Newsletter

Neutron Scattering Grou

IOP Institute of Physics | RSC | Advancing the Chemical Scie

October 2017

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NEWS

The prestigious ***BTM Willis*** neutron prize awarded to Dr Andrew Seel for his contributions to neutron scattering and studies of "beautiful" metal-amine solutions

This week saw the prestigious BTM Willis prize for outstanding neutron scattering science awarded to Dr Andrew Seel, from the University of Oxford and UCL. The prize is jointly awarded by the Royal Society of Chemistry and the Institute of Physics Neutron Scattering Groups to an early career researcher addressing a significant problem in physical, life or engineering science, or in recognition of a major development in a neutron scattering technique. Dr Seel is recognised in both these categories – he was instrumental in the further development and expansion of mass-resolved neutron spectroscopy in the chemical sciences, and he has used a wide range of neutron techniques to study a group of functional materials known as metal-amine solutions.

Dr Ian Tucker is the Chair of the IOP Neutron Scattering Group and presented the award to Dr Seel at the UK Neutron and Muon Science and User Meeting in Warwick. He says, "This was a remarkably difficult year for the committee as there were some outstanding applicants. However the committee's decision was unanimous and I am delighted to present Andrew with this award. His nomination was unique in that he could be equally recognised for his science and for his contributions to the neutron and muon techniques – very well deserved!"

Dr Seel completed both his undergraduate degree and DPhil at the University of Oxford under the supervision of Prof Peter Edwards FRS, before becoming an instrument scientist on the VESUVIO instrument at the ISIS Neutron and Muon Source. Here he was at the forefront of the development of DINS. Prof Neal Skipper from University College London nominated Andrew for the award. He says, "Andrew really helped to widen the application of this technique – for example via mass selective measurements – and to extend its use beyond studying quantum behaviour in the lightest elements to heavier elements such as lithium. Alongside this his research has exploited a wide range of neutron techniques, most recently to shed new light on the mechanisms behind electron localisation/delocalisation and trapping in new phases of metal-amine systems."

Dr Seel's recent paper these metal-amine systems was published in the journal Angewandte Chemie. Metal-amines solutions have a fascinating history. These strikingly colourful liquids were discovered by Sir Humphry Davy in 1808. Ammonia and amines are hydrogen-based solvents with a unique ability to accommodate high concentrations of metal solutes. They display some unusual characteristics, as Davy discovered while using a potassium-ammonia solution. He found that a concentrated potassium-ammonia solution has a striking bronze/gold appearance, whilst a more dilute solution has an intense blue colour. There is also a large increase in volume with metal concentration, meaning that, extraordinarily, a more concentrated solution will float above a more dilute one.

Metal-amine liquids are also remarkably tuneable – by varying the electron density it is possible to causes the solution to change from an electrolyte to a liquid demonstrating genuine metallic behaviour. Not only that the chemical properties can be tuned by varying the amine and metal used. In the 1940s, R. A. Ogg claimed to have discovered evidence of high-temperature superconductivity in glassy metal-amine solutions, although his results have never been consistently replicated.

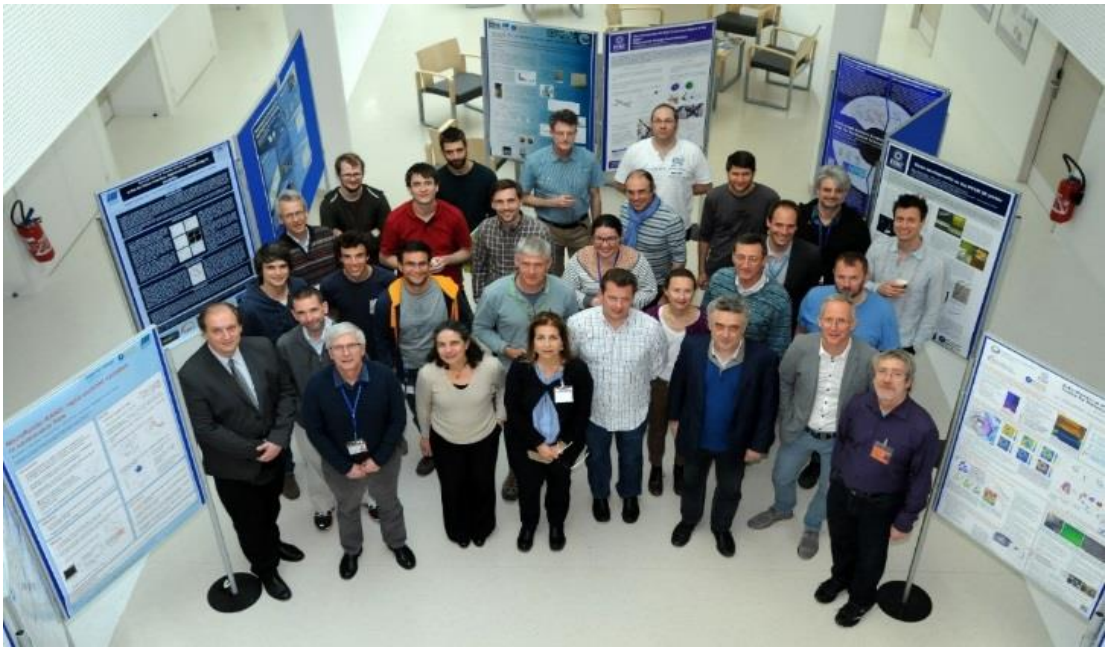
As part of the award Dr Seel presented at the NMSUM conference on the challenges of working with metal-amine solutions, and where he hopes the research will lead – including the potential to prove Ogg right in providing a new route to high temperature superconductors! He says, “The conference was a fantastic experience and I am genuinely honoured to receive this award. None of this work could have been done without the support of ISIS. Work of this exploratory nature, from someone in their early stages of their career required a real leap of faith on behalf of ISIS. Their confidence in my work and the supportive nature of the facility is what made this possible. I hope I can build on this work to develop our fundamental knowledge of these beautiful liquids and help us realise their full potential!”

Focus: Soft Matter at the ILL

1. Update on the facilities in the Partnership for Soft Condensed Matter

Report by Y. Gerelli/Institut Laue-Langevin

www.epn-campus.eu/users/pscm & gerelli@ill.eu



The Partnership for Soft Condensed Matter (PSCM) is a joint initiative established by the Institut Laue-Langevin (ILL) and the European Synchrotron Radiation Facility (ESRF) in Grenoble, France.

The main PSCM mission is to provide enhanced support services to ILL and ESRF users who address contemporary challenges in Soft Matter research including nanomaterials, environmental and energy sciences, biotechnology and related fields. Currently the PSCM offers access to 13 laboratories hosting 25 major pieces of equipment as well as distinct ILL and ESRF sample preparation facilities. Recently the PSCM instrumental suite was expanded by the incorporation of the ESRF-AFM platform and with the acquisition of a gas chromatography setup as well as of a zeta-sizer apparatus.

In addition to normal users operations, five long-term partnership programmes, devoted to the collaborative development of specialized sample environments and instruments, are currently established with University of Göttingen (DE), Technical University of Berlin (DE), Imperial College London (UK), University of Paderborn (DE) and University of Natural Resources and Life Sciences of Vienna (AT).

Examples of partner-driven science supported by the PSCM include complex self-assembly phenomena in polyelectrolyte–surfactant mixtures, a novel texture analysis method for nanocomposite materials, a multi-technique study of keratin bundles in cells, and the development of microfluidic devices for studies of complex fluids.

In 2017, the PSCM was subject to the first 5-year review conducted by a Panel of 4 experts from France, United Kingdom, Sweden and Italy, and recommendations from the Panel will serve as guidelines for the renewal of the 5-year agreement!

Focus: Soft Matter at the ILL

2. Advances in lipid deuteration and more realistic model membranes

Report by R. Morrison/Institut Laue-Langevin

www.sine2020.eu & morrison@ill.eu

As part of the SINE2020 grant, the ILL has employed a post-doctoral researcher, Rachel Morrison, to optimize the production of deuterated lipids for the re-creation of more realistic model membranes for use in neutron experiments.

Deuteration offers increased scattering contrast for neutron measurements. However, biologically relevant, deuterated lipids are difficult to synthesis chemically due to unsaturated fatty acid chains. At the PSCM, and with the help of the ILL's Deuteration Laboratory, we are investigating methods for the biological production, purification and analysis of deuterated lipids.

Deuterated lipids can be obtained by adapting organisms to grow on perdeuterated media. Using this approach, we have shown that yeast (Pichia Pastoris) lipid extracts contain similar phospholipid classes but altered fatty acids profiles when produced under deuterated conditions. We are currently optimizing growth conditions to ensure that hydrogenous and deuterated batches are comparable, and we are also investigating the effects of fatty acid incorporation into phospholipids with the hope to fine tune phospholipid production, for example, to obtain high yields of DOPC.

Once we have prepared the deuterated lipids, we can investigate how different lipid extraction methods affect the efficiency, lipid profiles and limit degradation of the produced lipids. We are also developing methods for the purification and analysis of the prepared lipids as well as currently optimizing the HPLC separation of lipid classes using a Diol column. Subsequent research will focus on the separation of lipids based on their fatty acid chains.

The ultimate aim of the project is for the large-scale production of purified and well-characterized deuterated lipids for use by the neutron community!

3. Current developments on the SANS instrument D11

Report by R. Schweins/Institut Laue-Langevin

www.ill.eu/d11 & schweins@ill.eu

D11 is one of three Small-Angle Neutron Scattering (SANS) instruments operated at the ILL and has been in user operation since 1972. The instrument has been continuously upgraded over the years, also with respect to sample environments. Three current sample environment projects, jointly pursued with ILL´s sample environment group, will be briefly detailed in the following.

Firstly, two new high pressure (hp) cells for SANS of solutions have been developed, one limited to 3 kbar with a large opening angle of 60° in order to illuminate fully the detector even at the shortest sample-detector distance of 1.4 m. In addition, a 5 kbar hp cell has been developed, with a restricted opening angle of 54°. Sapphire windows are used for both cells and yield a high neutron transmittance of more than 85% at 6 Å. Both have been available for hp-SANS experiments since 2016.

Secondly, a three-year project has started last year, in collaboration with TU Berlin, on a dedicated sample environment to monitor chemical reactions in-situ. A special chemical reactor with many access ports to execute in-situ complementary measurements, such as pH, turbidity and conductivity, is available. Syringe-pumps connected to the instrument control software allow automated and synchronised SANS measurements as a function of the complementary variables, and this was demonstrated for pH as proof-of-principle experiment in January 2017. In addition, an electric-field cell is currently being commissioned that will enable the alignment of lyotropic samples under an electric-field perpendicular to the neutron beam.

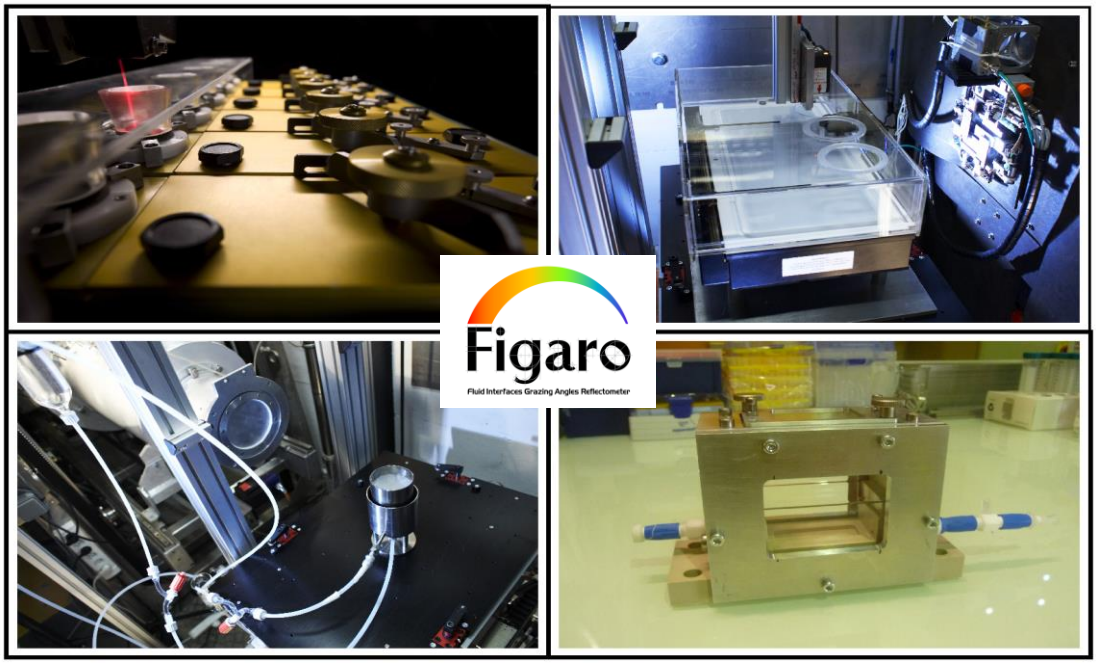
The latest project is the installation of an in-situ Dynamic Light Scattering (DLS) device, developed together with Cordouan and adapted to measure simultaneously two angles (90° and 170°) with standard cells within sample changers. The use of simultaneous SANS and DLS measurements yields complementary information: SANS enables the characterization of the size and shape, whereas DLS can be used to determine the diffusion coefficient and average hydrodynamic radius over a broad length scale from a few nanometers up to microns. The system will be available to users in 2018.

With these current developments on the ILL's most established SANS instrument, D11 is gearing up for even higher performance in the future!

4. New approach & new science from the FIGARO reflectometer

Report by R. Campbell/Institut Laue-Langevin

www.ill.eu/figaro & campbell@ill.eu



FIGARO was commissioned as a new neutron reflectometer for the study of liquid surfaces at the Institut Laue-Langevin in 2009. Since then it has gone from strength to strength as a leading experimental resource.

The instrument is both powerful and versatile. It relies on the constant high flux of neutrons from the ILL reactor and has features that allow seamless tuning of the balance between flux, resolution and dynamic range for every experiment. A combination of these options, with the highest available flux and a low incident angle, has been exploited in the study of fast kinetic processes. The surface excess of a deuterated monolayer can be determined in just one second, and this has facilitated research involving kinetic studies related to health and environment.

A brand new approach has been developed recently to resolve the interfacial composition of mixtures. First one measures the scattering excess of a macromolecule with surfactant and bulk water that are both matched in isotopic contrast to air, and then one measures an equivalent system that has deuterated surfactant. Simultaneous equations involving the two measured scattering excesses can then be solved to determine the surface excess of each component. This method has shortened the acquisition time needed to determine the interfacial composition of a mixture from around two hours to two minutes, and as the analysis does not require a structural model with some unknown input parameters it is even more accurate.

This advance has opened up research involving adsorption kinetics (e.g. peptide interactions with lipid monolayers) and film dynamics (e.g. polymer/surfactant films during repeated cycles of the surface area) that was not previously possible.

In fact this approach, unique to FIGARO at the ILL, is now being exploited by lots of user groups from the UK and other countries, which hints at the exciting scientific findings to be produced on the instrument in years to come!

Conference Report

International Soft Matter Conference in Grenoble, 12–16 September 2016

Report by G. Fragneto/Institut Laue-Langevin

www.ismc2016.org & fragneto@ill.eu

The 4th International Soft Matter Conference (ISMC2016) was held at the centre Alpes-Congrès at Alpexpo Grenoble, from 12th to 16th September 2016 under the auspices of the SoftComp consortium.

Three previous conferences were held in Aachen (2007), Granada (2010) and Rome (2013). Over those five sunny days in Grenoble, the conference has brought together nearly 700 experimentalists and theorists working in the soft matter field of which more than 200 students. Thirty-seven different nationalities were represented.

With 8 plenary and 21 keynote lectures, 116 contributed talks (selected from 800 submitted abstracts) and 480 posters, the conference has covered both the fundamental and applied aspects of soft matter and complex systems. The Institut Laue-Langevin took a leading role in the organization with ILL scientists chairing the conference and co-chairing the programme committee. Other local organisers of ISMC2016 have included scientists from the ESRF as well as from the Grenoble University and other research organisations such as CEA, CNRS, and INPG. 36 sponsors among institutions and private companies have allowed a smooth running of the programme with reasonable financial impact on the participants. The sponsorship received was very successful as compared to previous editions. In total 14 industrial companies presented themselves with booths in the central exhibition area and 6 industrial sponsors enriched the programme with the organisation of lunch seminars.

Overall, as underlined by many of the participants, the conference was a great success in terms of quality of scientific contributions, technical organisation, possibilities for discussions and exchanges, rewarding three years of hard work by the local organising committee.

A great publicity was made for the use of neutron scattering in soft matter!

Conference Report

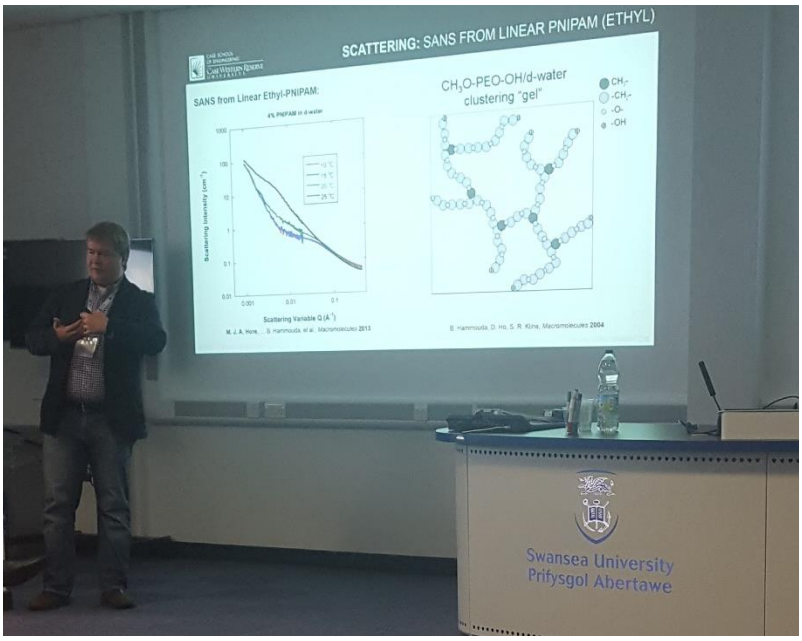
Physical Aspects of Polymer Science (Polymer Physics Group Biennial) Swansea, 13-15 September 2017;

Report by R. Thompson, Durham University **http://www.iop.org/calendar**

The polymer physics group biennial (now known as PAPS) is one of the key events in the IOP's Polymer physics group's calendar. While the focus is theory, and experimental polymer science, the contribution of neutron scattering techniques to this field was clear to see in a high proportion of the speakers' presentations. The opening session had a nanocomposites theme and most of the presentations (Clarke, Sheffield; Weir, Sheffield & Thompson, Durham) showed the value of SANS and QENS in understanding the structure and dynamics of filled polymer systems.

As well as several neutron reflection flavoured talks (Cabral, Parnell, Gutfreund, to name but a few) the poster session highlighted the many areas where neutron scattering plays an vital role, particularly for younger researchers in polymer science. This was exemplified by the excellent poster by Elizabeth Hynes on polymer/fullerene bilayers. An interesting an emerging feature is that neutron scattering is increasingly being applied to areas where restrictions on sample volume make this seem an unlikely choice. Marco Adamo (ICL) showed that SANS can now be applied to study materials in microfluidic devices.

One of the highlights of the conference was the (invited) DPOLY exchange visit lecture, given by Prof Michael Hore (pictured below), Case Western Reserve University entitled "Investigations of star, cyclic, and concatenated polymers with neutron scattering" which illustrated the fascinating insights that NS can offer on the influences of functionality and topology on solution structure.



The sun shone on Swansea Bay campus for most of the event, and what little rain came was fairly warm. Putting this event together is a colossal undertaking, and a huge "thank-you" is due to James Elliott, Joe Keddie, Michael Ries, University of Leeds, and particularly Anthony Higgins, Swansea University making it such a success. We look forward to the next PAPS meeting will be in Lincoln – September 2019.

15th Theoretical and Experimental Magnetism Meeting (TEMM), UK-Korea workshop on strongly correlated systems and IOP Magnetism-TCM joint group symposium

4-6 July 2017, The Cosener's House, Abingdon

Report by D.T. Adroja

The 15th Theoretical and Experimental Magnetism Meeting (TEMM) and UK-Korea workshop on strongly correlated electron systems was held at the Cosener's House, Abingdon UK from 5-6 July 2017. This year it was a fourth UK-Korea workshop on strongly correlated electron systems. The meeting was preceded by one day IOP Magnetism-TCM joint group symposium on 4th July 2017 and was followed by the Condensed Matter Physics in the City programme. As in the past this year's meeting was extremely successful and provided an opportunity for collaboration between top UK and Korean research groups. TEMM has become an important part of the UK and international scientific calendars for those interested in the field of magnetism. This year's two-day meeting was organised by the ISIS facility, IBS-CCES, ILL, DIAMOND, the IoP Magnetism and Neutron Scattering groups, SEPnet and the Hubbard Theory Consortium.

The meeting attracted total 110 registered participants from nine different countries. The participants included academics, senior researchers, post-doctoral fellows and PhD students. There were 25 invited talks and 8 poster presentations. In the opening session on unconventional superconductivity Prof. Toby Perring welcomed the participants. The meeting concluded with novel materials talks and opportunity for an inelastic x-ray instrument at the Diamond light source. The meeting presented an excellent opportunity to hear and discuss with leading experts from all over the world on topics of current research in magnetism. The topics included unconventional superconductivity, low dimensional and frustrated magnetism, effects of strong spin-orbit coupling, quantum spin liquids, strongly correlated electron systems, multiferroics, metal-organic frame work and skyrmions. The talks were focused on both theoretical and experimental condensed matter physics. The experimental talks were focused on neutron scattering, muon spin rotation and x-ray scattering investigations.

Events

The events listed may be of interest to NSG members. Please contact this group if you would like your event to be publicised through this newsletter.

Title & Link for more information	Date	Location
Neutrons and Global Challenges II: Health and Healthcare https://www.iopconferences.org/iop/frontend/reg/thome.csp?pageID=713867&eventID=1201&traceRedir=2&eventID=1201	9 February 2018 (Registration deadline 1 Feb)	IOP London

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If you would like to get in touch with a member of the committee please email the Science Support Officer at groups@iop.org

Newsletter Editor: Dr Richard Thompson, Please e-mail contributions for the next issue to: r.l.thompson@durham.ac.uk

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