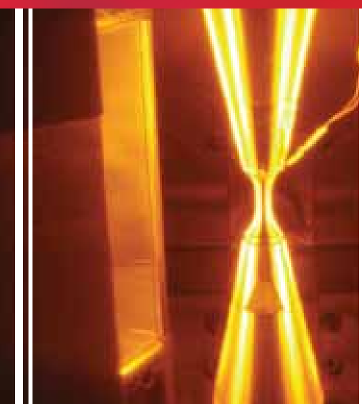
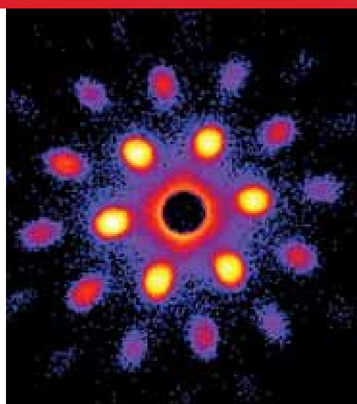
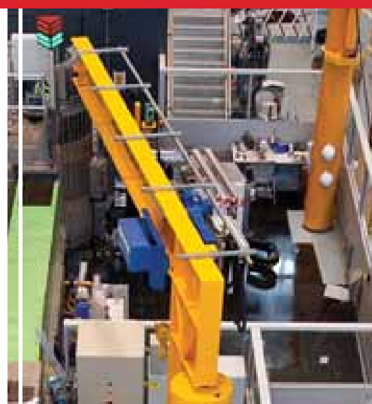
AUSTRALIA–JAPAN NEUTRON SCIENCE WORKSHOP

Sharing science with neutrons







5–6 NOVEMBER 2013 SYDNEY, AUSTRALIA

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Australian Academy of Science

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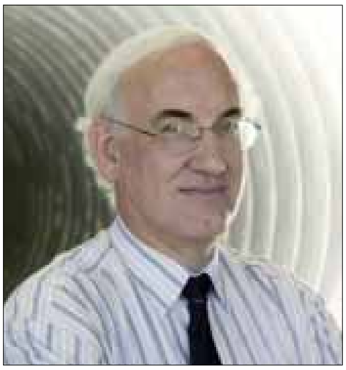
WELCOME

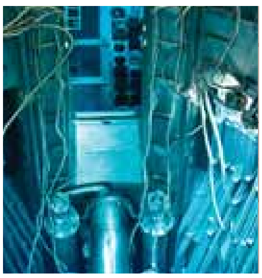
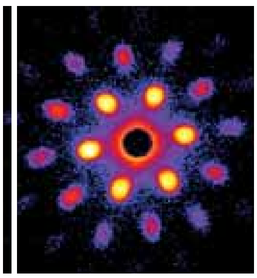
On behalf of the Australian research community and ANSTO I would like to welcome our Japanese friends and colleagues to this workshop on *Australia–Japan: sharing science with neutrons*. Of course, ANSTO also warmly welcomes the domestic delegates from around Australia to the meeting.

This workshop results from a joint Japan–Australia Science and Technology Meeting held in Tokyo in August 2012, in which Dr Masa Arai and I participated, and indeed from much longer-standing deep interactions and collaborations between Japan and Australia in crystallography, neutron scattering and synchrotron radiation. In the workshop, we are seeking to enhance and grow the long-term scientific interactions between the research communities of our two countries, and extend them to new areas. In particular, there is potential to greatly increase and strengthen the interactions between the new J-PARC spallation neutron source in Tokai, and our OPAL research reactor, here in Sydney, and to have higher levels of Australian usage at J-PARC along with greater Japanese involvement at OPAL and the Bragg Institute. We hope that, by highlighting the exciting new science and technology in both countries, new opportunities and ideas will emerge, which we will be able to pursue together over the coming years.

I would like to acknowledge the generous financial support provided by the Australian Government towards this event and the assistance of the Australian Academy of Science in relation to the management of the workshop.



Dr Rob Robinson
Head, Bragg Institute, ANSTO
President, Australian Institute of Physics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PROGRAM

TUESDAY 5 NOVEMBER

8.30 am Arrival at ANSTO Discovery Centre for security clearance

8.45 am Registration

9.00 am Official opening

Session 1

Introduction

Chair: Dr Rob Robinson

9.40 am **Professor Yasuhiko Fujii**, **CROSS**
Small science at large facilities in the Asia-Oceania region

10.00 am **Professor John White FAA FRS**, **Australian National University**
Sustainable cooperation in our region

10.20 am **Dr Masatoshi Arai, J-PARC**
What is J-PARC, and its Materials and Life Sciences facility?

10.40 – 11.00 am Morning tea

11.00 am Tour of the OPAL reactor's neutron beam facilities

Session 2

Soft matter and synergy with synchrotrons

Chair: Professor Mitsuhiro Shibayama

12.00 pm **Professor Toshiji Kanaya**, **Kyoto University**
Polymer crystallisation under flow

12.20 pm **Professor Michael James, Australian Synchrotron**
Studies of organic semiconducting devices using neutrons

12.40 – 1.40 pm Lunch

Session 3

Structural biology

Chair: Professor Frances Separovic

1.40 pm **Professor Jill Trewhella, The University of Sydney**
Neutron contrast variation: a powerful tool for studying biomolecular complexes

2.00 pm **Dr Satoru Fujiwara, QuBS/JAEA**
Protein dynamics studied by neutron scattering

2.20 pm **Professor John Carver, Australian National University**
Solution scattering investigations of protein–protein interactions

2.40 – 3.30 pm Break for Melbourne Cup festivities and afternoon tea

Session 4

Hard condensed matter

Chair: Professor Youichi Murakami

3.30 pm **Dr Garry McIntyre, ANSTO**
Modern neutron Laue diffraction: exotic physics, organometallic hydrides, and proteins

3.50 pm **Dr Masatomo Yashima, TITEC**
Precise crystal-structure analysis of ion-conducting ceramic materials and oxynitride photocatalysts by neutron powder diffraction

4.10 pm **Dr Frank Klose, ANSTO**
Opportunities for neutron scattering in spintronic thin film materials science

Session 5

Complementary use of neutron and synchrotron radiation

Chair: Professor Michael James

4.30 pm **Professor Youichi Murakami, IMSS, KEK**
Complementary use of neutron and synchrotron radiation beams

4.50 pm **Professor Keith Nugent FAA, La Trobe University**
Neutron and X-ray phase-contrast imaging

5.10 pm **Dr Yukinobu Kawakita, J-PARC**
Complementary use of neutron and synchrotron to study on ionic-conductors

7.00 – 10.00 pm Official workshop dinner, Rydges, Cronulla, Forby Sutherland Room

WEDNESDAY 6 NOVEMBER

Session 6

Soft matter 2

Chair: Dr Elliot Gilbert

Parallel workshops

Chair: Dr Hal Lee

9.00 – 10.00 am Japan–Australia cooperation on cold-neutron moderators
Dr Makoto Teshigawara, J-PARC
Moderator design and neutronic performance in JSNS

10.00 – 10.40 am Japan–Australia cooperation on helium-3 polarisers
Dr Takayuki Oku, J-PARC
Development and application of an in-situ SEOP ^{3}He neutron spin filter at J-PARC/MLF

9.00 am	**Professor Mitsuhiro Shibayama, ISSP/University of Tokyo** *Research activity and joint-use program of the Institute of Solid-State Physics, University of Tokyo*
9.20 am	**Professor Greg Warr, The University of Sydney** *Neutron scattering studies of ionic liquid*
09.40 am	**Professor Hideko Seto, KEK, J-PARC** *Recent activities on soft matter in J-PARC*
10.00 am	**Professor Frances Separovic FAA, The University of Melbourne** *Structural effects of the antimicrobial peptides on supported lipid bilayers*
10.20 am	**Professor Atsushi Takahara, Kyushu University** *Analyses of soft interfaces by neutron reflectivity*

10.40 – 11.00 am Morning tea

Session 7

Materials science

Chair: Professor Kiyoichiro Motoya

11.00 am	**Professor Mark Hoffman, University of New South Wales** *Effect of relaxor-ferroelectric transitions on fatigue of BNT-based lead-free piezoceramics*
11.20 am	**Professor Kiyoichiro Motoya, Tokyo University of Science** *Real-time observation of magnetic structural change in frustrated magnets*
11.40 am	**Dr Vanessa Peterson, ANSTO** *In situ analysis of energy materials at the Bragg Institute*
12.00 pm	**Professor Toshiya Otomo, KEK, J-PARC** *High intensity neutron scattering techniques for hydrogen materials studies*
12.20 pm	**Professor Craig Buckley, Curtin University** *Concentrated solar thermal energy storage using metal hydrides*
12.40 pm	**Dr Ryoichi Kajimoto, J-PARC** *Chopper spectrometers at J-PARC and their science*

1.00 – 1.40 pm Lunch

Session 8

Soft matter 3

Chair: Professor Atsushi Takahara

1.40 pm	**Dr Patrick Hartley, CSIRO** *Science with neutrons: examples and opportunities within CSIRO's Applied Research Programs*
2.00 pm	**Dr Junichi Suzuki, CROSS** *Development of the small and wide angle neutron scattering instrument TAIKAN at J-PARC*
2.20 pm	**Dr Elliot Gilbert, ANSTO** *Opportunities for neutron scattering in food materials science*

2.40 – 3.00 pm Afternoon tea

Session 9

Finale

Chair: Professor John White

3.00 pm	**Dr Garry Foran, CROSS** *CROSS-Tokai and the MLF: working together for the neutron user community*
3.20 pm	**Professor Takashi Kamiyama, KEK, J-PARC** *My experience in collaboration with Australian friends in materials science*
3.40 pm	**Professor Brendan Kennedy, Sydney University** *Reactor or accelerator? How I decide where to take my samples*
4.00 pm	Summary and wrap-up

SPEAKERS

DR MASATOSHI ARAI

Division Head, Japan Atomic Energy Agency

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PRESENT POSITION

Division Head, Senior Primary Researcher, Materials Life Science Division, J-PARC Center, Japan Atomic Energy Agency (JAEA)

EDUCATION

PhD, physics, Tohoku University

RESEARCH INTERESTS

- Neutron scattering instrumentation and technique
- Dynamics of disordered system
- High Tc superconductivity
- Low dimensional spin system

PROFESSIONAL EXPERIENCE

2010 – present Division Head; **2009** Deputy Division Head, Materials Life Science Division, J-PARC Center; **2007** Section Leader of the Neutron Science Section, Materials Life Science Division, J-PARC Center, JAEA; **2005** Senior Primary Researcher, Quantum Beam Science Directorate, JAEA; **1996** Professor, High Energy Accelerator Research Organisation (KEK); **1992** Associate Professor, Kobe University; **1985** Research Associate, National Laboratory for High Energy Physics (KEK); **1983.7** Postdoctoral fellow, Argonne National Laboratory, US.

WHAT IS J-PARC, AND ITS MATERIALS AND LIFE SCIENCES FACILITY

J-PARC MLF is designed to be a 1 MW spallation neutron source. The averaged neutron flux is about 1/4 of ILL research reactor, the world's best reactor. However, the pulse peak flux can exceed 100 times that of ILL. This factor gives a new paradigm for neutron scattering not only in basic science but also in applications such as industrial use of neutrons. Twenty instruments have been already funded, 16 are available for user programs and the four are either being commissioned or constructed. In Japan we have never had a world-class neutron facility and J-PARC/MLF is a new challenge for us to realise this goal. Since ANSTO/Bragg Institute is a world class facility, we have a lot of things to learn from ANSTO such as facility management, user programs, technology in instruments, sample environments, etc., as well as English, a common language in the world. For these reasons we decided to have a comprehensive collaboration with ANSTO.

PROFESSOR CRAIG BUCKLEY

Dean of Research Faculty of Science and Engineering, Curtin University

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Professor Craig Buckley is Dean of Research in the Faculty of Science and Engineering, Professor of Physics, Head of the Hydrogen Storage Research Group, and Deputy Director of the Fuels and Energy Technology Institute at Curtin University. Since being awarded his BSc (Honours 1st Class, 1989) and PhD (1994) from Griffith University he has held various research positions in the UK, US and Australia prior to being awarded tenure at Curtin. His research is focused on hydrogen storage materials and the investigation of the atomic and nanostructure of a wide range of materials. Professor Buckely has won several ARC Discovery, Linkage, LIEF (Linkage, Infrastructure, Equipment and Facilities) and Industry grants, and has published approximately 100 refereed journal publications. He is a member of several national and international science and advisory committees including as an Australian expert on the International

Energy Agency (IEA) Hydrogen Implementing Agreement: Task 32: Hydrogen-based energy storage.

CONCENTRATED SOLAR THERMAL ENERGY STORAGE USING METAL HYDRIDES

Solar energy is the most abundant renewable energy resource available to produce the planet's future electricity needs. The IEA roadmap for solar energy set a target of approximately 22% of global electricity production from solar energy by 2050, with 50% being produced from concentrating solar thermal power systems. Achieving this target will be possible only if the costs of producing electricity from solar energy are significantly reduced and cost effective energy storage technologies can be developed. A major challenge is to achieve continuous, low-variability power generation from renewable energy sources, for stand-alone applications or for integration with domestic power grids. Solar mirror collection fields can collect thermal energy during the day and run a heat engine to convert it into electricity, but cannot provide power at night. However, if some of the heat is used to remove hydrogen from a metal hydride, the reverse reaction where hydrogen absorbs back into the metal hydride can then occur at night, releasing heat for power generation. This allows solar energy to provide 24-hour power generation. By combining a high temperature metal hydride with a low temperature metal hydride a coupled pair reversible metal hydride thermochemical solar energy storage system is created.

PROFESSOR JOHN A CARVER

Director, Research School of Chemistry, The Australian National University

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Since July 2013, John Carver has been Director of the Research School of Chemistry at the Australian National University in Canberra. He undertook his honours degree in Chemistry at the University of Adelaide. In 1983, he was awarded his PhD from the ANU and subsequently undertook postdoctoral studies in biochemistry at the universities of Oxford and Adelaide. In 1988, Professor Carver took up a position as Lecturer in Chemistry at the University of Wollongong. In 2004, he returned to The University of Adelaide as Professor of Chemistry and Head of the School of Chemistry and Physics. For periods, he was also Deputy Executive Dean of the Faculty of Sciences and Head of the School of Molecular and Biomedical Science. Professor Carver's research interests are in protein structure, function and interactions, particularly relating to molecular chaperones and their mechanism of stabilising other proteins. He utilises a diversity of spectroscopic, biophysical and protein chemical techniques for his research. He has co-authored more than 140 research publications and has received a variety of fellowships.

SOLUTION SCATTERING INVESTIGATIONS OF PROTEIN–PROTEIN INTERACTIONS

Molecular chaperones are a diverse group of proteins that are involved in preventing protein misfolding and aggregation. They have an important role in preventing such protein–protein interactions that are characteristic of the proteinaceous deposits in diseases such as Alzheimer's, Parkinson's and cataract. In this talk, I shall present some of our work utilising small-angle X-ray and neutron scattering (SAXS and SANS respectively) techniques to investigate the mechanism of action of three types of mammalian molecular chaperones: small heat-shock proteins (e.g.αB-crystallin), 14-3-3ζ and β-casein. All three proteins share no sequence similarity. αB-crystallin and β-casein both exist as relatively unstructured, heterogeneous, dynamic and large oligomeric species. By contrast, 14-3-3ζ is found as a well-ordered, α-helical dimer. Despite all these differences, the three proteins exhibit marked similarities in their mechanism of chaperone action. A variety of target proteins, under diverse stress conditions (e.g. elevated temperature, reductive, chemical etc.), were used to provide detailed insight, via SAXS and SANS experiments, into how these molecular chaperones efficiently prevent large-scale protein aggregation.

DR GARRY FORAN

Comprehensive Research Organization for Science and Society

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After receiving his PhD from The University of Sydney in 1992, Dr Foran joined ANSTO as part of the fledgling Australian National Beamline Facility team and moved to Japan where he worked as a beamline scientist at the Photon Factory synchrotron radiation light source for 17 years. In 2009, on secondment from ANSTO, Dr Foran took up a position at the Australian Synchrotron where he was responsible for preparing the Australian Synchrotron Development Plan – a roadmap for the future of the AS. In 2011, Dr Foran returned to Japan to take up his current position at CROSS-Tokai, working chiefly in international relations.

CROSS-TOKAI AND THE MLF: WORKING TOGETHER FOR THE NEUTRON USER COMMUNITY

In July 2009, the Japanese government established at J-PARC the Public Neutron Beam Facility consisting of the accelerators used to generate the neutron beams and a proportion of the beamlines that exploit these beams for research purposes. In order that open access to major publicly-funded research facilities be guaranteed, the policy framework within which the Public Neutron Beam Facility was created required that an independent third-party organisation be responsible for the administration and support of the science program on the so-called Public Beamlines. CROSS-Tokai was appointed to this role by the Ministry of Education, Culture, Sports, Science and Technology in March 2011. Although CROSS-Tokai is structurally independent of JAEA and KEK – the co-owners and operators of J-PARC – it maintains a high level of cooperation and collaboration with the two founding organisations that is driven by the common objectives of all the stakeholders. In practical terms, the core functions of CROSS-Tokai can be summarised as follows:

- Proposal selection and beamtime allocation on the public beamlines
- User support on the public beamlines
- Provide an information resource for facility users
- Outreach and facility utilisation promotion
- Contract beamline assessment and selection

PROFESSOR YASUHIKO FUJII

Director, Research Centre for Neutron Science and Technology, Comprehensive Research Organization for Science and Society

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1970 Research Associate, ISSP, Tokyo University; **1979** Associate Physicist, Physics Department, Brookhaven National Laboratory; **1983** Associate Professor, Faculty of Engineering Science, Osaka University; **1988** Professor, Institute of Materials Science, University of Tsukuba; **1992** Professor, ISSP, Tokyo University; **1993** Chair, Neutron Scattering Lab., ISSP, Tokyo University; **2001** President, Japanese Society for Neutron Science; **2003** Director, Neutron Science Research Centre, JAERI; **2004** Emeritus Professor of Tokyo University; **2005** Deputy Director General, Quantum Beam Science Directorate, JAEA; **2007** Director General of the above; **2010** Director, Research Centre for Neutron Science and Technology, Comprehensive Research Organization for Science and Society (CROSS)

SMALL SCIENCE AT LARGE FACILITIES IN THE ASIA-OCEANIA REGION

For the past quarter of a century, the Asia-Oceania region has been growing energetically in the field of neutron science and technology based on completion of a series of new/refurbished neutron sources. In parallel user communities in each country/region started organising their own societies such as ANBUG (Australia), NSSI (India), JSNS (Japan), KNBUA (Korea), TWNSS (Taiwan) and CNSS (China), established so far. The culmination of such a trend in user communities resulted in the formation of the Asia-Oceania Neutron Scattering Association (AONSA) in August 2008, as an affiliation of neutron scattering societies. The establishment of AONSA complemented the tri-polar global network with the preceding ENSA in Europe and NSSA in North America. We will introduce details of

AONSA's activities and discuss the neutron community with synchrotron radiation, both of which are categorised as 'small science at large facilities', necessitating such large facilities as nuclear reactors and accelerators, costing a large amount of public money not only for construction but also for operation. Thus we share the same destiny and work cooperatively, particularly for our region.

DR SATORU FUJIWARA

Prime Scientist, Japan Atomic Energy Agency

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Professor Fujiwara earned a PhD from the Department of Biophysical Engineering, Osaka University, Japan, for a small-angle X-ray scattering study of protein-DNA complexes. After postdoctoral work at SERC Daresbury Laboratory, UK, University of California, San Francisco, US, and Brookhaven National Laboratory, US, on small-angle X-ray and neutron scattering studies of proteins, he moved to the Advanced Science Research Center, the Japan Atomic Energy Research Institute (now the Japan Atomic Energy Agency, JAEA), as a research scientist. Now as a prime scientist in the Neutron Biophysics Group in the Quantum Beam Science Directorate, JAEA, he continues research on proteins. His research interest is elucidation of the dynamics-structure-function relationship of the proteins. For this ultimate purpose, combination of structural studies using small-angle scattering and dynamics studies using neutron inelastic scattering has been carried out particularly on muscle proteins and proteins related to the amyloid diseases.

PROTEIN DYNAMICS STUDIED BY NEUTRON SCATTERING

Proteins constantly fluctuate under the influence of surrounding aqueous environments. These thermal fluctuations, or dynamics, of proteins are indispensable for the structural changes that make proteins function. Ultimate understanding of the protein functions thus requires characterisation of the dynamics of the proteins including hydration water and elucidation of how dynamics is related to the structures, and thereby functions, of the proteins. We have been studying this dynamics-structure-function relationship of the proteins using combination of neutron scattering, which can measure the dynamics of the proteins directly, and structural methods such as small-angle scattering. As an example, neutron scattering studies of actin are presented. Monomeric actin molecules (G-actin) polymerise into a filamentous complex (F-actin), and this F-actin plays important roles in various functions related to cell motility including muscle contraction. We carried out neutron scattering measurements on G-actin and F-actin, and detected the difference in the dynamics between G-actin and F-actin. It was shown that this difference is coupled to the difference in the dynamics of hydration water around G-actin and F-actin. The recent results on possible modulation of the dynamics of F-actin by the presence of the regulatory system (troponin and tropomyosin) are also presented.

DR ELLIOT GILBERT

Leader, Food Science; Instrument Scientist, Quokka (SANS), Australian Nuclear Science and Technology Organisation

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Dr Elliot Gilbert led the project for the design, construction and commissioning of the QUOKKA small-angle neutron scattering instrument at the OPAL facility and is currently instrument-responsible. In addition, Dr Gilbert is leader of the Food Science project that seeks to apply a materials science approach to the study of structure and dynamics in food-based systems. He received his PhD in chemistry from the Australian National University in 1998. Following an ARC/SPIRT Industrial Postdoctoral Fellowship, he joined the Small-Angle Scattering Group at the Intense Pulsed Neutron Source at Argonne National Laboratory, US, in 1999 where he provided scientific and technical assistance to users of the small-angle scattering instruments. Dr Gilbert's interests lie in soft condensed matter science and he has investigated such diverse areas as emulsion stabilisation, polymers in confined geometry and phase separation in paraffins, but now has an increasing focus on naturally occurring materials and has recently written a review on the application of neutron scattering in food science. He chaired the last international conference on small-angle scattering in Sydney in 2012, is Principal Guest Editor for the *Journal of Applied Crystallography* (SAS2012 Special Issue), currently serves on the International Programme Committee for the 23rd IUCr conference and, as well as reviewing for a large range of scientific journals, is on the editorial board of *Food Structure* (Elsevier).

OPPORTUNITIES FOR NEUTRON SCATTERING IN FOOD MATERIALS SCIENCE

The subject of food is certainly newsworthy, whether the story is associated with 'food security', the growing of food for fuel, or blurring the line between food and medicine. In Australia, we have developed a program of research in which we use nuclear-based methods to investigate fundamental and industrial problems of national significance in food science. One of the most ubiquitous forms of food is the biopolymer blend, starch. It is composed of amylose and amylopectin, packed into complex molecular arrangements that show a high level of organisation over several length scales from the atomic (yielding variations in crystal packing) to granular (on the micron scale). Amylopectin is assumed to contribute significantly towards the structural and physicochemical properties of starch, whereas the location and role of amylose is less understood. Recently, the amylose fraction has been under heavy scrutiny because of its resistance to enzymatic digestion driven by the potential use of high-amylose starches as ingredients in formulating foods rich in resistant starch. The consumption of such materials has been widely implicated to lead to reductions in the incidence of diet-related disease. The vast majority of the food consumed however is not composed of granular starch but is, in fact, processed – often gelatinised and retrograded – thus an understanding of starch structure must also extend to processing. The latter is well suited to neutron scattering due to the highly penetrating nature of the radiation enabling beam transmission through complex sample environments, opening up the opportunity to study industrially-relevant processes in real time. This presentation will briefly introduce the broad application of neutron (and X-ray) scattering methods to food-based systems within the 'Food Structure and Dynamics' group at ANSTO with a subsequent focus on our investigations of starch structure.

DR PATRICK HARTLEY

Research Theme Leader, CSIRO Energy Flagship, CSIRO

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Dr Patrick Hartley leads the Fuels and Products research theme within the CSIRO Energy Research Flagship, focusing on developing new technologies to transform Australia's energy and biomass resources into fuels and products. Dr Hartley's scientific background is in colloid and interface science and its application to the development of products and processes for biomedical, energy production, energy transport and energy transformation applications. Dr Hartley was awarded his PhD in 1994 from Imperial College, London. He was a Research Fellow at the Advanced Minerals Products Research Centre at The University of Melbourne from 1995–98, and joined CSIRO in 1998. Dr Hartley has received a number of awards, including the CSIRO Medal for Business Excellence (2009), the CSIRO Medal (2004) and the Grimwade Prize in Industrial Chemistry, The University of Melbourne (2004). He was Chair of the Colloids and Surface Chemistry Division of the Royal Australian Chemical Institute (2005–07). He has served as CSIRO's Councillor to the Australian Institute of Nuclear Science and Education since 2011.

SCIENCE WITH NEUTRONS: EXAMPLES AND OPPORTUNITIES FROM CSIRO'S APPLIED RESEARCH PROGRAMS

CSIRO, the Commonwealth Scientific and Industrial Research Organisation, is Australia's national science agency and one of the largest and most diverse research agencies in the world. CSIRO's role is to deliver applied science and innovation which supports Australia's industry sectors, society and environment. This presentation will provide examples and opportunities from CSIRO's research projects in the biomedical, resources, energy and manufacturing areas of how neutron science techniques can be used to deliver detailed understanding of material properties and behaviours which underpin applied science outcomes.

PROFESSOR MARK HOFFMAN

Pro Vice-Chancellor (Research), University of New South Wales

Email mark.hoffman@unsw.edu.au

Professor Hoffman is Pro Vice-Chancellor Research of the University of New South Wales. From 2007–12 he was Head of the School of Materials Science and Engineering at UNSW. He holds a BE (1989) and PhD (1994) from The University of Sydney and a Masters of Business and Technology from UNSW (2006). Professor Hoffman's research expertise is in the area of structural integrity of materials, specifically the design of materials for high reliability in complex environments. In recent years he has focused on piezoelectric materials. He has published more than 170 international journal papers and graduated 23 PhD and Masters students. Professor Hoffman is former Director of the International Congress on Fracture, a Research Program Leader for the ARC Centre of Excellence in Design in Light Metals, Fellow of the Institute of Engineers Australia and an Associate Editor of the *Journal of the American Ceramic Society*.

EFFECT OF RELAXOR-FERROELECTRIC TRANSITIONS ON FATIGUE OF BNT-BASED LEAD-FREE PIEZOCERAMICS

Piezoelectric devices are a key enabling technology in industrial, manufacturing and automotive industries. Piezoceramics are currently lead-based, causing toxic by-products, especially during manufacture and waste incineration. Consequently, the search for non-toxic piezoceramics that can replace lead-based materials such as Pb(Zr,Ti)O3 (PZT) is one of the major challenges in science and engineering and BNT-based systems show considerable promise as an alternative. The fatigue behavior of a ferroelectric composition 94BNT-6BT under bipolar and unipolar electrical cycling was investigated as a function of temperature from 25 to >100°C. For both bipolar and unipolar cycling a decrease of polarisation, mechanical strain, permittivity 33 and piezoelectric coefficient d33 are observed, with most of the degradation occurring within 104 cycles. In situ neutron diffraction in the unloaded state revealed a phase transformation and formation of ferroelectric order within 1000 cycles at room temperature but then a disappearance of the ferroelectric order with subsequent cycles, despite the retention of piezoelectric properties. However, as temperature increased observable ferroelectric order disappeared at all levels of cycling. The presentation will posit that fatigue behavior in these systems can be explained by an electric field-temperature (E-T) phase relationship with the loci of transitions between phases varying with composition.

PROFESSOR MICHAEL JAMES

Head of Science, Australian Synchrotron/Australian Nuclear Science and Technology Organisation

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Professor Michael James received his BSc from The University of Sydney, and PhD in inorganic chemistry from the University of Cambridge, UK, where he investigated new classes of magnetic and superconducting ceramics. He built Australia's first neutron reflectometer at the 10 MW HIFAR reactor, developed a SAXS and X-ray reflectometry facility, before building and operating the PLATYPUS time-of-flight neutron reflectometer at OPAL. Other roles at ANSTO included leading the Chemical Deuteration Laboratory and in 2007 he was appointed a visiting Professor with the School of Chemistry at the University of New South Wales. In January 2013, he took up the role of Head of Science at the Australian Synchrotron. During his career he has worked in numerous areas of neutron and X-ray scattering, including instrumentation, solid state chemistry, powder diffraction from molecular and magnetic materials; as well as reflectometry from nanoscale thin films, chemical and biological sensors, and molecular interactions with biomimetic cellular membranes. Other current research interests include the study of organic photovoltaics and organic light-emitting diodes. He has published more than 130 peer-reviewed scientific papers.

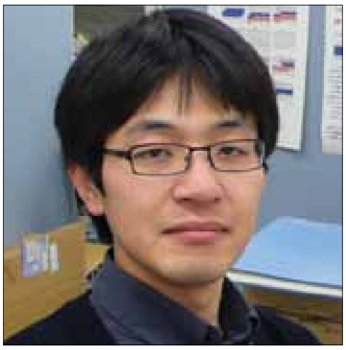
STUDIES OF ORGANIC SEMICONDUCTING DEVICES USING NEUTRONS

The operating efficiencies and lifetimes of thin-film optoelectronics are key performance metrics that require further optimisation before the widespread use of such devices. To better understand the morphologies and molecular interactions within nanoscale optoelectronic systems, as-prepared and annealed devices were investigated in a series of experiments using time-of-flight neutron reflectometry and in situ photoluminescence (PL) measurements. Scattering contrast between key molecular components of the discrete electronic layers was enhanced in a number of instances using chemical deuteration. Inter-diffusion processes between electron transport, hole transport and emissive layers in multilayer (OLEDs) were shown to occur after annealing beyond critical temperatures. Organic photovoltaic solar cells (OPVs) produced by solution processing methods typically show poor efficiencies in their as-cast state, despite substantial inter-mixing between sequentially processed electron donor and electron acceptor components. Devices annealed at temperatures up to 150 °C show complete inter-diffusion accompanied by substantial increases in their external quantum efficiencies; although large gains in efficiency seem not to require complete blending of the bilayer structure.

PHASE SEPARATION IN ANNEALED OLED

Molecular interactions and PL quenching in thin films of fluorescent carbazole-based dendrimers exposed to gaseous analogues of TNT can also be examined by time-correlated neutron reflectometry and in situ PL spectroscopy.

DR RYOICHI KAJIMOTO



Principal Researcher, J-PARC, Japan Atomic Energy Agency

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Dr Kajimoto received his Ph D in March 2000 with the thesis 'Neutron scattering study on charge ordering and magnetism in perovskite manganese oxides R1-xAxMnO3'. He was a Postdoctoral Fellow at Ochanomizu University in 2000–04 and a Postdoctoral Fellow at the High Energy Accelerator Research Organisation (KEK) in 2004–05. He has been at the Japan Atomic Energy Agency since 2005. His research field is neutron scattering studies on magnetism of transition metal oxides such as colossal magnetoresistive manganites, multiferroic manganites, layered perovskites nickelates, and triangular-lattices of chromium oxides.

CHOPPER SPECTROMETERS AT J-PARC AND THEIR SCIENCE

Chopper spectrometers are one of the typical inelastic neutron scattering instruments at a pulsed source. J-PARC already has three chopper spectrometers: BL01-4SEASONS, BL12-HRC, and BL14-AMATERAS in operation, and another one, BL23-POLANO, is under construction. They are complementary to each other, and the combination of these spectrometers enables flexible studies of dynamics of molecules, magnets, dielectrics, metals, superconductors etc. in the energy range of 10-2 – 102 meV. In the presentation, I will give a short review of the features of the spectrometers and show examples of their scientific outputs.

PROFESSOR TAKASHI KAMIYAMA

Professor, J-PARC / Institute of Materials Structure Science, High Energy Accelerator Research Organization

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Professor Kamiyama was awarded his PhD in physics by Tohoku University in 1987. He has worked at the Tohoku University and University of Tsukuba. He currently works for the High Energy Accelerator Organisation and J-PARC. He has been a leading scientist in powder diffraction instrumentation in both the former KENS and present J-PARC. He is a leader of the Neutron Science Section of the MLF Division in J-PARC and of the neutron scattering project in the new generation batteries project (RISING) of the New Energy and Industrial Technology Development Organization (NEDO). He is an adviser to iMATERIA, the Ibaraki prefecture materials diffractometer, and a leader of development of the neutron powder diffraction data analyses software suite, Z-Code, for all powder diffractometers at J-PARC.

MY EXPERIENCE IN COLLABORATION WITH AUSTRALIAN FRIENDS IN MATERIALS SCIENCE

I will talk about my experience in collaboration with Australian friends in material science.

PROFESSOR TOSHIJI KANAYA

Professor, Kyoto University

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Toshi Kanaya has been a Professor at the Institute for Chemical Research, Kyoto University, since 2003. He obtained his PhD in polymer chemistry from Kyoto University in 1981. He is now the President of the Japanese Society for Neutron Science (JSNS). His research interests are in soft matter science, in particular polymer science, using quantum beams such as neutrons and synchrotron X-ray radiation.

ABSTRACT

It is well known when polymers are crystallised under flows they show a very different morphology from that in quiescent crystallisation: the so-called shish-kebab structure, which consists of extended chain crystal (shish) and folded chain lamella crystals (kebabs) periodically attached along the shish. This structure is believed to be a structural origin of ultra-high modulus and ultra-high strength fibres. Therefore, extensive studies have been made on the shish-kebab structure, however its formation mechanism is still not clear. In this work we have studied the role of high and low molecular weight components for the shish-kebab formation. In a previous paper, we studied the role of high molecular weight components in the shish-kebab formation using SANS and SAXS, and found that the high molecular weight components were included in the shish. However, it was reported by another research group that low molecular weight components were included in the shish more than high molecular ones, which seemed to be completely opposite to our results. In order to disclose the contradiction we have studied again the effects of high and low molecular weight components for shish-kebab formation by SANS and SAXS.

DR YUKINOBU KAWAKITA

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EDUCATION

Kyoto University, **1989** BA, **1991** MS, **1997** D. Sci.; **1997** Doctor of Science, Electronic and Atomic Structures of Liquid Tellurium Containing Alkali Elements

RESEARCH CAREER

1994–2007 Research Associate, Faculty of Science, Kyushu University; **2007–2010** Assistant Professor, Faculty of Sciences, Kyushu University; **2010–11** Researcher, J-PARC/JAEA; **2011–13** Senior Researcher, J-PARC/JAEA; **2013 – present** Section Sub-Leader, J-PARC/JAEA

ADDITIONAL POSTS

1999–2000 Alexander von Humboldt Research Fellow, Philips University of Marburg, Germany; **2002–06** Project Leader of LAM-40 instrument at KENS, KEK; **2003–10** Entrusted Researcher of JAERI and JAEA

COMPLEMENTARY USE OF NEUTRON AND SYNCHROTRON TO STUDY ON IONIC-CONDUCTORS

CuI is a typical superionic conductor where iodine ions form a f.c.c. lattice and Cu ions migrate into interstices of the I sublattice. Since the anomalous diffusion process in CuI and the related superionic conductors, including noble-metal ions, is considered as partial melting of the cation sublattice and partial solidification of anion sublattice from the liquid side, it is interesting and important to grasp characteristic partial structures from their melts. The structural model of liquid CuI and AgI obtained by the reverse Monte Carlo simulation, reproducing good X-ray and neutron diffraction data,

revealed that cations form chain-like fragments in liquid, which suggests that cations move collectively even in the liquid. To understand such anomalous diffusion in molten salt, we performed quasielastic scattering measurements by using again both neutron and X-ray. Although I have not obtained full analyses, I will discuss ionic behavior in this molten salt.

DR BRENDAN KENNEDY

Professor of Chemistry, The University of Sydney

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Dr Kennedy is Professor of Solid State Chemistry at the University of Sydney. His research covers the areas of solid state and materials chemistry and crystallographic studies of structural phase transitions. His work ranges from fundamental experimental studies of 'interesting materials' to the design and optimisation of materials for specific application. This work, which has resulted in almost 300 papers, makes extensive use of high resolution neutron and synchrotron powder diffraction. Dr Kennedy is President of the Australian Institute of Nuclear Science and Engineering and a Past President of both the Australian Neutron Beam Users Group and the Society of Crystallographers in Australia and New Zealand.

REACTOR OR ACCELERATOR? HOW I DECIDE WHERE TO TAKE MY SAMPLES

For several years I have been interested in parametric studies of structural phase transitions. For much of this work neutron diffraction is critical, since the transitions are associated with oxygen displacements. But I am spoilt for choice, there is a reactor in my 'backyard' and a spallation source in Japan and so I need to decide which facility is appropriate. Each facility has strengths and weaknesses. In this presentation I will describe results from some of our recent work on perovskites and discuss where OPAL has answered all my questions and where the spallation source is better.

PROFESSOR FRANK KLOSE

Leader, Neutron Beam Instruments Program/Major Projects, Australian Nuclear Science and Technology Organisation

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Frank Klose completed his doctorate in experimental physics at the University of Goettingen, Germany. His science specialises in magnetic nanostructures with possible applications in data storage (e.g. spintronic and multiferroic materials) using neutron and synchrotron scattering methods. Before joining the Bragg Institute/ANSTO in 2007, Frank spent most of his career as a senior scientist in major US research facilities (Argonne and Oak Ridge National Laboratories). He is now leading the Neutron Beam Expansion Program at the Bragg Institute.

OPPORTUNITIES FOR NEUTRON SCATTERING IN SPINTRONIC THIN FILM MATERIAL SCIENCE

Basic science has revealed novel magnetic materials or magnetic effects which, in principle, show promise for being deployed in future magnetic electronics or storage devices. A particularly promising area is spintronic materials. However, many of the most promising materials only work under extreme conditions such as very low temperatures or large magnetic fields. The big challenge is to understand the physics of these often artificially structured and engineered materials at the atomic or nanometer level and to make them work at room temperature. In order to characterise new magnetic properties that are often caused by interface or finite size effects, neutron scattering techniques such as polarised neutron reflectometry, SANS and diffraction are very powerful tools. These techniques have the capability for characterising the magnetic structures of artificially layered films from the micron down to the sub-nanometre scale. Despite still being a relatively 'slow' magnetic measurement technique, neutron scattering experiments are often the key to explaining the underlying physics as they provide information that is only accessible using the unique combination of properties provided by the neutron particle. This talk will review the current state of the art and present striking examples which illustrate the usefulness of neutron beams in magnetic thin film and spintronics research.

PROFESSOR GARRY MCINTYRE

Research Leader, Hard Condensed Matter, Australian Nuclear Science and Technology Organisation

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Professor McIntyre's primary responsibilities are to provide scientific and strategic leadership to the Bragg Institute scientists who conduct research in hard condensed matter using neutron scattering at the OPAL reactor, to expand the OPAL user community, and to conduct neutron search and instrumental development. He is also the coordinator of the Magnetism Project that aims to raise the awareness of the many applications of neutron scattering to the study of magnetism and superconductivity. Professor McIntyre received his PhD in physics from the University of Melbourne. After postdoctoral positions in Uppsala and Edinburgh, he joined the diffraction group at the Institut Laue-Langevin in Grenoble, became an ILL Senior Fellow in 2005, and first head of the ILL Graduate School in 2008. He moved to the Bragg Institute as Research Leader in Hard Condensed Matter in October 2010. He also holds a Visiting Professorship in Chemistry at the University of Durham.

MODERN NEUTRON LAUE DIFFRACTION: EXOTIC PHYSICS, ORGANOMETALLIC HYDRIDES AND PROTEINS

Neutron Laue diffraction has been reborn thanks largely to the success of X-ray Laue diffraction for protein crystallography at synchrotrons and to the development of efficient large-area image-plate detectors. LADI (now LADI-III) located on a cold neutron beam at the Institut Laue-Langevin in Grenoble, France, continues to push the boundaries in neutron protein crystallography, while the Laue technique with thermal neutrons is proving very successful for small-molecule crystallography on crystals frequently no larger than 0.1 mm3, first on VIVALDI at the ILL and now on KOALA on the OPAL reactor at ANSTO. This is opening neutron diffraction to fields of structural chemistry previously deemed impossible, notably the precise identification and location of hydride species in organometallics. The high-resolution volumetric view of reciprocal space is particularly advantageous in the detection of phase changes, incommensurability and twinning, but does come at a price: all scattering from the sample, inelastic as well as elastic, contributes to the observed Laue patterns. This can however reveal valuable physical information about the sample beyond the crystal structure, but careful analysis is required to extract the details in the two-dimensional projection intrinsic to Laue patterns.

PROFESSOR KIYOICHIRO MOTOYA

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1977 D. Eng. Kyoto University; **1977–84** Research Associate, Institute for Solid State Physics, The University of Tokyo; **1984–94** Associate Professor, Department of Physics, Saitama University; **1994–** Professor, Department of Physics, Tokyo University of Science

REAL-TIME OBSERVATION OF MAGNETIC STRUCTURAL CHANGE IN FRUSTRATED MAGNETS

A ternary intermetallic compound CeIr3Si2 shows successive magnetic transitions at TN1=4.1 K and TN2=3.3 K. When the sample is cooled to the LT phase, magnetic Bragg peaks corresponding to the IT phase gradually decrease with time and another group of peaks corresponding to the LT phase structure grow up. Recently, we observed a rapid time variation of the line width utilising a high resolution set-up. Based on the time variations of the amplitude and line width of the LT and IT phase signals we constructed a model for the long-time variation of magnetic structure. Immediately after the sample is cooled below TN2, the entire sample volume is divided into many magnetic domains having the IT phase structure. These domains gradually transform to the LT phase domains. This transition in a particular domain is accomplished with nucleation and growth process. The overall time constant of the transition is governed by the nucleation rate of the LT phase structure (tN) which is nearly equal to t* determined by the time variation of the amplitudes. On the other hand, the characteristic time for the growth of LT phase volume in a particular domain (tG) is much shorter than tN.

PROFESSOR YOUICHI MURAKAMI

Deputy Director, Institute of Materials Structure Science High Energy Accelerator Research Organization

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EDUCATION

1980 Osaka University, School of Engineering Science Bachelor of Engineering; **1983** Osaka University, Graduate School of Engineering Science Master of Engineering; **1985** Osaka University, Graduate School of Engineering Science Doctor of Engineering

PROFESSIONAL CAREER

1986 University of Tsukuba, Graduate School of Pure and Applied Science, Lecturer; **1987** University of Tokyo, Faculty of Science, Department of Physics, Research Associate; **1994** National Laboratory for High Energy Physics, Associate Professor; **2001** Tohoku University, Graduate School of Science, Department of Physics Professor; **2009** High Energy Accelerator Research Organization, Professor, Head of Condensed Matter Research Centre; **2012** High Energy Accelerator Research Organization, Deputy Director of Institute of Materials Structure Science, Director of Photon Factory

COMPLEMENTARY USE OF NEUTRON AND SYNCHROTRON RADIATION BEAMS

Quantum beams (photon, neutron, and muon beams) are very powerful to elucidate the materials structure, which means crystal structure as well as electronic structure. The complementary use of these probes can explore a frontier of materials science. Recent developments of synchrotron, pulse- neutron, and -muon beam technologies have really made it possible to measure static and dynamic structures of materials particularly in various disciplines. In this talk the complementary use in strongly correlated electron systems will be presented. In particular, the detection of the ordering structures of electronic degrees of freedom (charge, spin, and orbital) will be reported.

The Institute of Materials Structure Science, High Energy Accelerator Research Organization joins in the cooperative effort of the MEXT Element Strategy Initiative to Form Core Research Center for Electronic Materials (Tokodai Institute for Element Strategy: TIES). Recent results of this project will be also presented.

PROFESSOR KEITH NUGENT FAA

Deputy Vice-Chancellor (Research), La Trobe University

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Professor Keith Nugent is Deputy Vice-Chancellor and Vice President (Research) at La Trobe University as well as Professor of Physics. Prior to joining La Trobe in January 2013, Professor Nugent was Laureate Professor of Physics and Federation Fellow at The University of Melbourne as well as Director of the Australian Synchrotron. He is a Fellow of the Australian Academy of Science and of the American Physical Society. His research interests lie at the interface of physics and biology with particular interest in the coherent X-ray science and the associated possibilities offered by the new X-ray free electron laser sources operating at SLAC and SPring8, and under construction in Germany, Switzerland and South Korea.

NEUTRON AND X-RAY PHASE CONTRAST IMAGING

In the mid-1990s, with the advent of third generation synchrotron sources, it was discovered that radiographs of samples showed an interesting new form of contrast. It was realised that this contrast arises from small variations in the thickness of a sample resulting in the refraction of the incident X-rays which, after propagating some distance, is revealed as significant intensity contrast. This form of imaging is now known as propagation-based phase-contrast imaging and was a largely unanticipated discovery. Other important forms of X-ray phase-contrast imaging have subsequently been developed. As the incident photon energy increases, the importance of phase contrast relative to absorption contrast increases exponentially so that phase contrast is much better suited to harder X-rays. In 2000, it was further realised that this contrast also applies to neutrons, opening up neutron phase-contrast radiography. In this presentation, I will describe the physics of phase-contrast imaging as it applies to both X-rays and neutrons. I will show some of the latest results including insights into a diverse range of physical phenomenon from biomedical imaging through to materials science. Phase contrast imaging is a central aspect of both the Dingo facility at OPAL as well as the Imaging and Medical Beamline at the Australian Synchrotron.

DR TAKAYUKI OKU

Principal Researcher, Japan Atomic Energy Agency

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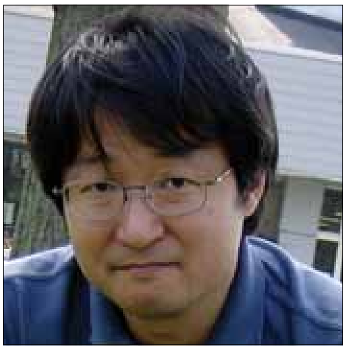
Takayuki Oku is the Principal Researcher at the Japan Atomic Energy Agency. He is a sub-leader of the Technology Development Section, Materials and Life Science Division, J-PARC Center. Dr Oku has more than 15 years experience of experimental work on neutron optical device development and small-angle neutron scattering (SANS). So far, he has developed sextupole magnet-based neutron lenses and quadrupole magnet-based neutron polarisers, and succeeded in applying them to SANS instruments for steady and pulse neutron sources. He is now engaged in the development of 3He neutron spin filter for neutron scattering experiments.

DEVELOPMENT AND APPLICATION OF AN IN-SITU SEOP 3HE NEUTRON SPIN FILTER AT J-PARC/MLF

We have been developing an in-situ SEOP 3He neutron spin filter to apply it to pulsed neutron experiments at J-PARC/MLF. The 3He based neutron polariser is useful in experiments such as polarised neutron scattering experiments in a wide q-range, inelastic scattering experiment with high energy magnetic and phonon excitation, magnetic field imaging etc, since it is effective for neutrons in a wide energy range. To introduce the in-situ SEOP polarised 3He neutron spin filter into the instruments of the pulsed neutron facility such as J-PARC/MLF, it is important to make the system compact and stable, because the system is located inside thick and bulky radiation shields for high energy gamma ray and neutrons. In this study, we have developed compact laser optics with a volume holographic grating (VHG) element, and composed an in-situ SEOP 3He neutron spin filter. We have started to apply the 3He spin filter as an analyser to polarised neutron small-angle scattering and reflection measurements. In this paper, we report the design of our SEOP 3He neutron spin filter system and some results of the related polarised neutron beam experiments.

PROFESSOR TOSHIYA OTOMO



Japan Atomic Accelerator Research Complex

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1993 Doctor of Engineering from Tohoku University and Postdoctoral fellow at Institute for Material Research, Tohoku University; **1994** Research Associate, High Energy Physics Laboratory (former name of High Energy Accelerator Research Organization, KEK); **2003** Associate Professor, KEK; **2008** Professor, KEK

HIGH INTENSITY NEUTRON SCATTERING TECHNIQUES FOR HYDROGEN MATERIALS STUDIES

A neutron total diffractometer, NOVA, was constructed at J-PARC to analyse the crystalline and non-crystalline structure of hydrogen storage materials. With the world's most intense pulsed neutron source of J-PARC, NOVA realises short-time total scattering measurement and low-resolution inelastic measurement. As a total diffractometer, NOVA covers a wide momentum transfer range, 0.01 Å-1 $\leq$ Q $\leq$ 100 Å-1 (Q = 2π/d, where d is a lattice constant) in one measurement. Based on the high neutron flux of J-PARC, real-time observation of the non-equilibrium state is feasible. One of the main objects of NOVA is hydrogen storage mechanism in materials. To observe hydrogen absorption and desorption processes, in-situ sample environments such as H2/D2 gas atmosphere (up to 10 MPa, temperature range can be controlled from 50 K to 473 K) and high-temperature (up to 1373 K) have been equipped on NOVA. Based on the high neutron flux of J-PARC, the real-time observation of non-equilibrium state is feasible. Another unique feature of NOVA is a capability of inelastic measurement to study the vibrational state of hydrogen, which closely relates to bonding to surrounding atoms. Some recent results of structural analysis on NOVA will be presented.

DR VANESSA PETERSON

Principal Research and Neutron Scattering Instrument Scientist, Australian Nuclear Science and Technology Organisation

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Dr Peterson leads the Energy Materials research project at ANSTO's Bragg Institute, focused on progressing environmentally-friendly and sustainable energy technologies through the use of neutron-scattering tools and expertise. The research is aimed at understanding and developing battery and fuel-cell materials, and porous framework materials for the capture and conversion of gases such as hydrogen and carbon dioxide. Dr Peterson is co-responsible for the Wombat and Echidna neutron powder diffractometers at the Bragg Institute.

IN SITU ANALYSIS OF ENERGY MATERIALS AT THE BRAGG INSTITUTE

Creating a global energy system that is both environmentally and economically sustainable is one of the largest challenges facing scientific and engineering communities. Alternative energy sources, new materials, and gas separation and sequestration technologies have risen as a result of the combined needs for energy and environmental sustainability. Neutron scattering represents a wide range of analysis techniques that have made important contributions to each of these areas. The Energy Materials project is a formal research project at the Bragg Institute focused on progressing new sustainable energy technologies through the coupling of neutron-scattering tools and experts at the Bragg Institute with external collaborators. Of experimental importance in such studies is the examination of materials while they are functioning, with both equilibrium and non-equilibrium studies being made. Non-equilibrium studies give detail that is representative of the real-world working conditions of the material, but are difficult to realise experimentally. Examples of recent neutron powder diffraction studies made by the Energy Materials research project on equilibrium and non-equilibrium systems will be presented. Examples will be taken from the project's two main research areas, materials being used for the separation and storage of gases of use in the energy sector, including hydrogen, carbon dioxide, and oxygen, as well as materials for use in batteries.

PROFESSOR FRANCES SEPAROVIC FAA

Head of School of Chemistry, The University of Melbourne

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Professor Separovic is a biophysical chemist who specialises in NMR spectroscopy, teaches chemistry, and is Head of School of Chemistry, with her lab based at the Bio21 Institute, The University of Melbourne. She has developed solid-state NMR techniques to determine the structure and dynamics of membrane components in situ, specialising in peptide antibiotics and toxins in phospholipid bilayers. As well as serving as General Treasurer of the Royal Australian Chemical Institute, she was elected to the Council of the Biophysical Society (US), the Council of the International Union for Pure and Applied Biophysics, President of the Australian Society for Biophysics, President of the Australian New Zealand Society for Magnetic Resonance; and is an editorial board member of *Accounts in Chemical Research* and editor of *Biochimica Biophysica Acta* and *European Biophysics Journal*. Professor Separovic was awarded the ASB Robertson Medal, the ANZMAG Medal and elected Fellow of the Biophysical Society (US), an ISMAR Fellow, and a Fellow of the Australian Academy of Science.

STRUCTURAL EFFECTS OF ANTIMICROBIAL PEPTIDES ON SUPPORTED LIPID BILAYERS

The membrane interactions of the antimicrobial peptides aurein 1.2 and maculatin 1.1 have been studied using a range of biophysical techniques to determine the location and mechanism of action in DMPC (dimyristoylphosphatidylcholine) and DMPC/DMPG (dimyristoylphosphatidylglycerol) model membranes that mimic characteristics of eukaryotic and prokaryotic membranes, respectively. Neutron reflectometry, solid-state NMR and dual polarisation interferometry revealed subtle changes in membrane structure caused by the peptides. Quartz crystal microbalance with dissipation, vesicle dye leakage and atomic force microscopy measurements were used to investigate the global mode of peptide interaction. Aurein 1.2 displayed an enhanced interaction with the anionic DMPC/DMPG membrane while exhibiting primarily a surface interaction with both types of model membranes, which led to bilayer disruption and membrane lysis. The mode of action is consistent with the carpet mechanism for aurein 1.2. In DMPC bilayers, maculatin 1.1 displayed a concentration dependent binding and an increasing perturbation of bilayer order. Maculatin 1.1 interacted more strongly with mixed DMPC/DMPG bilayers with retention of bilayer lipid order and structure, consistent with pore formation. These results emphasise the importance of membrane charge in mediating antimicrobial peptide activity and highlight the importance of using complementary methods of analysis in probing their mode of action.

PROFESSOR HIDEKI SETO

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Dr Seto received his PhD from Osaka University in 1989. **1989–2002** Research Associate, Faculty of Integrated Arts and Sciences, Hiroshima University; **2002–08** Associate Professor, Department of Physics, Kyoto University; **2008** Professor, Institute of Materials Structure Science (IMSS), High Energy Accelerator Research Organization (KEK); **2009–12** Head of Neutron Science Division, IMSS, KEK; **2010** Deputy Division Head, Materials and Life Science Experimental Facility, J-PARC; **2013** Deputy Director, IMSS, KEK

RECENT ACTIVITIES ON SOFT MATTER IN J-PARC

Soft matter is a subfield of condensed matter comprising a variety of physical states that are easily deformed by thermal stresses or thermal fluctuations. They include liquids, colloids, polymers, liquid crystals, amphiphilic molecules, and a number of biological materials. These materials often self-organise into mesoscopic structures that are much larger than the microscopic scale, and yet are much smaller than the macroscopic scale of the material. The properties and interactions of these mesoscopic structures may determine the macroscopic behaviour of the material. In spite of the various forms of these materials, many of their properties have common physicochemical origins, such as a large number of internal degrees of freedom, weak interactions between structural elements, and a delicate balance between entropic and enthalpic contributions to the free energy. These properties lead to large thermal fluctuations, a wide variety of forms, sensitivity of equilibrium structures to external conditions, macroscopic softness, and metastable states.

Because the main elements of soft matter are light atoms such as hydrogen, carbon, nitrogen, etc., neutron is one of the most powerful tools to investigate structural and dynamical properties of soft matter. In this respect, various kinds of experiments on soft matter are conducted in J-PARC/MLF.

PROFESSOR MITSUHIRO SHIBAYAMA

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PRESENT POSITION

Director, Neutron Science Laboratory, The Institute for Solid State Physics, The University of Tokyo

EDUCATION

Kyoto University, 1977, BA, 1979, MS., 1983, D. Eng.

RESEARCH CAREER

1983–84 Research Associate, (Polymer Research Institute, University of Massachusetts, US; **1984–2000** Associate Professor, Professor, Department of Polymer Science and Engineering, Faculty of Textile Science, Kyoto Institute of Technology; **2000 – present** Institute for Solid State Physics, The University of Tokyo

HONOURS

Sakurada Takeshi Memorial Award, The Society of Fiber Science and Technology, Japan, **1991**; Wiley Polymer Science Award, The Society of Polymer Science, Japan, **2000**; The Chemical Society of Japan Award for Creative Work, **2004**; The Award of the Society of Polymer Science, Japan, **2010**; Paper Award, Physical Society of Japan, **2012**

RESEARCH ACTIVITY AND JOINT-USE PROGRAM OF THE INSTITUTE OF SOLID-STATE PHYSICS, THE UNIVERSITY OF TOKYO

The Neutron Science Laboratory (NSL) has been playing a central role in neutron scattering activities in Japan since 1961 by performing its own research programs as well as providing a strong General User Program for the university-owned various neutron scattering spectrometers installed at the JRR-3 (20MW) operated by the Japan Atomic Energy Agency (JAEA) in Tokai. In 2003, the Neutron Scattering Laboratory was reorganised as the Neutron Science Laboratory to further promote neutron science with use of the instruments in JRR-3. Under the General User Program supported by NSL, 14 university-group-owned spectrometers in the JRR-3 reactor are available for a wide scope of research on materials science, close to 300 proposals are submitted each year, and the number of visiting users under this program reaches more than 6000 person-day/year. In 2009, NSL and Neutron Science Laboratory (KENS), High Energy Accelerator Research Organization (KEK) built a chopper spectrometer, High Resolution Chopper Spectrometer, HRC, at the beamline BL12 of MLF/J-PARC. HRC is complementary to the existing inelastic spectrometers at JRR-3.

The current status of JRR-3 and the research activities of the General User Program will be reported with an emphasis on the future direction of the program.

DR JUNICHI SUZUKI

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Dr Suzuki joined the Japan Atomic Energy Research Institute as a researcher in 1992 and since then has been mainly working in the area of development and application of SANS instruments at the JRR-3 and at the MLF at the Japan Proton Accelerator Research Complex. Dr Suzuki has contributed to the development of neutron optical devices such as magnetic neutron lenses and applied them to SANS instruments. He has also studied magnetic materials, superconducting materials, and alloys including steels and is responsible for the small and wide angle neutron scattering instrument TAIKAN at the MLF.

DEVELOPMENT OF THE SMALL AND WIDE ANGLE NEUTRON SCATTERING INSTRUMENT TAIKAN AT J-PARC

The design and performance of the small and wide angle neutron scattering instrument (TAIKAN) at the Materials and Life Science Experimental Facility (MLF) at the Japan Proton Accelerator Research Complex (J-PARC) will be introduced. A time-of-flight (TOF) small angle neutron scattering instrument with a pulsed neutron source generally offers a wide simultaneous q range with high q resolution, but TAIKAN, with an intense pulsed neutron source and a wide angle detector, is offering a very wide q range (q ~ 0.0005-20A-1) with high q resolution.

PROFESSOR ATSUSHI TAKAHARA

Professor and Director, Kyushu University

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Professor Takahara earned his DEng (1983) in the field of polymer science. He worked at the Faculty of Engineering, Kyushu University, as an Assistant Professor and then Associate Professor from 1983 to 1999. He was a full Professor of IFOC, Kyushu University, from 1999 to 2003. Since 2003, he has been a Professor at the Institute for Materials Chemistry and Engineering, Kyushu University. He is an associate editor of *Polymer* journal and has served as editorial board member of several international journals, including *Progress in Polymer Science* and *Biointerphases*. From 2005 to 2008, and 2011 to the present, he has been elected as a member of the Science Council of Japan. From 2013, he has been a director of the Institute for Materials Chemistry and Engineering, Kyushu University. His research interests are focused on polymer surfaces and interfaces, polymer nanocomposites, and development of new techniques for polymer surface characterisation.

ABSTRACT

Neutron reflectivity (NR) measurement is one of the most powerful tools for characterising soft materials interfaces. The authors have installed a horizontal-type time-of-flight neutron reflectometer SOFIA at J-PARC. The performance of NR was confirmed by measuring the NR of deuterated polystyrene (d-PS) thin films on a silicon wafer and multilayers of cadmium stearate prepared by the Langmuir-Blodgett method. NR at the deuterium oxide (D2O)/silicon disk showed specular reflection down to 10–6–10-7 and q up to 2.0 nm–1, which improved the precise structure analysis of swollen polyelectrolyte brush at the D2O interface. The salt-concentration dependences of the chain dimensions and swollen brush structures of polyzwitterions, namely poly(2-methacryloyloxyethylp hosphorylcholine) (PMPC) and poly[3-(N-2-methacryloyloxyethyl-N,N-dimethyl) ammonatopropanesulfonate] (PMAPS) in aqueous solutions of various ionic strengths were characterised by atomic force microscopy (AFM), and NR. AFM and NR measurements showed the independence of NaCl concentration of the swollen thickness of the PMPC brush in aqueous solution, and significant changes in the swollen thickness of the PMAPS brush in aqueous NaCl solution.

PROFESSOR JILL TREWHELLA

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Jill Trewhella is a Professor in the School of Molecular Bioscience and Deputy Vice-Chancellor (Research) at the University of Sydney. As DVC Research (since 2009) she has overseen the development of major cross-disciplinary research initiatives; such as the Charles Perkins Centre that focuses on preventing and alleviating the impacts on individuals and communities of the increasing incidence of obesity. She earned BSc and MSc degrees in mathematics and physics (UNSW) and a PhD in Chemistry (The University of Sydney) before moving to the US for 25 years where she held significant leadership positions while pursuing her research. She was the founding Leader of the multi-disciplinary Bioscience Division at Los Alamos, with more than 300 researchers working on projects such as the Human Genome Project, Structural Genomics of TB, the HIV/AIDS Gene Data Base, and NIH research resources for flow cytometry and stable isotopes. She returned to Australia in 2005 as an ARC Federation Fellow having gained international recognition for her contributions to our understanding of biomolecular signalling.

NEUTRON CONTRAST VARIATION: A POWERFUL TOOL FOR STUDYING BIOMOLECULAR COMPLEXES

Neutron scattering and contrast variation are powerful methods that can contribute to our understanding of the structures of biomolecules, especially biomolecular complexes and assemblies. Since the mid-20th century, structural biology has evolved from focusing on understanding the chemistry underpinning biological processes such as enzyme activation, recognition, and

binding to seeking to understanding how assemblies and networks of biological molecules act in concert to accomplish biological outcomes such as protein synthesis, movement in muscle cells, and replication. This talk will focus on contributions of neutron scattering and contrast variation to studies of regulatory proteins, the complexes they form and how these results have contributed to our understanding of biological function. Examples will be highlighted to stimulate discussion of future challenges in structural biology where neutrons and contrast variation can contribute.

PROFESSOR GREGORY WARR

Professor of Chemistry, The University of Sydney

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Professor Gregory Warr is Professor of Physical Chemistry at The University of Sydney, and was Head of School from 2007 until March 2013. He completed his B.Sc. (Hons I) (1982) and Ph.D. (1986) at The University of Melbourne. He has held postdoctoral and visiting appointments at the University of Minnesota, Princeton University, the Centre d'Etudes Nucléaires, Saclay, the NIST Centre for Neutron Research, and the CNRS Centre de Recherche Paul Pascale in Bordeaux. He has more than 150 peer-reviewed publications, and presented his work in more than 80 seminars and conference papers around the world. He is a former chair of the RACI Colloids Division, and has served on the Editorial Advisory Boards of *Langmuir*, *The Journal of Colloid and Interface Science*, and *The Australian Journal of Chemistry*. He collaborates with researchers in Australia, Japan, France, the USA, and Sweden, focusing on using neutron beam techniques to understand structure in soft matter systems.

NEUTRON SCATTERING STUDIES OF IONIC LIQUID NANOSTRUCTURES

Ionic liquids (ILs) have become objects of great interest over the past decade or so. Spanning applications from catalysis and synthesis to heat transfer and lubrication, as solvents for novel synthetic and biological polymers, ILs seem to be invading all facets of the chemical and physical sciences. Recently, a number of studies have revealed new insights into the structure of ionic liquids and their solutions.

This talk will discuss the use of neutron scattering techniques to elucidate the bulk structure of ILs themselves, as well as increasingly complex mixtures and solutions with ILs as critical components. These include simple solutes and water-IL mixtures, homo- and amphiphilic polymers, as well as a variety of surfactant self-assembly phases including micellar solutions, microemulsions and lyotropic liquid crystals.

PROFESSOR JOHN WHITE FAA FRS

Professor, Research School of Chemistry, Australian National University

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Professor White is acknowledged for his development of neutron contrast variation in structure determination. His current work is in 'pillared' graphite intercalation compounds and the fundamentals of nano-toxicology. In the first, the objective is to cheaply store hydrogen, and in the second to understand the chemical and physiological properties of the 'nanoparticle-corona' – proposed as the means of facilitated entry of nanoparticles into cells. Professor White is currently a Distinguished Visiting Professor at the CSIRO and Professor of Chemistry at the Australian National University. He has been Director, Institute Laue-Langevin, Grenoble, France; Pro-Vice Chancellor and Chair, Board of the Institute of Advanced Studies, Australian National University (ANU); Chairman, Oxford-Australia Scholarships Committee; Chairman, International Advisory Committee, J-PARC Project, Tokai, Japan. President, Royal Australian Chemical Institute (RACI); President Australian Institute of Nuclear Science and Engineering (AINSE); President Asia-Oceania Neutron Scattering Association ,(AONSA). Recent recognition of the work includes the Leighton Medal (RACI) 2005; Craig Medal – Australian Academy of Science 2006; Founder's lecturer St Johns College, Oxford 2007; Liversidge Lecture (Royal Society of NSW) Sydney 2010; and Kashiwa Lecture Tokyo University 2011.

SUSTAINABLE COOPERATION IN OUR REGION

About $US1.5 billion has been spent on new neutron sources in Asia-Oceania over the past 10 years – chiefly in Japan, Australia, Korea and China. Many other countries have high capability also. These sources have diverse applications. The Asia-Oceania region now closely resembles that in Europe in 1970 when the Institut Laue Langevin, ILL, was built in Grenoble by the French and German governments as a symbol of amity. That multinational institute is now the world leader in using neutron scattering for physics, chemistry, biology, materials science and engineering. Our region's very modern facilities provide the opportunity to rank equally with ILL in science and technology using nuclear methods and the same strategic possibilities to bring together, in a sustainable and lasting way, our scientists and nations as happened after 1970 for the European Scientific Community. The Asia-Oceania Neutron Scattering Association (AONSA) and the Facility Directors have established a working relationship to support this long-term collaboration. The lecture will identify national and international 'drivers' for such collaboration, the likely outcomes and some principles to ensure sustainability.

DR MASATOMO YASHIMA

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Professor Yashima has been a Professor in the Department of Chemistry and Materials Science at the Tokyo Institute of Technology since April 2011. Professor Yashima received a BS in physics from Tsukuba University in 1986 and obtained a PhD in materials science and engineering from the Tokyo Institute of Technology in 1991. He was a Research Associate of Titech from 1991–97 and an Associate Professor of Titech from 1997 to March 2011. His current research interests: precise crystal structure analysis with high-temperature neutron and synchrotron powder diffraction, electron/nuclear density analysis and design of inorganic crystalline materials (ionic conductors, catalysts, ferroelectrics, photocatalysts, and biomaterials). He has published more than 490 papers, including more than 185 original research papers (cited more than 5102 times, ISI, October 3, 2013). He has received 17 awards including the Award of the Ceramic Society of Japan (2009) and the Award of the Crystallographic Society of Japan (2008).

PRECISE CRYSTAL-STRUCTURE ANALYSIS OF ION-CONDUCTING CERAMIC MATERIALS AND OXYNITRIDE PHOTOCATALYSTS BY NEUTRON POWDER DIFFRACTION

We review our recent work on the visualisation of diffusional pathways of mobile ions and chemical bonding in ceramic materials through neutron and synchrotron powder diffraction experiments of ceramic materials. Crystal structure and oxide-ion diffusional pathways of $PrBaCo_2O_{5+\delta}$ at 1000 oC have been investigated by high-temperature neutron (HERMES) diffraction and maximum-entropy-method (MEM)-based nuclear-density analysis. The oxide ions of $PrBaCo_2O_{5+\delta}$ two-dimensionally and anisotropically diffuse through equatorial and deficient apical oxygen sites in Pr-Co-O ion-conducting slabs. We also report a high-temperature neutron (HEREMS) diffraction study of nano-crystalline (10.1(7) nm), compositionally homogeneous, tetragonal $Ce_{0.5}Zr_{0.5}O_2$. Contrary to the previous work, we have observed no tetragonal-to-cubic phase transition in the nano-crystalline $Ce_{0.5}Zr_{0.5}O_2$ up to 1176 K. Possible oxygen diffusion pathways along the fluorite <100> and <110> directions were visualised in the spatial distribution of bond valence sums calculated using the present refined crystal structure of nano-crystalline $Ce_{0.5}Zr_{0.5}O_2$ at 1023 K and 3DBVSMapper. Novel calcium strontium tungsten oxynitrides $Ca_xSr_{1-x}WO_2N$ ($x = 0.25$ and 0.5) have been synthesised. The existence of nitrogen in $Ca_xSr_{1-x}WO_2N$ was confirmed by the refined occupancy factor in the Rietveld analysis of neutron data measured by the Echidna diffractometer@ANSTO. We acknowledge the co-authors and great help in the neutron works at ANSTO, JRR-3, J-PARC and HANARO.

EARLY AND MID CAREER RESEARCHERS

DR SARA CALLORI

Postdoctoral Research Fellow, Australian Nuclear Science and Technology Organisation

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Dr Callori is a joint postdoctoral research fellow at the Bragg Institute at ANSTO and at the University of New South Wales. Her current research focuses on the investigation of magnetic thin films and multilayers using neutron scattering techniques. She earned her PhD in May 2013 at Stony Brook University in New York, US. Her dissertation work concentrated on the growth and characterisation of ferroelectric heterostructures, namely the comparison of PbTiO3 based heterostructures with conventional and novel dielectric components. In addition to research, she is also interested in physics education and outreach.

DR MOHAMMAD CHOUCAIR

Research Fellow, The University of Sydney

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Dr Choucair is currently a Research Fellow of the School of Chemistry at The University of Sydney. He previously held an Experienced Researcher role within the Department of Physics in Parma University, Italy, before moving to The University of Sydney. He was awarded the Cornforth Medal in 2011 and is currently a Chartered Member of the Royal Australian Chemical Institute, recently being elected to the RACI NSW Branch Committee. Dr Choucair's researched is focused on the physical chemistry of carbon nano-materials.

DR JOHN DANIELS

Senior Lecturer, the University of New South Wales

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Dr Daniels is in the School of Materials Science and Engineering at UNSW as a Senior Lecturer and Australian Institute of Nuclear Science and Engineering research fellow. He was awarded his PhD in 2007 from the School of Physics at Monash University, Melbourne, for work in the field of time-resolved neutron scattering in ferroelectric materials. After his PhD, he spent three years as a postdoctoral researcher within the Structure of Materials group at the European Synchrotron Radiation Facility, Grenoble, France. During this time he specialised in the application of high-energy X-ray scattering techniques to the study of functional and mechanical properties of materials, in particular electro-ceramics.

DR TAMIM DARWISH

Team Leader: Chemical Deuteration, Australian Nuclear Science and Technology Organisation

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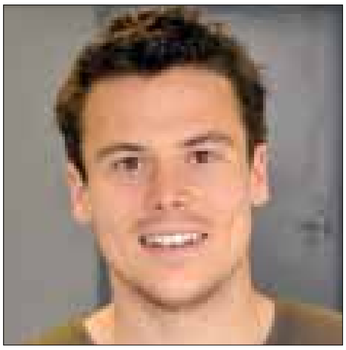
Dr Darwish leads the chemical deuteration team at the National Deuteration Facility at ANSTO. In 1998, he graduated with a Maîtrise degree in chemistry from the Lebanese University Beirut. In 2006, he obtained his PhD degree in chemistry from the University of New South Wales, Australia. Subsequently, he undertook postdoctoral appointments at The University of Sydney and then at the Institute of Materials Engineering at ANSTO. In 2010 he received an invitation fellowship from the Japan Society for the Promotion of Science. His research interests are in developing new methods for the synthesis and characterisation of deuterium labelled compounds for neutron scattering, NMR, IR and other techniques.

MR TERENCE HARTNETT



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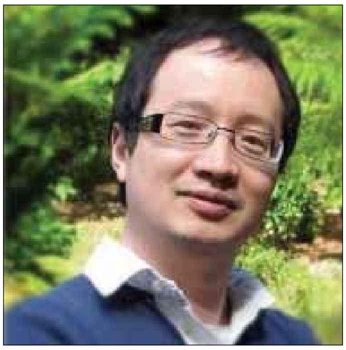
Mr Hartnett is a PhD student working in The University of Melbourne and CSIRO collaboration on biomaterials. In early 2013, he visited the SOFIA beamline at the Materials and Life Science Experimental Facility (MLF) in Tokai-Mura, Japan, to conduct experiments designed to improve understanding of the phase behaviour of thin-film lyotropic liquid crystals. His wider PhD project focuses on finding solutions to drug delivery problems in the treatment of macular degeneration and investigates the use of self-assembled nanoparticle drug delivery systems for the delivery of bioactive therapeutics to the posterior segment of the eye.

DR LIZHONG HE



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Dr He is a Senior Lecturer at the Department of Chemical Engineering, Monash University. He completed his Bachelor of Science in applied chemistry and Master of Engineering in biochemical engineering at Tianjin University, China. He then carried out his PhD research at GKSS Research Centre, Germany, working on self-assembly and affinity adsorption of glycoconjugates. Dr He spent two years as a postdoctoral researcher at the Max-Planck-Institute for Polymer Research. Before joining Monash University, he was an AINSE Research Fellow and Deputy Director at the Centre for Biomolecular Engineering, Australian Institute for Bioengineering and Nanotechnology, at The University of Queensland.

DR RICHARD MOLE

Instrument Scientist: Pelican, Australian Nuclear Science and Technology Organisation

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Dr Mole completed a PhD in inorganic chemistry at the University of Cambridge in 2006. This focused on studying a series of molecule based magnetic systems with a range of complementary techniques including amongst others elastic and inelastic neutron scattering. He subsequently moved to the FRM II in Munich where he worked on the thermal neutron triple axis spectrometer PUMA. Finally he moved to his current position at ANSTO in late 2010 where he is co-responsible for the cold neutron time-of-flight spectrometer, Pelican. He has a strong interest in instrument development, in particular in looking at focusing methods that allow the study of small samples and the use of polarised neutron techniques. His current research interests are in the field of molecular magnetism; in particular applications of neutron scattering techniques to complex systems including lanthanide based single molecule magnets and switchable porous magnetic networks.

DR ANNA PARADOWSKA

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Dr Anna Paradowska is co-responsible for the KOWARI Strain Scanner at ANSTO. The main focus of her research activities are in residual-stress analysis using neutron and synchrotron X-ray diffraction with the goal of relating them to manufacturing procedures and integrity requirements for various types of engineering components. Additionally she has a strong interest in neutron in-situ study of thermo-mechanical properties of engineering materials and engineering application of imaging diffraction techniques.

DR KIRRILY RULE

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After completing her PhD from Monash University with Trevor Hicks in 2004, Kirrily undertook a postdoctoral fellowship in Canada with Bruce Gaulin investigating frustrated pyrochlores. She then spent six years at the Helmholtz-Zentrum-Berlin as instrument scientist on the cold neutron TAS, Flex. In 2012 Kirrily returned to ANSTO as an instrument scientist on Taipan, the thermal TAS. Kirrily's current research includes using neutron scattering techniques, coupled with extreme environments (high magnetic fields and low temperatures) to investigate novel and low dimensional magnetic materials. Right now her focus is on spin = ½, quantum magnets – particularly the natural minerals azurite and linarite.

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Dr Sani obtained his Masters in physical-chemistry science with distinctions at the University of Bordeaux. He moved to Sweden to complete a co-tutoring PhD held in the Department of Chemistry at the University of Umea. After receiving his PhD in November 2008, in 2009 he moved to Australia in Professor Frances Separovic's group at The University of Melbourne. His field of expertise is biophysics with special interest in biological solid-state NMR spectroscopy, with the aim to develop in situ techniques to study living cells and elucidate the role of membrane lipids in the molecular mechanism of diseases.

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Dr Petra Ágota Szilágyi received her PhD in 2007 from the University Eötvös Loránd (Budapest, Hungary) and the University Paul Sabatier (Toulouse, France). Since then she has worked as a postdoctoral fellow at the Laboratory of Coordination Chemistry of the CNRS (Toulouse, France), Edinburgh University (Edinburgh, UK) and the Delft University of Technology (Delft, the Netherlands). She is currently a lecturer at Curtin University. She has authored and co-authored more than 20 manuscripts. Her current research interest lies in the application of coordinate compounds for energy conversion and storage.