^{\text{III}}\}$ (Ln = Gd, Tb, Ho and Er) complexes in a bent geometry. Field-induced single-ion magnetic behavior of the Er^{III} and Tb^{III} analogues. **Dalton Trans** **45**, no. 22 (2016): 9235-9249. doi:10.1039/C5DT03871E.

F Grazi et al. Determination of the manufacturing methods of Indian swords through neutron diffraction. **Microchemical Journal** **125** (2016): 273-278. doi:10.1016/j.microc.2015.11.035.

M Green et al. Defining the intrinsically disordered C-terminal domain of SSB reveals DNA-mediated compaction. **J Mol Biol** **428**, no. 2 (2016): 357-364. doi:10.1016/j.jmb.2015.12.007.

M Griesser et al. New insights into the manufacturing technique and corrosion of high leaded antique bronze coins. **Microchemical Journal** **126** (2016): 181-193. doi:10.1016/j.microc.2015.12.002.

LR Griffin et al. Multilayering of Calcium Aerosol-OT at the Mica/water interface studied with neutron reflection – formation of a condensed lamellar phase at CMC. **Langmuir** **32**, no. 49 (2016): 13054-13064. doi:10.1021/acs.langmuir.6b03601.

- LR Griffin et al. A comparison of didodecyldimethylammonium bromide adsorbed at mica/water and silica/water interfaces using neutron reflection. *J Coll Int Sci* **478** (2016): 365-373. doi:10.1016/j.jcis.2016.06.015.
- M Gupta et al. Phonons and stability of infinite-layer iron oxides SrFeO₂ and CaFeO₂. *Solid State Commun* **241** (2016): 43-55. doi:10.1016/j.ssc.2016.05.010.
- G Guélou et al. The impact of charge transfer and structural disorder on the thermoelectric properties of cobalt intercalated TiS₂. *J Mater Chem C* **4**, no. 9 (2016): 1871-1880. doi:10.1039/c5tc04217h.
- T Haku et al. Crystal Field Excitations in the Breathing Pyrochlore Antiferromagnet Ba₃Yb₂Zn₅O₁₁. *J Phys Soc Jpn* **85**, no. 3 (2016): 034721. doi:10.7566/JPSJ.85.034721.
- OS Hammond, DT Bowron and KJ Edler. Liquid structure of the choline chloride-urea deep eutectic solvent (reline) from neutron diffraction and atomistic modelling. *Green Chem* **18**, no. 9 (2016): 2736-2744. doi:10.1039/c5gc02914g.
- G Hannappel et al. Stability of a spin-triplet nematic state near to a quantum critical point. *Phys Rev B* **93**, no. 23 (2016): 235105. doi:10.1103/PhysRevB.93.235105.
- AC Hannon. Bonding and structure in network glasses. *J Non-Cryst Solids* **451** (2016): 56-67. doi:10.1016/j.jnoncrysol.2016.04.035.
- DR Harcombe et al. One-dimensional magnetic order in the metal-organic framework Tb(HCOO)₃. *Phys Rev B* **94**, no. 17 (2016): 174429. doi:10.1103/PhysRevB.94.174429.
- DMH Harryman and AP Pertica. Online Total Ionisation Dosimeter (TID) Monitoring Using Semiconductor Based Radiation Sensors in the ISIS Proton Synchrotron. In *International Beam Instrumentation Conference (IBIC), Barcelona, Spain*, 12-15 Sep 2016, (2016). <http://jacow.web.psi.ch/conf/y16/ibic16n5alba/prepress/TUPG24.PDF>.
- JM Hart et al. Spontaneous Nanoparticle Dispersal in Polybutadiene by Brush-Forming End-Functional Polymers. *Macromolecules* **49**, no. 4 (2016): 1434-1443. doi:10.1021/acs.macromol.5b02318.
- G Hazell et al. Langmuir monolayers composed of single and double tail sulfobetaine lipids. *J Coll Int Sci* **474** (2016): 190-198. doi:10.1016/j.jcis.2016.04.020.
- G Hazell et al. Evidence of lipid exchange in styrene maleic acid lipid particle (SMALP) nanodisc systems. *Langmuir* **32**, no. 45 (2016): 11845-11853. doi:10.1021/acs.langmuir.6b02927.
- MS Hellsing et al. Sorption of perfluoroalkyl substances to two types of minerals. *Chemosphere* **159** (2016): 385-391. doi:10.1016/j.chemosphere.2016.06.016.
- CI Hiley et al. Ba₄Ru₃O₁₀2(OH)_{1.8}: a new member of the layered hexagonal perovskite family crystallised from water. *Chem Commun* **52**, no. 38 (2016): 6375-6378. doi:10.1039/C6CC02121B.
- CR Hill et al. Neutron scattering analysis of water's glass transition and micropore collapse in amorphous solid water. *Phys Rev Lett* **116**, no. 21 (2016): 215501. doi:10.1103/PhysRevLett.116.215501.
- A Hillier, D Paul and K Ishida. Probing beneath the surface without a scratch — Bulk non-destructive elemental analysis using negative muons. *Microchemical Journal* **125** (2016): 203-207. doi:10.1016/j.microc.2015.11.031.
- J Ho et al. STAT2 Is a pervasive Cytokine regulator due to its inhibition of STAT1 in multiple signaling pathways. *PLoS Biology* **14**, no. 10 (2016): e2000117. doi:10.1371/journal.pbio.2000117.
- I Hoffmann et al. Kinetics of oil exchange in nanoemulsions prepared with the phase inversion concentration method. *Langmuir* **32**, no. 46 (2016): 12084-12090. doi:10.1021/acs.langmuir.6b03009.
- MJ Hollamby et al. Simultaneous SAXS and SANS analysis for the detection of toroidal supramolecular polymers composed of noncovalent supermacrocycles in solution. *Angew Chem* **128**, no. 34 (2016): 10044-10047. doi:10.1002/ange.201603370.
- MJ Hollamby et al. Fluorescent liquid pyrene derivative-in-water microemulsions. *Chem Commun* **52**, no. 46 (2016): 7344-7347. doi:10.1039/c6cc01517d.
- D Hollas, E Muchova and P Slavicek. In the shadow of electrons : nuclear quantum effects in chemistry. *Chemické Listy* **110**, no. 5 (2016): 394-403. http://www.chemicke-listy.cz/docs/full/2016_05_394-403.pdf.
- J Holmberg et al. Residual stress state in an induction hardened steel bar determined by synchrotron- and neutron diffraction compared to results from lab-XRD. *Mater Sci Eng A* **667** (2016): 199-207. doi:10.1016/j.msea.2016.04.075.
- Y Hosaka et al. Charge and spin order in the perovskite CaFe_{0.5}Mn_{0.5}O₃: charge disproportionation behavior of randomly arranged Fe₄₊. *Phys Rev B* **94**, no. 10 (2016): 104429. doi:10.1103/PhysRevB.94.104429.
- V Hounkpati et al. *In situ* neutron measurements and modelling of the intergranular strains in the near-beta titanium alloy Ti-beta21S. *Acta Mater* **109** (2016): 341-352. doi:10.1016/j.actamat.2016.02.065.
- JE Houston et al. Charge-Mediated Localization of Conjugated Polythiophenes in Zwitterionic Model Cell Membranes. *Langmuir* **32**, no. 32 (2016): 8141-8153. doi:10.1021/acs.langmuir.6b01828.

C Howard et al. X-ray and neutron powder diffraction analyses of $\text{Gly} \cdot \text{MgSO}_4 \cdot 5\text{H}_2\text{O}$ and $\text{Gly} \cdot \text{MgSO}_4 \cdot 3\text{H}_2\text{O}$, and their deuterated counterparts. *Acta Crystallogr C* **72** (2016): 203-216. doi:10.1107/S2053229616001200.

RF Howe et al. Application of inelastic neutron scattering to the methanol-to-gasoline reaction over a ZSM-5 catalyst. *Catal Lett* **146**, no. 7 (2016): 1242-1248. doi:10.1007/s10562-016-1742-5.

D Hu et al. Spin excitations in optimally P-doped $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$ superconductor. *Phys Rev B* **94** (2016): 094504. doi:10.1103/PhysRevB.94.094504.

AV Hughes et al. On the interpretation of reflectivity data from lipid bilayers in terms of molecular-dynamics models. *Acta Crystallographica Section D Structural Biology* **72**, no. 12 (2016): 1227-1240. doi:10.1107/S2059798316016235.

HM Hunter et al. Demonstrating hydrogen production from ammonia using lithium imide – Powering a small proton exchange membrane fuel cell. *J Power Sources* **329** (2016): 138-147. doi:10.1016/j.jpowsour.2016.08.004.

JR Hönnige et al. Residual Stress Characterization and Control in the Additive Manufacture of Large Scale Metal Structures. In *10th International Conference on Residual Stresses (ICRS-10), Sydney, Australia*, 3-7 July, 2016, (2016): 455-460. http://www.mrforum.com/wp-content/uploads/open_access/9781945291173.pdf.

I Iriarte-Carretero et al. The rich phase behavior of the thermopolarization of water: from a reversal polarization to large enhancement near criticality conditions. *Phys Chem Chem Phys* **18**, no. 29 (2016): 19894-19901. doi:10.1039/C6CP03082C.

S Isaksson et al. Protein-containing lipid bilayers intercalated with size-matched mesoporous silica thin films. *Nano Lett* **17**, no. 1 (2016): 476-485. doi:10.1021/acs.nanolett.6b04493.

S Istomin et al. Tuning the high-temperature properties of $\text{Pr}_2\text{NiO}_4+\text{O}$ by simultaneous Pr- and Ni- cations replacement. *RSC Adv* **6**, no. 40 (2016): 33951-33958. doi:10.1039/C6RA03099H.

UA Jayasooriya et al. Rate of molecular transfer of allyl alcohol across an AOT surfactant layer using muon spin spectroscopy. *Langmuir* **32**, no. 3 (2016): 664-672. doi:10.1021/acs.langmuir.5b03482.

H Jazaeri et al. Study of cavities in a creep crack growth test specimen. *Procedia Structural Integrity* **2** (2016): 942-949. Is in proceedings of: *21st European Conference on Fracture (ECF), Catania, Italy*, 20-24 Jun 2016. doi:10.1016/j.prostr.2016.06.121.

D Jia et al. Re-entrance of poly(N,N-diethylacrylamide) in $\text{D}_2\text{O}/\text{d}$ -ethanol mixture at 27 °C. *Macromolecules* **49**, no. 14 (2016): 5152-5159. doi:10.1021/acs.macromol.6b00785.

RD Johnson et al. Modulated spin helicity stabilized by incommensurate orbital density waves in a quadruple perovskite manganite. *Phys Rev B* **93**, no. 18 (2016): 180403. doi:10.1103/PhysRevB.93.180403.

AJ Johnston et al. On the atomic structure of cocaine in solution. *Phys Chem Chem Phys* **18**, no. 2 (2016): 991-999. doi:10.1039/c5cp06090g.

B Jones, DJ Adams and HV Smith. Initial Experience with Carbon Stripping Foils at ISIS. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 1378-1380. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/tupmr053.pdf>.

DR Jones et al. An investigation of the effect of carbon support on ruthenium/carbon catalysts for lactic acid and butanone hydrogenation. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17259-17264. doi:10.1039/c6cp01311b.

MO Jones, J Hartley and A Porch. Simultaneous neutron diffraction and microwave dielectric characterisation of ammine materials – a non-destructive, non-contact characterisation tool for determining ammonia content in solids. *Phys Chem Chem Phys* **18**, no. 33 (2016): 23340-23347. doi:10.1039/c6cp04249j.

X Just-Baringo et al. Selective synthesis of cyclooctanoids by radical cyclization of seven-membered lactones : neutron diffraction study of the stereoselective deuteration of a chiral organosamarium intermediate. *Angew Chem Int Ed* **55**, no. 40 (2016): 12499-12502. doi:10.1002/anie.201606792.

S Kabra et al. Energy-dispersive neutron imaging and diffraction of magnetically driven twins in a Ni_2MnGa single crystal magnetic shape memory alloy. *J Phys Conf Ser* **746**, no. 1 (2016): 012056. doi:10.1088/1742-6596/746/1/012056.

L Kalland et al. C-type related order in the defective fluorites $\text{La}_2\text{Ce}_2\text{O}_7$ and $\text{Nd}_2\text{Ce}_2\text{O}_7$ studied by neutron scattering and ab initio MD simulations. *Phys Chem Chem Phys* **18**, no. 34 (2016): 24070-24080. doi:10.1039/c6cp04708d.

EL Kamil, HW Morgan and MA Hayward. “ $\text{Ba}_6\text{Nb}_4\text{RuO}_{18}$ ” and “ $\text{LaBa}_4\text{Nb}_3\text{RuO}_{15}$ ” – the structural consequences of substituting paramagnetic cations into AnBn-1O3n cation-deficient perovskite oxides. *J Solid State Chem* **238** (2016): 267-272. doi:10.1016/j.jssc.2016.03.040.

T Kandemir et al. Different routes to methanol: inelastic neutron scattering spectroscopy of adsorbates on supported copper catalysts. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17253-17258. doi:10.1039/c6cp00967k.

EB Karlsson et al. The hydrogen anomaly in neutron Compton scattering: new experiments and a quantitative theoretical explanation. *Measurement Sci Technol* **27**, no. 8 (2016): 085501. doi:10.1088/0957-0233/27/8/085501.

M Karlsson. Proton dynamics in oxides: an insight into the mechanics of proton conduction from quasielastic neutron scattering. In Structural Characterization Techniques - *Advances and Applications in Clean Energy*. Edited by L Malavasi, 125-160. Singapore: Pan Stanford Publishing, 2016. <http://www.panstanford.com/books/9789814669344.html>.

M Kassem et al. Mercury sulfide dimorphism in thioarsenate glasses. *J Phys Chem B* **120**, no. 23 (2016): 5278-5290. doi:10.1021/acs.jpcc.6b03382.

E Kastrisianaki-Guyton et al. Adsorption of sodium dodecylsulfate on single-walled carbon nanotubes characterised using small-angle neutron scattering. *J Coll Int Sci* **472** (2016): 1-7. doi:10.1016/j.jcis.2016.03.026.

DA Keen. Perovskites take the lead in local structure analysis. *IUCr* **3**, no. 1 (2016): 8-9. doi:10.1107/S2052252515024033.

DD Khalyavin et al. Spin and orbital ordering in TlMnO₃: neutron diffraction study. *Phys Rev B* **94**, no. 13 (2016): 134412. doi:10.1103/PhysRevB.94.134412.

JC Khong et al. Design and characterisation of metallic glassy alloys of high neutron shielding capability. *Sci Rep* **6** (2016): 36998. doi:10.1038/srep36998.

AFR Kilpatrick et al. Synthesis and Characterization of Solid Polymethylaluminumoxane: A Bifunctional Activator and Support for Slurry-Phase Ethylene Polymerization. *Chem Mater* **28**, no. 20 (2016): 7444-7450. doi:10.1021/acs.chemmater.6b03009.

S Kim et al. Spin State As a Probe of Vesicle Self-Assembly. *J Am Chem Soc* **138**, no. 8 (2016): 2552-2555. doi:10.1021/jacs.6b00537.

K Kimura et al. Magnetodielectric detection of magnetic quadrupole order in Ba(TiO)Cu₄(PO₄)₄ with Cu₄O₁₂ square cupolas. *Nat Commun* **7** (2016): 13039. doi:10.1038/ncomms13039.

CJ Kinane et al. Influence of the liquid helium meniscus on neutron reflectometry data. *Low Temp Phys* **42**, no. 2 (2016): 152-155. <http://dx.doi.org/10.1063/1.4941005>.

FG Kinyanjui et al. Crystal structure and proton conductivity of BaSn_{0.6}Sc_{0.4}O₃-delta: insights from neutron powder diffraction and solid-state NMR spectroscopy. *J Mater Chem A* **4**, no. 14 (2016): 5088-5101. doi:10.1039/c5ta09744d.

O Kirichek et al. Segregated water observed in a putative fish embryo cryopreservative. *Royal Society Open Science* **3**, no. 3 (2016): 150655. doi:10.1098/rsos.150655.

FKK Kirschner et al. Robustness of superconductivity to competing magnetic phases in tetragonal FeS. *Phys Rev B* **94**, no. 13 (2016): 134509. doi:10.1103/PhysRevB.94.134509.

M Knaapila et al. Incorporation of a cationic conjugated polyelectrolyte CPE within an aqueous poly(vinyl alcohol) sol. *Macromolecules* **49**, no. 23 (2016): 9119-9131. doi:10.1021/acs.macromol.6b01895.

KS Knight. High-pressure thermoelastic and structural properties of KCaF₃ perovskite in the low temperature Pbnm phase. *J Alloys Comp* **693** (2016): 1305-1314. doi:10.1016/j.jallcom.2016.09.285.

KS Knight and CL Bull. Low temperature and high pressure thermoelastic and crystallographic properties of SrZrO₃ perovskite in the Pbnm phase. *Solid State Sci* **62** (2016): 90-104. doi:10.1016/j.solidstatesciences.2016.11.002.

I Knyght et al. Interaction of the antimicrobial peptides rhesus theta-Defensin and porcine protegrin-1 with anionic phospholipid monolayers. *Langmuir* **32**, no. 29 (2016): 7403-7410. doi:10.1021/acs.langmuir.6b01688.

PL Knöchel et al. Synthesis, structural characterisation and proton conduction of two new hydrated phases of barium ferrite BaFeO_{2.5-x}(OH)_(2x). *J Mater Chem A* **4**, no. 9 (2016): 3415-3430. doi:10.1039/c5ta06383c.

AI Kolesnikov et al. Quantum Tunneling of Water in Beryl: A New State of the Water Molecule. *Phys Rev Lett* **116**, no. 16 (2016): 167802. doi:10.1103/PhysRevLett.116.167802.

A Konstantatos et al. In-depth magnetic characterization of a [2 × 2] Mn(III) square grid using SQUID magnetometry, inelastic neutron scattering, and high-field electron paramagnetic resonance spectroscopy. *Inorg Chem* **55**, no. 20 (2016): 10377-10382. doi:10.1021/acs.inorgchem.6b01634.

H Kroll et al. CoMg olivine: cation partitioning, thermal expansion and structural variation studied by *in situ* neutron and synchrotron powder diffraction. *Eur J Miner* **28**, no. 4 (2016): 703-719. doi:10.1127/ejm/2016/0028-2554.

P Krooß et al. Cyclic Degradation of Co₄₉Ni₂₁Ga₃₀ High-Temperature Shape Memory Alloy: On the Roles of Dislocation Activity and Chemical Order. *Shape Memory and Superelasticity* **2**, no. 1 (2016): 37-49. doi:10.1007/s40830-015-0049-5.

J-B Lagrange et al. nuSTORM FFAG Decay Ring. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 3369-3371. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/thpmb053.pdf>.

J-B Lagrange et al. FFAG Beam Line for nuPIL - Neutrinos from Plon Beam Line. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 3372-3374. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/thpmb054.pdf>.

J-B Lagrange, C Hunt and J Pasternak. The MICE Demonstration of Muon Ionization Cooling. In *7th International Particle Accelerator Conference (IPAC'16)*, Busan, Korea, 8-13 May 2016, (2016): 1547-1549. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/tupmy004.pdf>.

G Lamura et al. Role of magnetic dopants in the phase diagram of Sm 1111 pnictides: The case of Mn. *Phys Rev B* **94**, no. 21 (2016): 214517. doi:10.1103/PhysRevB.94.214517.

T Lancaster et al. Transverse field muon-spin rotation measurement of the topological anomaly in a thin film of MnSi. *Phys Rev B* **93**, no. 14 (2016): 140412. doi:10.1103/PhysRevB.93.140412.

F Lang et al. Unconventional magnetism on a honeycomb lattice in alpha-RuCl₃ studied by muon spin rotation. *Phys Rev B* **94**, no. 2 (2016): 020407. doi:10.1103/PhysRevB.94.020407.

D Lançon et al. Magnetic structure and magnon dynamics of the quasi-two-dimensional antiferromagnet FePS₃. *Phys Rev B* **94**, no. 21 (2016): 214407. doi:10.1103/PhysRevB.94.214407.

D Lançon et al. MnO nanoparticles as the cause of ferromagnetism in bulk dilute Mn-doped ZnO. *Appl Phys Lett* **109**, no. 25 (2016): 252405. doi:10.1063/1.4972956.

SR Lawrie et al. Detailed beam and plasma measurements on the vessel for extraction and source plasma analyses (VESPA) Penning H(-) ion source. Rev Sci Instrum **87**, no. 2 (2016): 02B122. Is in proceedings of: *16th International Conference on Ion Sources (ICIS), New York, New York, USA*, 23-28 Aug 2015. doi:10.1063/1.4934580.

A Lazzarini et al. A comprehensive approach to investigate the structural and surface properties of activated carbons and related Pd-based catalysts. *Catalysis Science & Technology* **6**, no. 13 (2016): 4910-4922. doi:10.1039/C6CY00159A.

A Lazzarini et al. Graphitization of activated carbons : a molecular-level investigation by INS, DRIFT, XRD and Raman techniques. *Phys Procedia* **85** (2016): 20-26. Is in proceedings of: E-MRS Spring Meeting, Lille, France, 2-4 May 2016. doi:10.1016/j.phpro.2016.11.076.

GM Lazzarini et al. Traceable atomic force microscopy of high-quality solvent-free crystals of [6,6]-phenyl-C₆₁-butyric acid methyl ester. *Appl Phys Lett* **108**, no. 5 (2016): 053303. doi:10.1063/1.4941227.

AP Le Brun et al. Deuterium Labeling Strategies for Creating Contrast in Structure–Function Studies of Model Bacterial Outer Membranes Using Neutron Reflectometry. *Method Enzymol* **566** (2016): 213-252. doi:10.1016/bs.mie.2015.05.020.

S Le Roux et al. Structure of amorphous GeSe₃ by neutron diffraction and first-principles molecular dynamics: Impact of trajectory sampling and size effects. *J Chem Phys* **145**, no. 8 (2016): 084502. doi:10.1063/1.4961265.

S Lee et al. Multistage symmetry breaking in the breathing pyrochlore lattice Li(Ga, In)Cr₄O₈. *Phys Rev B* **93**, no. 17 (2016): 174402. doi:10.1103/PhysRevB.93.174402.

A Leineweber. Thermal expansion anisotropy as source for microstrain broadening of polycrystalline cementite, Fe₃C. *J Appl Crystallogr* **49**, no. 5 (2016). doi:10.1107/S1600576716012383.

K Lejaeghere et al. Reproducibility in density functional theory calculations of solids. *Science* **351**, no. 6280 (2016): 1415-U81. doi:10.1126/science.aad3000.

SJ Lenton et al. Structural evidence for solvent-stabilisation by aspartic acid as a mechanism for halophilic protein stability in high salt concentrations. *Phys Chem Chem Phys* **18**, no. 27 (2016): 18054-18062. doi:10.1039/C6CP02684B.

J Lettry et al. Linac4 H- ion sources. Rev Sci Instrum **87**, no. 2 (2016): 02B139. Is in proceedings of: *16th International Conference on Ion Sources (ICIS), New York, New York, USA*, 23-28 Aug 2015. doi:10.1063/1.4936120.

LH Lewis, CH Marrows and S Langridge. Coupled magnetic, structural, and electronic phase transitions in FeRh. *J Phys D Appl Phys* **49**, no. 32 (2016): 323002. doi:10.1088/0022-3727/49/32/323002.

P Li et al. Analysis of the Asymmetric Synergy in the Adsorption of Zwitterionic–Ionic Surfactant Mixtures at the Air–Water Interface below and above the Critical Micelle Concentration. *J Phys Chem B* **120**, no. 15 (2016): 3677-3691. doi:10.1021/acs.jpcc.6b00762.

Y Li et al. Muon Spin Relaxation Evidence for the U(1) Quantum Spin-Liquid Ground State in the Triangular Antiferromagnet YbMgGaO₄. *Phys Rev Lett* **117**, no. 9 (2016): 097201. doi:10.1103/PhysRevLett.117.097201.

X Liao et al. An in-depth understanding of the bimetallic effects and coked carbon species on an active bimetallic Ni(Co)/Al₂O₃ dry reforming catalyst. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17311-17319. doi:10.1039/C6CP01089J.

CD Ling et al. Experimental observation and computational study of the spin-gap excitation in Ba₃BiRu₂O₉. *Phys Rev B* **94**, no. 17 (2016): 174401. doi:10.1103/PhysRevB.94.174401.

J Liu et al. Antiferromagnetism in a Family of S=1 Square Lattice Coordination Polymers NiX₂(pyz)₂ (X = Cl, Br, I, NCS; pyz = Pyrazine). *Inorg Chem* **55**, no. 7 (2016): 3515-3529. doi:10.1021/acs.inorgchem.5b02991.

C Loong, A Scherillo and G Festa. Scattering techniques : small- and wide-angle neutron diffraction. in *Neutron Methods for Archaeology and Cultural Heritage. Neutron Scattering Applications and Techniques* edited by N Kardjilov, G Festa, part 2, 183-207. Springer International Publishing, 2016. doi:10.1007/978-3-319-33163-8_9.

P Lopez-Crespo et al. Characterisation of overloads in fatigue by 2D strain mapping at the surface and in the bulk. *Fatigue & Fracture of Engineering Materials & Structures* **39**, no. 8 (2016): 1040-1048. doi:10.1111/ffe.12463.

SW Lovesey, DD Khalyavin and G van der Laan. Neutron diffraction and the electronic properties of BaFe₂Se₃. *Phys Scripta* **91**, no. 1 (2016): 015803. doi:10.1088/0031-8949/91/1/015803.

SW Lovesey. Zeeman spectrum, magnetic neutron diffraction pattern, and Dirac multipoles for a multiferroic material CuB₂O₄. *Phys Rev B* **94**, no. 9 (2016): 094422. doi:10.1103/PhysRevB.94.094422.

SW Lovesey. Electronic and magnetic properties of orthorhombic iron selenide. *Phys Rev B* **93**, no. 8 (2016): 085126. doi:10.1103/PhysRevB.93.085126.

Z Lu et al. Unusual surface and solution behaviour of keratin polypeptides. *RSC Adv* **6**, no. 107 (2016): 105192-105201. doi:10.1039/C6RA15817J.

A Luchini et al. Functionalized SPIONs: the surfactant nature modulates the self-assembly and cluster formation. *Phys Chem Chem Phys* **18**, no. 27 (2016): 18441-18449. doi:10.1039/c6cp01694d.

A Ludl et al. Probing ice VII crystallization from amorphous NaCl-D₂O solutions at gigapascal pressures. *Phys Chem Chem Phys* **19** (2016): 1875-1883. doi:10.1039/C6CP07340A.

K Luo et al. Anion Redox Chemistry in the Cobalt Free 3d Transition Metal Oxide Intercalation Electrode Li[Li_{0.2}Ni_{0.2}Mn_{0.6}]O₂. *J Am Chem Soc* **138**, no. 35 (2016): 11211-11218. doi:10.1021/jacs.6b05111.

K Luo et al. One-pot synthesis of Lithium-rich cathode material with hierarchical morphology. *Nano Lett* **16**, no. 12 (2016): 7503-7508. doi:10.1021/acs.nanolett.6b03296.

K Ma et al. Unusual adsorption at the air-water interface of a zwitterionic carboxybetaine with large charge separation. *Langmuir* **32**, no. 14 (2016): 3340-3347. doi:10.1021/acs.langmuir.6b00074.

S Machida et al. Intensity Effects in the Formation of Stable Islands in Phase Space During the Multi-Turn Extraction Process at the CERN PS. In *57th ICFA Advanced Beam Dynamics Workshop on High-Intensity, High Brightness and High Power Hadron Beams (HB2016)*, Malmö, Sweden, 3-8 Jul 2016, (2016).

S Machida et al. Intensity Effects in the Formation of Stable Islands in Phase Space During the Multi-Turn Extraction Process at the CERN PS. Presented at *57th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams (HB2016)*, Malmö, Sweden, 3-8 July, 2016. http://accelconf.web.cern.ch/AccelConf/hb2016/talks/tuam7x01_talk.pdf.

E Mahdi and J Tan. Mixed-matrix membranes of zeolitic imidazolate framework (ZIF-8)/Matrimid nanocomposite: Thermo-mechanical stability and viscoelasticity underpinning membrane separation performance. *J Membrane Sci* **498** (2016): 276-290. doi:10.1016/j.memsci.2015.09.066.

E Mahdi and J Tan. Dynamic molecular interactions between polyurethane and ZIF-8 in a polymer-MOF nanocomposite: Microstructural, thermo-mechanical and viscoelastic effects. *Polymer* **97** (2016): 31-43. doi:10.1016/j.polymer.2016.05.012.

EM Mahdi, AK Chaudhuri and J Tan. Capture and immobilisation of iodine (I₂) utilising polymer-based ZIF-8 nanocomposite membranes. *Molecular Systems Design & Engineering* **1**, no. 1 (2016): 122-131. doi:10.1039/C5ME00008D.

JW Makepeace et al. Ammonia decomposition catalysis using lithium-calcium imide. *Faraday Discuss* **188** (2016): 525-544. doi:10.1039/C5FD00179J.

MG Makowska et al. *In situ* time-of-flight neutron imaging of NiO-YSZ anode support reduction under influence of stress. *J Appl Crystallogr* **49**, no. 5 (2016): 1674-1681. doi:10.1107/S1600576716012668.

F Malamud et al. Texture analysis of Napoleonic War Era copper bolts. *Appl Phys A* **122**, no. 4 (2016): 276. doi:10.1007/s00339-016-9835-y.

P Mandal et al. Controlling phase assemblage in a complex multi-cation system: phase-pure room temperature multiferroic (1-x)BiTi_{(1-y)/2}Fe_yMg_{(1-y)/2}O_{3-x}CaTiO₃. *Adv Funct Mater* **26**, no. 15 (2016): 2523-2531. doi:10.1002/adfm.201504911.

JL Manson et al. Bimetallic MOFs (H₂O)_x[Cu(MF₆)(pyrazine)₂](4-x)H₂O (M = V⁴⁺, x=0; M = Ga³⁺, x=1): co-existence of ordered and disordered quantum spins in the V⁴⁺ system. *Chem Commun* **52** (2016): 12653-12656. doi:10.1039/C6CC05873F.

HR Marchbank et al. Structure of nano-sized CeO₂ material : a combined scattering and spectroscopic investigation. *ChemPhysChem* **17**, no. 21 (2016): 3494-3503. doi:10.1002/cphc.201600697.

MPM Marques et al. Osteometrics in burned human skeletal remains by neutron and optical vibrational spectroscopy. *RSC Adv* **6**, no. 73 (2016): 68638-68641. doi:10.1039/C6RA13564A.

T Marrow et al. *In situ* measurement of the strains within a mechanically loaded polygranular graphite. *Carbon* **96** (2016): 285-302. doi:10.1016/j.carbon.2015.09.058.

D Martynov et al. Sensitivity of the Advanced LIGO detectors at the beginning of gravitational wave astronomy. *Phys Rev D* **93**, no. 11 (2016): 112004. doi:10.1103/PhysRevD.93.112004.

- JA McEwan et al. Diffusion at interfaces in OLEDs containing a doped phosphorescent emissive layer. *Adv Mater Inter* **3**, no. 17 (2016). doi:10.1002/admi.201600184.
- AR McFarlane et al. The application of inelastic neutron scattering to investigate the interaction of methyl propanoate with silica. *Phys Chem Chem Phys*, no. 18 (2016): 26, 17210-17216. doi:10.1039/C6CP01276K.
- V Merlo et al. Superconducting thermal neutron detectors. *J Phys Conf Ser* **746**, no. 1 (2016): 012019. doi:10.1088/1742-6596/746/1/012019.
- F Mezzadri et al. Structural and magnetic characterization of the double perovskite $\text{Pb}_2\text{FeMoO}_6$. *J Mater Chem C* **4**, no. 7 (2016): 1533-1542. doi:10.1039/C5TC03529E.
- X Miao et al. Tuning the magnetoelastic transition in $(\text{Mn,Fe})_2(\text{P,Si})$ by B, C, and N doping. *Scripta Mater* **124** (2016): 129-132. doi:10.1016/j.scriptamat.2016.07.015.
- XF Miao et al. Kinetic-arrest-induced phase coexistence and metastability in $(\text{Mn,Fe})_2(\text{P,Si})$. *Phys Rev B* **94**, no. 9 (2016): 094426. doi:10.1103/PhysRevB.94.094426.
- CA Middleton, PM Grindrod and PR Sammonds. The effect of rock particles and D_2O replacement on the flow behaviour of ice. *Philos T Roy Soc A* **375**, no. 2086 (2016): 20150349. doi:10.1098/rsta.2015.0349.
- T Minniti et al. Materials analysis opportunities on the new neutron imaging facility IMAT@ISIS. *JINST* **11** (2016): C03014. Is in proceedings of: *International Workshop on Imaging, Varenna, Italy*, 7-10 Sep 2015. doi:10.1088/1748-0221/11/03/C03014.
- S Mirfayzi et al. Detector for imaging and dosimetry of laser-driven epithermal neutrons by alpha conversion. *JINST* **11**, no. 10 (2016): C10008. Is in proceedings of: *4th International Conference on Frontiers in Diagnostics Technologies, Frascati, Italy*, 30 Mar - 1 Apr 2016. doi:10.1088/1748-0221/11/10/C10008.
- S Mitra et al. Enhancement of lateral diffusion in catanionic vesicles during multilamellar-to-unilamellar transition. *J Phys Chem B* **120**, no. 15 (2016): 3777-3784. doi:10.1021/acs.jpcc.6b02997.
- KMH Mohammed et al. Design and control of Lewis acid sites in Sn-substituted microporous architectures. *J Mater Chem A* **4**, no. 15 (2016): 5706-5712. doi:10.1039/C5TA10283A.
- SD Mohan, GR Mitchell and FJ Davis. Development of molecular anisotropy in centrifugally spun fibers as compared to electrospun fibers. *Macromolecular Materials and Engineering* **301**, no. 11 (2016): 1313-1319. doi:10.1002/mame.201600275.
- TA Mohayai, C Rogers and P Snopok. Simulated Measurements of Cooling in Muon Ionization Cooling Experiment. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 1565-1567. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/tupmy011.pdf>.
- TA Mohayai, C Rogers and P Snopok. Simulated Measurements of Beam Cooling in Muon Ionization Cooling Experiment. In *North American Particle Accelerator Conference 2016 (NAPAC'16), Chicago, IL USA*, 9-14 Oct 2016, (2016): 771-774. <http://accelconf.web.cern.ch/AccelConf/napac2016/papers/wepoa36.pdf>.
- A Montes-Arango et al. Discovery of process-induced tetragonality in equiatomic ferromagnetic FeNi. *Acta Mater* **116** (2016): 263-269. doi:10.1016/j.actamat.2016.06.050.
- N Mufti et al. Unique magnetic structure of YbCo_2Si_2 . *Phys Rev B* **94**, no. 4 (2016): 045116. doi:10.1103/PhysRevB.94.045116.
- AD Mulliner et al. Dimer-mediated cation diffusion in the stoichiometric ionic conductor Li_3N . *Phys Chem Chem Phys* **18**, no. 7 (2016): 5605-5613. doi:10.1039/c5cp07625k.
- A Muraro et al. Performance of the full size nGEM detector for the SPIDER experiment. *Nucl Instrum Meth A* **813** (2016): 147-152. doi:10.1016/j.nima.2015.12.015.
- A Muraro et al. Neutron radiography as a non-destructive method for diagnosing neutron converters for advanced thermal neutron detectors. *JINST* **11** (2016): C03033. Is in proceedings of: *International Workshop on Imaging, Varenna, Italy*, 7-10 Sep 2015. doi:10.1088/1748-0221/11/03/C03033.
- T Murphy et al. Dissolved chloride markedly changes the nanostructure of the protic ionic liquids propylammonium and ethanolanmonium nitrate. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17169-17182. doi:10.1039/c5cp06947e.
- T Murphy et al. Ionic liquid nanostructure enables alcohol self assembly. *Phys Chem Chem Phys* **18**, no. 18 (2016): 12797-12809. doi:10.1039/c6cp01739h.
- T Murphy et al. Bulk nanostructure of the prototypical 'good' and 'poor' solvate ionic liquids $[\text{Li}(\text{G4})][\text{TFSI}]$ and $[\text{Li}(\text{G4})][\text{NO}_3]$. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17224-17236. doi:10.1039/c6cp00176a.
- A Nag et al. Origin of the Spin-Orbital Liquid State in a Nearly $J=0$ Iridate $\text{Ba}_3\text{ZnIr}_2\text{O}_9$. *Phys Rev Lett* **116**, no. 9 (2016): 097205. doi:10.1103/PhysRevLett.116.097205.
- Z Nedelkoski et al. Realisation of magnetically and atomically abrupt half-metal/semiconductor interface: $\text{Co}_2\text{FeSi}_{0.5}\text{Al}_{0.5}/\text{Ge}(111)$. *Sci Rep* **6** (2016): 37282. doi:10.1038/srep37282.
- T Nguyen-Thanh et al. Lattice dynamics and elasticity of SrCO_3 . *J Appl Crystallogr* **49**, no. 6 (2016): 1982-1990. doi:10.1107/S1600576716014205.
- EJ Nilsson et al. A neutron scattering and modelling study of aqueous solutions of tetramethylammonium and tetrapropylammonium bromide. *Phys Chem Chem Phys* **18**, no. 16 (2016): 11193-11201. doi:10.1039/c6cp01389a.

N Ning Li, RK Thomas and AR Rennie. Neutron reflectometry of anionic surfactants on sapphire: a strong maximum in the adsorption near the critical micelle concentration. *J Coll Int Sci* **471** (2016): 81-88. doi:10.1016/j.jcis.2016.03.014.

HJ Niu et al. Room temperature magnetically ordered polar corundum GaFeO₃ displaying magnetoelectric coupling. *J Am Chem Soc* **139**, no. 4 (2016): 1520-1531. doi:10.1021/jacs.6b11128.

S Nneji et al. Modelling and control of neutron and synchrotron beamline positioning systems. *Nucl Instrum Meth A* **813** (2016): 123-131. doi:10.1016/j.nima.2015.12.067.

ST Norberg et al. *In situ* neutron powder diffraction study of the reaction $M_2O_3 \leftrightarrow M_3O_4 \leftrightarrow MO$, $M = (Fe_{0.2}Mn_{0.8})$: implications for chemical looping with oxygen uncoupling. *CrystEngComm* **18**, no. 29 (2016): 5537-5546. doi:10.1039/C6CE00784H.

SE Norman et al. Solvation structure of uracil in ionic liquids. *ChemPhysChem* **17**, no. 23 (2016): 3923-3931. doi:10.1002/cphc.201600984.

AJ O'Malley et al. Ammonia mobility in chabazite: insight into the diffusion component of the NH₃-SCR process. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17159-17168. doi:10.1039/C6CP01160H.

AJ O'Malley et al. Room temperature methoxylation in zeolites: insight into a key step of the methanol-to-hydrocarbons process. *Chem Commun* **52**, no. 14 (2016): 2897-2900. doi:10.1039/c5cc08956e.

AJ O'Malley et al. Methanol diffusion in zeolite HY: a combined quasielastic neutron scattering and molecular dynamics simulation study. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17294-17302. doi:10.1039/C6CP01151A.

AJ O'Malley et al. Modelling metal centres, acid sites and reaction mechanisms in microporous catalysts. *Faraday Discuss* **188** (2016): 235-255. doi:10.1039/C6FD00010J.

J Oh et al. Spontaneous decays of magneto-elastic excitations in non-collinear antiferromagnet (Y,Lu) MnO₃. *Nat Commun* **7** (2016): 13146. doi:10.1038/ncomms13146.

K Ohara et al. Structural and electronic features of binary Li₂S-P₂S₅ glasses. *Sci Rep* **6** (2016): 21302. doi:10.1038/srep21302.

C Olsson et al. Structure of aqueous trehalose solution by neutron diffraction and structural modeling. *J Phys Chem B* **120**, no. 49 (2016): 12669-12678. doi:10.1021/acs.jpcc.6b10556.

F Orlandi et al. Long-range antiferromagnetic interactions in Ni-Co-Mn-Ga metamagnetic Heusler alloys: A two-step ordering studied by neutron diffraction. *Phys Rev B* **94**, no. 14 (2016): 140409. doi:10.1103/PhysRevB.94.140409.

F Orlandi et al. Improper Ferroelectric Contributions in the Double Perovskite Pb₂Mn_{0.6}Co_{0.4}WO₆ System with a Collinear Magnetic Structure. *Inorg Chem* **55**, no. 9 (2016): 4381-4390. doi:10.1021/acs.inorgchem.6b00117.

AR Overy et al. Design of crystal-like aperiodic solids with selective disorder-phonon coupling. *Nat Commun* **7** (2016): 10445. doi:10.1038/ncomms10445.

L Owen et al. A new approach to the analysis of short-range order in alloys using total scattering. *Acta Mater* **115** (2016): 155-166. doi:10.1016/j.actamat.2016.05.031.

JAM Paddison et al. Emergent order in the kagome Ising magnet Dy₃Mg₂Sb₃O₁₄. *Nat Commun* **7** (2016): 13842. doi:10.1038/ncomms13842.

EV Pagano et al. Status and perspective of FARCOS: A new correlator array for nuclear reaction studies. EPJ Web of Conferences 117 (2016): 10008. Is in proceedings of: *12th International Conference on Nucleus-Nucleus Collisions (NN2015), Catania, Italy*, 21-26 Jun 2015. doi:10.1051/epjconf/201611710008.

E Pambou et al. Structural features of reconstituted wheat wax films. *J R Soc Interface* **13**, no. 120 (2016): 20160396. doi:10.1098/rsif.2016.0396.

E Panabièrre et al. Structural reinvestigation of Li₃FeN₂: Evidence of cationic disorder through XRD, solid-state NMR and Mössbauer spectroscopy. *J Phys Chem Solids* **95** (2016): 37-42. doi:10.1016/j.jpcs.2016.03.016.

J Park et al. Robust singlet dimers with fragile ordering in two-dimensional honeycomb lattice of Li₂RuO₃. *Sci Rep* **6** (2016): 25238. doi:10.1038/srep25238.

K Park et al. Magnon-phonon coupling and two-magnon continuum in the two-dimensional triangular antiferromagnet CuCrO₂. *Phys Rev B* **94**, no. 10 (2016): 104421. doi:10.1103/PhysRevB.94.104421.

SF Parker et al. Structural and spectroscopic characterisation of C₄ oxygenates relevant to structure/activity relationships of the hydrogenation of alpha,beta-unsaturated carbonyls. *Spectrochim Acta Part A* **153** (2016): 289-297. doi:10.1016/j.saa.2015.08.034.

SF Parker et al. Methyl tunnelling of adsorbed methoxy on alumina catalysts. *Chem Commun* **52**, no. 2 (2016): 366-369. doi:10.1039/c5cc08223d.

SF Parker and D Lennon. Applications of neutron scattering to heterogeneous catalysis. *J Phys Conf Ser* **746**, no. 1 (2016): 012066. doi:10.1088/1742-6596/746/1/012066.

SF Parker et al. Structural and spectroscopic characterisation of C₄ oxygenates relevant to structure/activity relationships of the hydrogenation of alpha,beta-unsaturated carbonyls. *Spectrochim Acta Part A* **153** (2016): 289-297. <http://purl.org/net/epubs/manifestation/29541368>.

- SF Parker and P Collier. Applications of neutron scattering in catalysis. *Johnson Matthey Technology Review* **60**, no. 2 (2016): 132-144. <http://www.technology.matthey.com/pdf/132-144-jmtr-apr16.pdf>.
- SF Parker et al. Characterisation of the surface of freshly prepared precious metal catalysts. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17196-17201. doi:10.1039/c6cp01027j.
- AJ Parnell et al. Physical Mechanisms Responsible for the Water-Induced Degradation of PC₆₁BM P3HT Photovoltaic Thin Films. *J Polym Sci Part B* **54**, no. 2 (2016): 141-146. doi:10.1002/polb.23902.
- SR Parnell et al. Porosity of silica Stöber particles determined by spin-echo small angle neutron scattering. *Soft Matter* **12**, no. 21 (2016): 4709-4714. doi:10.1039/c5sm02772a.
- TR Patel, DJ Winzor and DJ Scott. Analytical ultracentrifugation: A versatile tool for the characterisation of macromolecular complexes in solution. *Methods* **95** (2016): 55-61. doi:10.1016/j.ymeth.2015.11.006.
- GM Paternò et al. Neutron polarisation analysis of Polymer : Fullerene blends for organic photovoltaics. *Polymer* **105** (2016): 407-413. doi:10.1016/j.polymer.2016.07.079.
- GM Paternò et al. Tuning fullerene intercalation in a poly (thiophene) derivative by controlling the polymer degree of self-organisation. *Sci Rep* **6** (2016): 34609. doi:10.1038/srep34609.
- MA Patino et al. Coupled Electronic and Magnetic Phase Transition in the Infinite-Layer Phase LaSrNiRuO₄. *Inorg Chem* **55**, no. 17 (2016): 9012-9016. doi:10.1021/acs.inorgchem.6b01484.
- J Penfold, RK Thomas and P Li. Anionic surfactant – Biogenic amine interactions : The role of surfactant headgroup geometry. *J Coll Int Sci* **466** (2016): 213-219. doi:10.1016/j.jcis.2015.12.030.
- J Penfold et al. Nature of the Intermicellar Interactions in Ethoxylated Polysorbate Surfactants with High Degrees of Ethoxylation. *Langmuir* **32**, no. 5 (2016): 1319-1326. doi:10.1021/acs.langmuir.5b04642.
- J Penfold et al. Tuning Polyelectrolyte–Surfactant Interactions: Modification of Poly(ethylenimine) with Propylene Oxide and Blocks of Ethylene Oxide. *Langmuir* **32**, no. 4 (2016): 1073-1081. doi:10.1021/acs.langmuir.5b04419.
- J Penfold, RK Thomas and P Li. Impact of biogenic amine molecular weight and structure on surfactant adsorption at the air–water interface. *J Coll Int Sci* **463** (2016): 199-206. doi:10.1016/j.jcis.2015.10.058.
- G Pepe et al. Rationalizing the suitability of rhodamines as chromophores in dye-sensitized solar cells : a systematic molecular design study. *Molecular Systems Design & Engineering* **1** (2016): 416-435. doi:10.1039/C6ME00076B.
- G Pepe et al. Molecular engineering of fluorescein dyes as complementary absorbers in dye co-sensitized solar cells. *Molecular Systems Design & Engineering* **1**, no. 4 (2016): 402-415. doi:10.1039/C6ME00075D.
- SJ Perkins et al. Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). *J Appl Crystallogr* **49**, no. 6 (2016): 1861-1875. doi:10.1107/S160057671601517X.
- B Perumal et al. The effect of hot deformation parameters on microstructure evolution of the alpha-phase in Ti-6Al-4V. *Metall Mater Trans A* **47**, no. 8 (2016): 4128-4136. doi:10.1007/s11661-016-3552-1.
- L Pfeifer et al. Hydrogen-bonded homoleptic Fluoride–Diarylurea complexes : structure, reactivity and coordinating power. *J Am Chem Soc* **138**, no. 40 (2016): 13314-13325. doi:10.1021/jacs.6b07501.
- T Pham et al. Dynamics of H₂ adsorbed in porous materials as revealed by computational analysis of inelastic neutron scattering spectra. *Phys Chem Chem Phys* (2016). doi:10.1039/c6cp01863g.
- S Pili et al. Proton Conduction in a Phosphonate-Based Metal–Organic Framework Mediated by Intrinsic “Free Diffusion inside a Sphere”. *J Am Chem Soc* **138**, no. 20 (2016): 6352-6355. doi:10.1021/jacs.6b02194.
- R Pilotti et al. High-temperature long-lasting stability assessment of a single-crystal diamond detector under high-flux neutron irradiation. *Europhys Lett* **116**, no. 4 (2016): 42001. doi:10.1209/0295-5075/116/42001.
- P Pizzol et al. CVD Deposition of Nb Based Materials for SRF Cavities. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 2241-2244. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/wepmb056.pdf>.
- C Plostinar et al. Studies of Ultimate Intensity Limits for High Power Proton Linacs. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 951-954. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/mopoy047.pdf>.
- D Polishchuk et al. Charge ordering in Nd_{2/3}Ca_{1/3}MnO₃: ESR and magnetometry study. *J Magnetism Magnetic Mater* **410** (2016): 109-115. doi:10.1016/j.jmmm.2016.03.022.
- DG Porter et al. Magnetostriction-driven ground-state stabilization in 2H perovskites. *Phys Rev B* **94**, no. 13 (2016): 134404. doi:10.1103/PhysRevB.94.134404.
- DW Posthuma de Boer and A Pertica. Thermal Simulations of Wire Profile Monitors in ISIS Extracted Proton Beamline 1. In *International Beam Instrumentation Conference (IBIC), Barcelona, Spain*, 12-15 Sep 2016, (2016). <http://jacow.web.psi.ch/conf/y16/ibic16n5alba/prepress/WEFG59.PDF>.

- H Postma and P Schillebeeckx. Neutron Resonance Analysis. in *Neutron Methods for Archaeology and Cultural Heritage. Neutron Scattering Applications and Techniques* edited by N Kardjilov, G Festa, part 2, 235-283. Springer International Publishing, 2016. doi:10.1007/978-3-319-33163-8_12.
- ME Potter et al. Spectroscopic investigation into the design of solid-acid catalysts for the low temperature dehydration of ethanol. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17303-17310. doi:10.1039/C6CP01209D.
- FM Pouzols et al. Neutron imaging data processing using the Mantid framework. *J Phys Conf Ser* **746**, no. 1 (2016): 012017. doi:10.1088/1742-6596/746/1/012017.
- SS Pramana et al. Correlation of Local Structure and Diffusion Pathways in the Modulated Anisotropic Oxide Ion Conductor CeNbO_{4.25}. *J Am Chem Soc* **138**, no. 4 (2016): 1273-1279. doi:10.1021/jacs.5b11373.
- F Pratt. Superconductivity and Magnetism in Organic Materials Studied with mu SR. *J Phys Soc Jpn* **85**, no. 9 (2016): 091008. doi:10.7566/JPSJ.85.091008.
- FL Pratt et al. Nanoscale depth-resolved polymer dynamics probed by the implantation of low energy muons. *Polymer* **105** (2016): 516-525. doi:10.1016/j.polymer.2016.07.078.
- CR Prior. Studies of High Intensity Proton FFAGs at RAL. In *57th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams (HB2016), Malmö, Sweden*, 3-8 Jul 2016, (2016): 379-384. <http://accelconf.web.cern.ch/AccelConf/hb2016/papers/weam6x01.pdf>.
- CR Prior. Studies of High Intensity Proton FFAGs at RAL. Presented at *57th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams (HB2016), Malmö, Sweden*, 3-8 Jul 2016. http://accelconf.web.cern.ch/AccelConf/hb2016/talks/weam6x01_talk.pdf.
- K Prša et al. Perspectives on neutron scattering in lanthanide-based single-molecule magnets and a case study of the Tb₂ (mu-N₂) system. *Magnetochemistry* **2**, no. 4 (2016): 45. doi:10.3390/magnetochemistry2040045.
- C Qiu et al. An experimental investigation into the stress and strain development of a Ni-base single crystal superalloy during cooling from solidification. *Mater Des* **114** (2016): 475-483. doi:10.1016/j.matdes.2016.10.072.
- M Rebai et al. Response function of single crystal synthetic diamond detectors to 1-4 MeV neutrons for spectroscopy of D plasmas. *Rev Sci Instrum* **87**, no. 11 (2016): 11D823. doi:10.1063/1.4960490.
- M Rebai et al. Time-stability of a Single-crystal Diamond Detector for fast neutron beam diagnostic under alpha and neutron irradiation. *Diam Relat Mater* **61** (2016): 1-6. doi:10.1016/j.diamond.2015.11.002.
- NH Rhys et al. On the structure of an aqueous propylene glycol solution. *J Chem Phys* **145**, no. 22 (2016): 224504. doi:10.1063/1.4971208.
- IM Riddlestone et al. Isolation of [Ru(IPr)(2)(CO)H](+) (IPr=1,3-Bis(2,6-diisopropylphenyl)imidazol-2-ylidene) and Reactivity toward E-H (E = H, B) Bonds. *Organometallics* **35**, no. 9 (2016): 1301-1312. doi:10.1021/acs.organomet.6b00173.
- E Rodrigo da Silva et al. Structural behaviour and gene delivery in complexes formed between DNA and arginine-containing peptide amphiphiles. *Soft Matter* **12**, no. 45 (2016): 9158-9169. doi:10.1039/C6SM01618A.
- CT Rogers and S Sheehy. Update on OPAL. Presented at *21st International Conference on Cyclotrons and their applications (CYC2016), Zurich, Switzerland*, 11-16 Sep 2016. http://accelconf.web.cern.ch/AccelConf/cyclotrons2016/talks/wea04_talk.pdf.
- S Rogers et al. The adsorbed state of a thiol on palladium nanoparticles. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17265-17271. doi:10.1039/C6CP00957C.
- G Romanelli et al. Soft confinement of water in graphene-oxide membranes. *Carbon* **108** (2016): 199-203. doi:10.1016/j.carbon.2016.07.021.
- G Romanelli and M Krzystyniak. On the line-shape analysis of Compton profiles and its application to neutron scattering. *Nucl Instrum Meth A* **819** (2016): 84-88. doi:10.1016/j.nima.2016.02.089.
- M Ruminy et al. Crystal-field parameters of the rare-earth pyrochlores R₂Ti₂O₇ (R = Tb, Dy, and Ho). *Phys Rev B* **94**, no. 2 (2016): 024430. doi:10.1103/PhysRevB.94.024430.
- M Ruminy et al. First-principles calculation and experimental investigation of lattice dynamics in the rare-earth pyrochlores R₂Ti₂O₇ (R = Tb, Dy, Ho). *Phys Rev B* **93**, no. 21 (2016): 214308. doi:10.1103/PhysRevB.93.214308.
- T Rutter et al. The mechanical design and simulation of a scaled H-Penning ion source. *Rev Sci Instrum* **87**, no. 2 (2016): 02B131. Is in proceedings of: *16th International Conference on Ion Sources (ICIS), New York, NY*, 23-28 Aug 2015. doi:10.1063/1.4934815.
- M Sagisaka et al. New class of amphiphiles designed for use in water-in-supercritical CO₂ microemulsions. *Langmuir* **32**, no. 47 (2016): 12413-12422. doi:10.1021/acs.langmuir.6b01670.
- R Saha et al. Neutron scattering study of the crystallographic and spin structure in antiferromagnetic EuZrO₃. *Phys Rev B* **93**, no. 1 (2016): 014409. doi:10.1103/PhysRevB.93.014409.
- A Sanchez-Fernandez et al. Micellization of alkyltrimethylammonium bromide surfactants in choline chloride : glycerol deep eutectic solvent. *Phys Chem Chem Phys* **18**, no. 48 (2016): 33240-33249. doi:10.1039/C6CP06053F.

A Sanchez-Fernandez et al. Micelle structure in a deep eutectic solvent: a small-angle scattering study. *Phys Chem Chem Phys* **18**, no. 20 (2016): 14063-14073. doi:10.1039/c6cp01757f.

L Sanchez-Garcia et al. Size determination and quantification of engineered cerium oxide nanoparticles by flow field-flow fractionation coupled to inductively coupled plasma mass spectrometry. *Journal of Chromatography A* **1438** (2016): 205-215. doi:10.1016/j.chroma.2016.02.036.

MR Sanders et al. Role of Lipid Composition on the Interaction between a Tryptophan-Rich Protein and Model Bacterial Membranes. *Langmuir* **32**, no. 8 (2016): 2050-2057. doi:10.1021/acs.langmuir.5b04628.

WF Sanjuan-Szklarz et al. Yes, one can obtain better quality structures from routine X-ray data collection. *IUCr* **3**, no. 1 (2016): 61-70. doi:10.1107/S2052252515020941.

T Santini et al. Reliability analysis of operating systems and software stack for embedded systems. *IEEE Trans Nucl Sci PP*, no. **99** (2016): 1-1. doi:10.1109/TNS.2015.2513384.

M Sapinski et al. Ionization Profile Monitor Simulations - Status and Future Plans. In 2016 *International Beam Instrumentation Conference (IBIC 2016), Barcelona, Spain*, 11-15 Sep 2016, (2016): 520-523. <http://accelconf.web.cern.ch/AccelConf/ibic2016/papers/tupg71.pdf>.

M Savage et al. Selective adsorption of Sulfur Dioxide in a robust metal-organic framework material. *Adv Mater* (2016). doi:10.1002/adma.201602338.

M Savage et al. Observation of binding and rotation of Methane and Hydrogen within a functional metal-organic framework. *J Am Chem Soc* **138**, no. 29 (2016): 9119-9127. doi:10.1021/jacs.6b01323.

M Schlegel et al. Conformation-controlled hydrogen storage in the CAU-1 metal-organic framework. *Phys Chem Chem Phys* **18**, no. 42 (2016): 29258-29267. doi:10.1039/C6CP05310F.

D Schmidiger et al. Emergent interacting spin islands in a depleted strong-leg Heisenberg ladder. *Phys Rev Lett* **116**, no. 25 (2016): 257203. doi:10.1103/PhysRevLett.116.257203.

EM Schooneveld et al. Radiative neutron capture as a counting technique at pulsed spallation neutron sources: a review of current progress. *Rep Prog Phys* **79**, no. 9 (2016): 094301. doi:10.1088/0034-4885/79/9/094301.

M Schumacher et al. Structural, electronic and kinetic properties of the phase-change material $\text{Ge}_2\text{Sb}_2\text{Te}_5$ in the liquid state. *Sci Rep* **6** (2016): 27434. doi:10.1038/srep27434.

DJ Scott. Accounting for thermodynamic non-ideality in the Guinier region of small-angle scattering data of proteins. *Biophysical Reviews* **8**, no. 4 (2016): 441-444. doi:10.1007/s12551-016-0235-5.

M Senn et al. Emergence of Long-Range Order in BaTiO_3 from Local Symmetry-Breaking Distortions. *Phys Rev Lett* **116**, no. 20 (2016): 207602. doi:10.1103/PhysRevLett.116.207602.

R Serra-Gómez et al. Structure and rheology of Poloxamine T1107 and its nanocomposite hydrogels with Cyclodextrin-modified Barium Titanate nanoparticles. *Langmuir* **32**, no. 25 (2016): 6398-6408. doi:10.1021/acs.langmuir.6b01544.

E Shalaev and AK Soper. Water in a soft confinement : structure of water in amorphous sorbitol. *J Phys Chem B* **120**, no. 29 (2016): 7289-7296. doi:10.1021/acs.jpcc.6b06157.

SL Sheehy et al. Overview of the Design of the IBEX Linear Paul Trap. In *7th International Particle Accelerator Conference (IPAC'16), Busan, Korea*, 8-13 May 2016, (2016): 3104-3106. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/wepoy048.pdf>.

Y Shen et al. Evidence for a spinon Fermi surface in a triangular-lattice quantum-spin-liquid candidate. *Nature* **540** (2016): 559-562. doi:10.1038/nature20614.

JJ Shephard et al. Microstructures of negative and positive azeotropes. *Phys Chem Chem Phys* **18**, no. 28 (2016): 19227-19235. doi:10.1039/C6CP02450E.

IP Silverwood et al. Evidence for a Surface Gold Hydride on a Nanostructured Gold Catalyst. *Chem Commun* **52**, no. 3 (2016): 533-536. doi:10.1039/C5CC06118K.

IP Silverwood et al. Correction: Evidence for a surface gold hydride on a nanostructured gold catalyst. *Chem Commun* **52**, no. 11 (2016): 2412-2412. doi:10.1039/c6cc90049f.

IP Silverwood et al. Towards microfluidic reactors for *in situ* synchrotron infrared studies. *Rev Sci Instrum* **87**, no. 2 (2016): 024101. Is in proceedings of: *16th International Conference on Ion Sources (ICIS), New York, New York, USA*, 23-28 Aug 2015. doi:10.1063/1.4941825.

IP Silverwood, SF Parker and CRA Catlow. Neutron scattering in catalysis and energy materials. *Phys Chem Chem Phys* **18**, no. 26 (2016): 17140-17140. doi:10.1039/c6cp90150f.

H Sim et al. Spontaneous structural distortion of the metallic Shastry-Sutherland system DyB_4 by quadrupole-spin-lattice coupling. *Phys Rev B* **94**, no. 19 (2016): 195128. doi:10.1103/PhysRevB.94.195128.

D Singh et al. Superconducting properties of the noncentrosymmetric superconductor Re_0Hf . *Phys Rev B* **94**, no. 5 (2016): 054515. doi:10.1103/PhysRevB.94.054515.

WA Slawinski, AO Sjästad and H Fjellvåg. Stacking faults and polytypes for layered double hydroxides : what can we learn from simulated and experimental X-ray powder diffraction data?. *Inorg Chem* **55**, no. 24 (2016): 12881-12889. doi:10.1021/acs.inorgchem.6b02247.

GN Smith et al. The internal structure of poly(methyl methacrylate) latexes in nonpolar solvents. *J Coll Int Sci* **479** (2016): 234-243. doi:10.1016/j.jcis.2016.06.027.

GN Smith et al. The effect of solvent and counterion variation on inverse micelle CMCs in hydrocarbon solvents. *Coll Surf A* **494** (2016): 194-200. doi:10.1016/j.colsurfa.2016.01.020.

GN Smith et al. The effects of counterion exchange on charge stabilization for anionic surfactants in nonpolar solvents. *J Coll Int Sci* **465** (2016): 316-322. doi:10.1016/j.jcis.2015.11.062.

J Smith et al. Probing crystallisation of a fluoro-apatite - mullite system using neutron diffraction. *J Non-Cryst Solids* **451** (2016): 84-88. doi:10.1016/j.jnoncrysol.2016.05.019.

E Solana-Madruga et al. Double double cation order in the high-pressure perovskites MnRMnSbO₆. *Angew Chem Int Ed* **55**, no. 32 (2016): 9340-9344. doi:10.1002/anie.201603526.

I Sovago et al. Electron density, disorder and polymorphism: high-resolution diffraction studies of the highly polymorphic neuralgic drug carbamazepine. *Acta Crystallogr B* **72** (2016): 39-50. doi:10.1107/S2052520615019538.

I Sovago et al. High resolution X-ray and neutron diffraction studies on molecular complexes of chloranilic acid and lutidines. *CrystEngComm* **18**, no. 30 (2016): 5697-5709. doi:10.1039/c6ce01065b.

A Sridhar et al. The solvation structure of alprazolam. *Phys Chem Chem Phys* **18**, no. 32 (2016): 22416-22425. doi:10.1039/C6CP02645A.

A Stadler et al. Picosecond to nanosecond dynamics provide a source of conformational entropy for protein folding. *Phys Chem Chem Phys* **18**, no. 31 (2016): 21527-21538. doi:10.1039/C6CP04146A.

K Stefanopoulos et al. Anomalous Depletion of Pore-Confined Carbon Dioxide upon Cooling below the Bulk Triple Point: An *In Situ* Neutron Diffraction Study. *Phys Rev Lett* **116**, no. 2 (2016): 025502. doi:10.1103/PhysRevLett.116.025502.

N Steinke et al. Atomic scale insights into urea-peptide interactions in solution. *Phys Chem Chem Phys* **18**, no. 5 (2016): 3862-3870. doi:10.1039/c5cp06646h.

C Stock et al. Solitary magnons in the S=52 antiferromagnet CaFe₂O₄. *Phys Rev Lett* **117**, no. 1 (2016): 017201. doi:10.1103/PhysRevLett.117.017201.

U Subbarao et al. Swinging symmetry, multiple structural phase transitions, and versatile physical properties in RECuGa₃ (RE = La-Nd, Sm-Gd). *Inorg Chem* **55**, no. 2 (2016): 666-675. doi:10.1021/acs.inorgchem.5b02023.

ND Subramanian et al. Optimised hydrogen production by aqueous phase reforming of glycerol on Pt/Al₂O₃. *Int J Hydrogen Energ* **41**, no. 41 (2016): 18441-18450. doi:10.1016/j.ijhydene.2016.08.081.

JP Sutter et al. Three-energy focusing Laue monochromator for the diamond light source x-ray pair distribution function beamline I15-1. In *12th International Conference on Synchrotron Radiation Instrumentation (SRI2015)*, New York, USA, 6-10 July 2015, AIP Conf Proc 1741 (2016): 040005. doi:10.1063/1.4952877.

JP Sutter et al. Rotation of X-ray polarization in the glitches of a silicon crystal monochromator. *J Appl Crystallogr* **49**, no. 4 (2016): 1209-1222. doi:10.1107/S1600576716009183.

V Sánchez-Gil et al. Evidence of a Structural Change in Pure-Silica MEL upon the Adsorption of Argon. *J Phys Chem C* **120**, no. 4 (2016): 2260-2270. doi:10.1021/acs.jpcc.5b11264.

AS Tascini et al. Thermal transport across nanoparticle-fluid interfaces: the interplay of interfacial curvature and nanoparticle-fluid interactions. *Phys Chem Chem Phys* **19** (2016): 3244-3253. doi:10.1039/C6CP06403E.

V Taufour et al. Ferromagnetic Quantum Critical Point Avoided by the Appearance of Another Magnetic Phase in LaCrGe₃ under Pressure. *Phys Rev Lett* **117**, no. 3 (2016): 037207. doi:10.1103/PhysRevLett.117.037207.

MTF Telling et al. Correction: Spectroscopic characteristics of the OSIRIS near-backscattering crystal analyser spectrometer on the ISIS pulsed neutron source. *Phys Chem Chem Phys* **18**, no. 11 (2016): 8243-8243. doi:10.1039/C6CP90057G.

N Terada et al. Magnetic ordering in pressure-induced phases with giant spin-driven ferroelectricity in multiferroic TbMnO₃. *Phys Rev B* **93**, no. 8 (2016): 081104. doi:10.1103/PhysRevB.93.081104.

Noriki Terada. High-pressure neutron diffraction with Hybrid-Anvil-Cell on cold neutron TOF diffractometer WISH: Application for multiferroics. *Japanese Society for Neutron Science* **26**, no. 2 (2016): 91-94.

L Timm et al. Exploration of antiferromagnetic CoO and NiO using reverse Monte Carlo total neutron scattering refinements. *Phys Scripta* **91**, no. 11 (2016): 114004. doi:10.1088/0031-8949/91/11/114004.

Y Tokudome et al. Layered double hydroxide nanoclusters: aqueous, concentrated, stable, and catalytically active colloids toward green chemistry. *ACS Nano* **10**, no. 5 (2016): 5550-5559. doi:10.1021/acs.nano.6b02110.

F Tonus et al. Redox behavior of the SOFC electrode candidate NdBaMn₂O₅⁺ investigated by high-temperature *in situ* neutron diffraction: first characterisation in real time of an LnBaMn(2)O(5.5) intermediate phase. *J Mater Chem A* **4**, no. 30 (2016): 11635-11647. doi:10.1039/C6TA03224A.

F Tonus and S Skinner. In-situ neutron diffraction study of cathode/electrolyte interactions under electrical load and elevated temperature. *Solid State Sci* **55** (2016): 88-92. doi:10.1016/j.solidstatesciences.2016.02.012.

S Toth et al. Frustrated Ising chains on the triangular lattice in $\text{Sr}_3\text{NiIrO}_6$. *Phys Rev B* **93**, no. 17 (2016): 174422. doi:10.1103/PhysRevB.93.174422.

JJ Towey and ER Barney. Multi-composition-EPSR : towards transferable potentials to model Chalcogenide glass structures. *J Phys Chem B* **120**, no. 51 (2016): 13169-13183. doi:10.1021/acs.jpcc.6b08793.

JJ Towey, AK Soper and L Dougan. Low-Density Water Structure Observed in a Nanosegregated Cryoprotectant Solution at Low Temperatures from 285 to 238 K. *J Phys Chem B* **120**, no. 19 (2016): 4439-4448. doi:10.1021/acs.jpcc.6b01185.

AS Tremsin et al. Investigation of microstructure within metal welds by energy resolved neutron imaging. *J Phys Conf Ser* **746** (2016): 012040. doi:10.1088/1742-6596/746/1/012040.

AS Tremsin, TY Yau and W Kockelmann. Non-destructive examination of loads in regular and self-locking Spiralock® threads through energy-resolved neutron imaging. *Strain* **52**, no. 6 (2016): 548-558. doi:10.1111/str.12201.

I Tucker et al. Adsorption of hydrophobin/beta-casein mixtures at the solid-liquid interface. *J Coll Int Sci* **478** (2016): 81-87. doi:10.1016/j.jcis.2016.06.002.

P Uresha et al. Calcium/strontium substituted phosphate based glasses for orthopaedic applications. *Frontiers in Bioengineering and Biotechnology* **4** (2016). Is in proceedings of: **10th World Biomaterials Congress, Montreal, Canada**, 17-20 May 2016. doi:10.3389/conf.FBIOE.2016.01.01175.

V Vaissier et al. How mobile are dye adsorbates and acetonitrile molecules on the surface of TiO_2 nanoparticles? A quasi-elastic neutron scattering study. *Sci Rep* **6** (2016): 39253. doi:10.1038/srep39253.

M Valero et al. Competitive and synergistic interactions between polymer micelles, drugs, and cyclodextrins : the importance of drug solubilization locus. *Langmuir* **32**, no. 49 (2016): 13174-13186. doi:10.1021/acs.langmuir.6b03367.

K Venkata et al. Characterising electron beam welded dissimilar metal joints to study residual stress relaxation from specimen extraction. *Int J Pres Ves Pip* **139-140** (2016): 237-249. doi:10.1016/j.ijpvp.2016.02.025.

RBL Vieira et al. Isolated hydrogen configurations in zirconia as seen by muon spin spectroscopy and ab initio calculations. *Phys Rev B* **94**, no. 11 (2016): 115207. doi:10.1103/PhysRevB.94.115207.

A Vispa et al. A robust comparison of dynamical scenarios in a glass-forming liquid. *Phys Chem Chem Phys* **18**, no. 5 (2016): 3975-3981. doi:10.1039/C5CP05143F.

HC Walker et al. Spin wave excitations in the tetragonal double perovskite Sr_2CuWO_6 . *Phys Rev B* **94**, no. 6 (2016): 064411. doi:10.1103/PhysRevB.94.064411.

JJ Walsh et al. Controlling Visible Light Driven Photoconductivity in Self-Assembled Perylene Bisimide Structures. *J Phys Chem C* **120**, no. 33 (2016): 18479-18486. doi:10.1021/acs.jpcc.6b06222.

J Wang et al. Tuning self-assembled morphology of the A β (16-22) peptide by substitution of Phenylalanine residues. *Colloids and Surfaces B: Biointerfaces* **147** (2016): 116-123. doi:10.1016/j.colsurfb.2016.07.052.

K Wang et al. Temporal mapping of photochemical reactions and molecular excited states with carbon specificity. *Nat Mater* **14**, no. 6 (2016): 467-473. doi:10.1038/nmat4816.

Q Wang et al. Magnetic ground state of FeSe. *Nat Commun* **7** (2016): 12182. doi:10.1038/ncomms12182.

CM Warsop et al. Simple models for beam loss near the half integer resonance with space charge. In **57th ICFA Advanced Beam Dynamics Workshop on High-Intensity and High-Brightness Hadron Beams (HB2016), Malmo, Sweden**, 3-8 Jul 2016, (2016): MOPR030. <https://hb2016.esss.se/prepress/papers/mopr030.pdf>.

N Waterfield Price et al. Coherent magnetoelastic domains in multiferroic BiFeO_3 films. *Phys Rev Lett* **117**, no. 17 (2016): 177601. doi:10.1103/PhysRevLett.117.177601.

MP Weir et al. Extrinsic Wrinkling and Single Exfoliated Sheets of Graphene Oxide in Polymer Composites. *Chem Mater* (2016). doi:10.1021/acs.chemmater.5b04502.

MP Weir et al. Distortion of Chain Conformation and Reduced Entanglement in Polymer-Graphene Oxide Nanocomposites. *ACS Macro Letters* **5**, no. 4 (2016): 430-434. doi:10.1021/acsmacrolett.6b00100.

F Weiss et al. Metastable nitric acid trihydrate in ice clouds. *Angew Chem Int Ed* **55**, no. 10 (2016): 3276-3280. doi:10.1002/anie.201510841.

CC Wilcox et al. An investigation into the behaviour of residual gas ionisation profile monitors in the ISIS extracted beamline. In **International Beam Instrumentation Conference 2016 (IBIC 2016), Barcelona, Spain**, 11-15 Sep 2016, (2016): WEPG68. <http://jacow.web.psi.ch/conf/y16/ibic16n5alba/prepress/WEPG68.PDF>.

RC Williams et al. Magnetic phase diagram of $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$ revised using muon-spin relaxation. *Phys Rev B* **93**, no. 14 (2016): 140406. doi:10.1103/PhysRevB.93.140406.

S Williams et al. Incommensurate counterrotating magnetic order stabilized by Kitaev interactions in the layered honeycomb $\alpha\text{-Li}_2\text{IrO}_3$. *Phys Rev B* **93**, no. 19 (2016): 195158. doi:10.1103/PhysRevB.93.195158.

RE Williamson, CM Warsop and B Jones. Development of physics models of the ISIS head-tail instability. In **57th ICFA Advanced Beam Dynamics Workshop on High-Intensity, High Brightness and High Power Hadron Beams (HB2016), Malmo, Sweden**, 3-8 Jul 2016, (2016). <http://purl.org/net/epubs/manifestation/26215994>.

JDS Witt et al. Magnetic phases of sputter deposited thin-film erbium. *Sci Rep* **6** (2016): 39021. doi:10.1038/srep39021.

T Wood et al. The ISIS pre-injector reconfiguration. *Rev Sci Instrum* **87**, no. 2 (2016): 02B121. doi:10.1063/1.4934658.

DN Woodruff et al. The Parent Li(OH)FeSe Phase of Lithium Iron Hydroxide Selenide Superconductors. *Inorg Chem* **55**, no. 19 (2016): 9886-9891. doi:10.1021/acs.inorgchem.6b01734.

RJ Woolfson et al. $[\text{CrF}(\text{O}_2\text{CtBu})_2]_9$: Synthesis and characterization of a regular homometallic ring with an odd number of metal centers and electrons. *Angew Chem Int Ed* **55**, no. 31 (2016): 8856-8859. doi:10.1002/anie.201601734.

JA Wright et al. Muonium chemistry at diiron subsite analogues of [FeFe]-Hydrogenase. *Angew Chem Int Ed* **55**, no. 47 (2016): 14580-14583. doi:10.1002/anie.201607109.

JA Wright et al. Muonium Chemistry at Diiron Subsite Analogues of [FeFe]-Hydrogenase. *Angew Chem* **128**, no. 47 (2016): 14800-14803. doi:10.1002/ange.201607109.

BM Wyvrat et al. Reactivity of Hydrogen on and in nanostructured Molybdenum Nitride : Crotonaldehyde Hydrogenation. *ACS Catalysis* **6**, no. 9 (2016): 5797-5806. doi:10.1021/acscatal.6b00936.

Q Xia et al. Direct hydrodeoxygenation of raw woody biomass into liquid alkanes. *Nat Commun* **7** (2016): 11162. doi:10.1038/ncomms11162.

L Xu et al. Self-Assembly of Magnetic Bacillus-Shaped Bilayer Vesicles in Catanionic Surfactant Solutions. *Langmuir* **32**, no. 40 (2016): 10226-10234. doi:10.1021/acs.langmuir.6b01564.

X Xu et al. Structural characterization of phase separation in Fe-Cr : a current comparison of experimental methods. *Metall Mater Trans A* **47**, no. 12 (2016): 5942-5952. doi:10.1007/s11661-016-3800-4.

C Yan et al. Shape Modification of Water-in- CO_2 Microemulsion Droplets through Mixing of Hydrocarbon and Fluorocarbon Amphiphiles. *Langmuir* **32**, no. 6 (2016): 1421-1428. doi:10.1021/acs.langmuir.5b03630.

S Yang and M Schröder. Tracking charge in metal organic frameworks promises to improve fuel cell materials. *Fuel Cells Bulletin* **2016**, no. 6 (2016): 12-13. doi:10.1016/S1464-2859(16)30158-4.

K Yokoyama et al. The new high field photoexcitation muon spectrometer at the ISIS pulsed neutron and muon source. *Rev Sci Instrum* **87**, no. 12 (2016): 125111. doi:10.1063/1.4972827.

D Yoo et al. High-Throughput Fabrication of Resonant Metamaterials with Ultrasmall Coaxial Apertures via Atomic Layer Lithography. *Nano Lett* **16**, no. 3 (2016): 2040-2046. doi:10.1021/acs.nanolett.6b00024.

H Zhang et al. Multiferroicity broken by commensurate magnetic ordering in Terbium Orthomanganite. *ChemPhysChem* **17**, no. 8 (2016): 1098-1103. doi:10.1002/cphc.201501188.

L Zhang and JM Cole. Can nitro groups really anchor onto TiO_2 ? Case study of dye-to- TiO_2 adsorption using azo dyes with NO_2 substituents. *Phys Chem Chem Phys* **18**, no. 28 (2016): 19062-19069. doi:10.1039/c6cp02294d.

R Zhang et al. $\text{La}_2\text{SrCr}_2\text{O}_7$: Controlling the Tilting Distortions of $n = 2$ Ruddlesden–Popper Phases through A-Site Cation Order. *Inorg Chem* **55**, no. 17 (2016): 8951-8960. doi:10.1021/acs.inorgchem.6b01445.

R Zhang et al. $\text{La}_2\text{SrCr}_2\text{O}_7\text{F}_2$: A Ruddlesden–Popper Oxyfluoride Containing Octahedrally Coordinated Cr^{4+} Centers. *Inorg Chem* **55**, no. 6 (2016): 3169-3174. doi:10.1021/acs.inorgchem.6b00114.

R Zhang, MS Senn and MA Hayward. Directed lifting of inversion symmetry in Ruddlesden–Popper Oxide–Fluorides : toward Ferroelectric and Multiferroic behavior. *Chem Mater* **28**, no. 22 (2016): 8399-8406. doi:10.1021/acs.chemmater.6b03931.

SL Zhang et al. Engineering helimagnetism in MnSi thin films. *AIP Adv* **6**, no. 1 (2016): 015217. doi:10.1063/1.4941316.

Y Zhao et al. Tuning one-dimensional nanostructures of bola-like peptide amphiphiles by varying the hydrophilic amino acids. *Chem Eur J* **22**, no. 32 (2016): 11394-11404. doi:10.1002/chem.201601309.

DAG de Oliveira et al. Evaluation and mitigation of radiation-induced soft errors in graphics processing units. *IEEE Transactions on Computers* **65**, no. 3 (2016): 791-804. doi:10.1109/TC.2015.2444855.

L del Rosso et al. Refined structure of metastable ice XVII from neutron diffraction measurements. *J Phys Chem C* **120**, no. 47 (2016): 26955-26959. doi:10.1021/acs.jpcc.6b10569.

L van Eijck et al. Design and performance of a novel neutron powder diffractometer : PEARL at TU Delft. *J Appl Crystallogr* **49**, no. 5 (2016): 1398-1401. doi:10.1107/S160057671601089X.

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L Stimpson. Novel properties of the layered material Ca₂Mn₃O₈. PhD, 2016.

M Tokac. Investigation of Interfacial Effects in Ferromagnetic Thin-Films. PhD, 2016.

AH Turner. Investigations of ionic liquid-solute interactions towards applications. PhD, 2016.

A Vispa. Dynamics of disordered systems. Phd, 2016.

E Wann. The Core Composition of Terrestrial Planets: A Study of the Ternary Fe-Ni-Si System. PhD, 2016.

R Welbourn. Adsorbed layers under challenging conditions at the solid-liquid interface. PhD, 2016.

R Williams. Correlated magnetic oxides studied using muon-spin spectroscopy. PhD, 2016.

M Wood. Adsorption at the metal/liquid interface. PhD, 2016.

F Yuen . A physicochemical analysis of the stabilising function of LEA proteins in conditions of abiotic stress. PhD, 2016.

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