



## FROM THE CHAIR

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Autumn 2014 Newsletter! This issue brings you a number of meeting reports, information about future events and calls for nominations for awards – I hope you enjoy browsing through it.

I would like to start by thanking the people that nominated me and then voted me in as the new Chair of the PCG-SCMP at this year's BCA spring meeting. It is a great honour and I will try to build on the great foundation my predecessors have laid down. For those of you that do not know me, I am an instrument scientist at ISIS and Diamond and I have been involved with the PCG-SCMP group off and on since I was awarded the Physical Crystallography Prize in 2006.

I would like to thank Ivana Evans for all her hard work during her time on the committee and particular during the last three years as our Chair. I will do my best to build on and not unravel her good work! I also strongly support Ivana's suggestion that we need to find new ways to make the PCG-SCMP Group the natural home for the structural condensed matter physics community, as well as for our existing membership. To this end, I would welcome any suggestion on how we might encourage engagement with the physics community.

Since our last newsletter the International Year of Crystallography has moved on and there have been several meetings not least the annual BCA Spring meeting, which I unfortunately could not attend but I enjoyed reading the review contained later in this newsletter. My personal high point so far this year was the very enjoyable 23<sup>rd</sup> congress and general assembly of the IUCr in Montreal; a view echoed by the reviews later in this issue. I think the conference really showed the strength of the physical crystallography community both by reflecting on where we have come from but also by the exciting developments that are keeping us at the heart of solving the current and future challenges that society faces as a whole.

Looking ahead to rest of this year, our Winter Meeting once again keeps the successful and popular format of the last few years, and will be held in conjunction with the ISIS Crystallography User Group Meeting, at the Cosener's House, Abingdon, 10-11<sup>th</sup> November 2014. As in previous years, the meeting will be supported by ISIS Crystallography Group and the Institute of Physics. Matthias Guttman (ISIS Facility) is in charge of putting together the scientific programme for the meeting. Some details can be found in this Newsletter, but a complete scientific programme and an online registration form will soon appear on the meeting website: <http://www.pcg-scmp.org/Meetings/Winter2014>. I hope you will be able to join us for what has become a very successful, intensive two-day meeting.

In addition to myself joining the PCG-SCMP committee as Chair there have been a couple of other changes. I'd like to thank Dave Allan who has retired from the committee following many years of service. Also I would like to formally welcome Anthony Philips (QMUL) who is now a full member of committee and treasurer of the group (having been our YCG rep) and Mark Senn (University of Oxford) as an ordinary member.

Finally, I'd like to draw to your attention to the call for nominations that is being announced in this Newsletter. Owing to the continued generous support by PANalytical, we are inviting nominations for the PANalytical Thesis Prize 2015. This year the rules have changed slightly and in particular theses from a two year period are now eligible, so we hope this will make the competition even stronger than in previous years and give more great PhD students a chance at the prize.

Matt Tucker

PCG-SCMP Chair

## ANNOUNCEMENTS

### PANalytical Thesis Prize 2015

#### Call for Nominations



The Physical Crystallography Group is pleased to invite entries for the PANalytical Thesis Prize in Physical Crystallography. The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a successfully examined thesis submitted in the period from 1<sup>st</sup> January 2013 to 31<sup>st</sup> December 2014.

To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IoP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA/PCG at the student rate to progress their nomination further (current rate £10 per annum or £35 for 4 years of the PhD degree). Please see the PCG-SCMP website ([http://www.pcg-scmp.org/Prizes#PANalytical\\_Thesis\\_Prize\\_for\\_Physical\\_Crystallography](http://www.pcg-scmp.org/Prizes#PANalytical_Thesis_Prize_for_Physical_Crystallography), [http://www.pcg-scmp.org/images/Fhj/0/0e/The\\_PANalytical\\_Thesis\\_Prize\\_rules\\_v2.pdf](http://www.pcg-scmp.org/images/Fhj/0/0e/The_PANalytical_Thesis_Prize_rules_v2.pdf)) for full details and conditions.

To enter the competition, candidates must submit:

- (a) a copy of the thesis in electronic format.
- (b) a personal statement of not more than 500 words explaining why the thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as defined on the website [www.pcg-scmp.org](http://www.pcg-scmp.org) or otherwise) in the research.
- (c) the names and contact details of two academic referees, one of whom may be the thesis supervisor, who will be able to comment on the thesis research of the candidate.

In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Nominations for the prize must be submitted to the PCG-SCMP Chair, Dr. Matt Tucker ([matt.tucker@stfc.ac.uk](mailto:matt.tucker@stfc.ac.uk)), by 31<sup>st</sup> January 2015 and the Prize will be awarded at the 2015 BCA Spring Meeting at University of York, 30<sup>th</sup> March – 2<sup>nd</sup> April 2015.

## EDUCATION AND OUTREACH

There have been a number of educational and training events that members of the PCG-SCMP community have been involved with and benefitted from (including the ISIS neutron training course, Powder diffraction and Rietveld refinement school, ISIS muon training school), please see the reports towards the end of this newsletter for a flavour of these events.

A **new film** has been launched earlier this month that “premieres the sparkling history of crystallography” (<http://www.diamond.ac.uk/Home/News/LatestNews/02-09-14.html>). It has been produced by the Diamond Light Source in collaboration with the Royal Institution of Great Britain and will be an excellent resource for education and outreach activities.

The Royal Albert Hall will soon host a **photography exhibition “Illuminating Atoms”** (4<sup>th</sup> November – 7<sup>th</sup> December) which explores the science and people behind crystallography in the UK. The exhibition aims to reflect the vibrancy of UK crystallography, featuring established scientists and young crystallographers and includes crystallography in academic and industrial settings and at central facilities. The exhibition has been very kindly sponsored by STFC, Wellcome Trust, GlaxoSmithKline, Astra Zeneca and Diamond Light Source, and we are very grateful to them for their assistance.

The photographs will be on display to concert attendees between 4<sup>th</sup> November and 7<sup>th</sup> December and there will be three open days (Saturday 15<sup>th</sup>, Sunday 16<sup>th</sup> and Saturday 29<sup>th</sup> November) for the public (including curious crystallographers!) to view portraits and reportage shot by photographer Max Alexander. A “wine and talk” evening (£10 including glass of wine, tickets available from Royal Albert Hall website soon) will take place on 9<sup>th</sup> November (in the Berry Bros & Rudd no. 3 Bar at the Royal Albert Hall) with exhibition viewing from 6pm followed by a talk (7pm) by Professor Elspeth Garman on the Braggs’ legacy and how crystallography has enabled the molecular understanding of diseases, viruses and bacteria.

It is hoped that after November, the exhibition will tour the UK – keep an eye on the BCA website and Crystallography News for details!

Claire Murray (Diamond)

It was mentioned at a recent PCG-SCMP AGM that there may be some archive material relating to the Braggs’ involvement in establishing the Physical Crystallography Group. If anyone can shed any light on this, please do get in touch ([e.e.mccabe@kent.ac.uk](mailto:e.e.mccabe@kent.ac.uk)).

## FUTURE MEETINGS

### Meeting Calendar

- PCG Winter Meeting and ISIS Crystallography Users Meeting, 10-11<sup>th</sup> November 2014, Cosener's House, Abingdon (<http://www.pcg-scmp.org/Meetings/Winter2014>)
- Solid State Group (of the Royal Society of Chemistry) Christmas meeting, 18-19<sup>th</sup> December 2014, University of Glasgow (<http://sscg2014.wordpress.com/>)
- BCA Spring Meeting, 30<sup>th</sup> March – 2<sup>nd</sup> April 2015, University of York (<http://crystallography.org.uk/bca-spring-meeting-2015-date-for-the-diaries/>), (<http://york2015.crystallography.org.uk/>)
- 12<sup>th</sup> International Conference on Materials Chemistry (MC12), 20 – 23<sup>rd</sup> July 2015, University of York (<http://www.rsc.org/ConferencesAndEvents/RSCConferences/MC12/>)

### PCG Winter Meeting, 10-11<sup>th</sup> November 2014, Cosener's House, Abingdon

Following the success of the format used the last couple of years, the PCG Winter meeting will take place at the Cosener's House, Abingdon, 10-11<sup>th</sup> November 2014 (lunchtime-to-lunchtime), in conjunction with the ISIS Crystallography Users Meeting.

Registration for the meeting is free. For participants working at UK-based research institutions who attend both meetings or the Users meeting only, the usual allowable travel costs and overnight accommodation will be reimbursed. A limited number of rooms have been pre-booked at the Cosener's House for the meeting. The rooms will be allocated on a first come first served basis.

We hope that the meeting will be of interest to a wide audience, from experienced researchers to PhD students. Following last year's success, the meeting will include a focus on the work of early career researchers so PhD students and postdocs are encouraged to submit abstracts for oral presentations.

A poster session will take place in the evening of 10<sup>th</sup> November 2014.

The full scientific programme and the timetable will be posted on the PCG-SCMP wiki (<http://www.pcg-scmp.org/Meetings/Winter2014>). To register for the meeting, please follow the link given on the website, registrations will close in late October.

### BCA Spring Meeting, 30<sup>th</sup> March – 2<sup>nd</sup> April 2015, University of York



The BCA Spring Meeting 2015 will take place from Monday 30<sup>th</sup> March to Thursday 2<sup>nd</sup> April 2015 at University of York. The PCG plenary will be given by **Prof. Tony Cheatham** from University of Cambridge, UK, and is entitled "Phase transitions in metal organic frameworks".

PCG sessions at the meeting will include:

- Beyond the elastic line –resonant and inelastic diffraction  
(Chair: Mark Senn)  
Keynote: Steve Collins (Diamond)
- Challenges and technical advances in powder diffraction  
(Chair: Paul Saines)  
Keynote: Pascal Manuel (ISIS)
- Structural insights into ferroic materials  
(Chair: Phil Lightfoot)  
Keynote: Pam Thomas (Warwick)
- Computational methods in materials discovery and crystallography (joint with CCG)  
(Chairs: John Claridge and Simon Parsons)  
Keynote: Keith Refson (STFC)
- Liquids, amorphous and nanomaterials (double session joint with IG)  
(Chairs: Christoph Salzmann and Spoorthi Dharmayat)  
Keynotes: Fiona Meldrum (Leeds) and Sam Callear (ISIS)

The deadline for abstract submission for oral and poster contributions is 12<sup>th</sup> January 2015.

The scientific programme and further details about the conference will appear at: <http://crystallography.org.uk/bca-spring-meeting-2015-date-for-the-diaries/>, (<http://york2015.crystallography.org.uk/>) .

## NEWS

### RECENT EVENTS

#### **Functional Inorganic Materials Symposium, 8<sup>th</sup> September 2014, Liverpool, UK**

On Monday 8<sup>th</sup> September the Department of Chemistry at the University of Liverpool hosted a one day symposium titled advanced inorganic materials: synthesis, processing, measurement and computation. It was chaired by Professor Matt Rosseinsky, Professor Michael Hayward and Dr John Claridge. Content covered oxide- and sulphide-based thermoelectrics, organic-inorganic perovskites, non-stoichiometric perovskites as catalysts, iron-based superconductors, spin filters, domain manipulation in ferroelectrics, and synthesis methods amongst other things. These topics were approached in terms of computational and experimental chemistry, physics and materials science by internationally leading researchers including Professors Antoine Maignan, Duncan Gregory, Aron Walsh, Simon Clarke, John Irvine, Mark Blamire, Marty Gregg and Bala Vaidhyanathan. The poster session at lunch gave the opportunity to network with attendants from 16 different universities and a number of other research institutions and businesses. The event featured some wonderful, new, thought-provoking science. It's a shame it was only the one day!

Harry Sansom (Kent then Liverpool)

#### **23<sup>rd</sup> congress and general assembly of the IUCr, 5-12<sup>th</sup> August 2014, Montreal, Canada**

This year saw my first time attending the International Union of Crystallography (IUCr) Congress and General Assembly, which was hosted by Montreal for its 23<sup>rd</sup> edition. The meeting started even before I had boarded my flight, running into David Keen and the Goodwin group at the check-in at Heathrow, and I got a small taste of the camaraderie that comes from making new friends and catching up with old ones in the crystallography community (a feeling that would last through the entire conference).

IUCr 2014 was certainly a daunting conference on paper – 7 full days featuring over 750 oral presentations and 1500 poster presentations – one of the biggest conferences I have ever been to. At the same time, it was a fantastic opportunity to hear about crystallography from a diverse set of vantage points: chemical, biological, mathematical and even astrophysical, and to see how this central scientific principle unites such a disparate group of researchers.

It is hard to do justice to the high quality of innovative and intriguing science that was presented over the week, but I will do my best to recount some personal highlights. John

Evans showed us the vast amount of information that can be derived from powder diffraction data; Branton Campbell gave an excellent overview of the use of symmetry mode analysis to analyse lower symmetry structures in terms of a higher symmetry structure's distortion modes; David Bish recounted his journey building the CheMin instrument on the Curiosity Rover that resulted in the first x-ray powder diffraction measurements on Mars; and Ray Withers gave us (in his usual entertaining style) a look into the world of modulated structures, and how sometimes you just have to get your hands dirty and diagonalise a 9 x 9 matrix yourself. There were also a large number of talks reflecting on newer ideas in the crystallography community, including quasicrystals and disordered materials, pushing the boundaries of even the very definition of crystals and order.

It wasn't all work and no play though, and in the evenings we got a chance to explore the vibrant nightlife of Montreal, including its lively Latin Quarter and Harbour districts. I also finally capitulated and tried the local delicacy of poutine, essentially a dish comprising of French fries, gravy and cheese curds, which tasted pretty much as good as it sounds (thankfully I waited until after I had given my talk to try it!).

In the end, the conference was a very rewarding experience, especially when reflecting on the friends I have made in the crystallography community from all over the world, and the truly excellent science I was exposed to. As such, I would like to thank the IUCr Congress for the award of a travel bursary to attend the conference, as well as funding from the Cambridge Trusts and Trinity College, without which I would not have been able to attend.

Matthew Dunstan (Cambridge)

It's a good thing that the IUCr Congress comes but every three years as – with over 200 hours of micro-symposia (not to mention keynotes, plenaries, workshops, and satellites!) – it is exhausting: of course in a good way! The 23<sup>rd</sup> IUCr was held in Montréal, a city with at least two must-see attractions for the structural scientist: Buckminster Fuller's geodesic dome – visible in the distance from the waterside near the conference venue; and 20,000 pink balls in The Village – a fantastic cross-over with Montréal Pride!

This being my first IUCr I was struck by the size and diversity of the meeting. As well as seeing many fantastic talks, a few of which I will mention below, the software sessions given by Branton Campbell on ISODISTORT and by Arkadiy Simonov on the diffuse scattering interpretation program Yell were both exciting and useful.

The importance of understanding local structure was a common theme in much of the physical crystallography whether for fundamental or practical interest. In the field of energy materials Phoebe Allan, among others, spoke eloquently on antimony anodes for Na-ion batteries and demonstrated the utility of PDF techniques for some extremely complicated systems. In another session, Karena Chapman gave a wide-ranging talk on developing in-situ studies of energy storage and conversion materials at the Argonne National Laboratory. Elsewhere, Marek Paściak spoke about modelling the diffuse scattering of the important relaxor and incipient ferroelectrics barium titanate and strontium titanate, respectively.

It was a great pleasure to hear the inimitable Ray Withers talk. One of the systems he spoke about in his keynote on hidden long range order in nominally 'disordered systems' were NaCl-type magnesium doped rare-earth sulfides. The signature of the 6-body correlations of one particular member of this family manifest not as 'diffuse' scattering but as sharp, continuous 3D shapes in reciprocal space – encoding both long- and short-range order in these non-Bragg features.

Alexander Shtukenberg gave an overview of some other neglected sharp 3D objects – twisted crystals. These crystals shun long-range translational order, twisting and bending as they grow. While most crystallographers would avoid such materials, Shtukenberg showed the great diversity of distortions possible as well as the beauty of the resulting crystals.

Talks were not without humour – even if sometimes lost on the international audience – perhaps most notably Phil Lightfoot double-act with Eric Morecambe explaining mode analysis of some ferroic Perovskites.

A trip to Montréal would not be complete without a serving of poutine - though perhaps not the best food to calm your nerves before giving a talk. I am very grateful to the SCMP for their support in my attendance of the 23rd IUCr Congress (through the SCMP/IOP research student conference fund). This enabled me to give a talk in MS83 entitled *Mapping topology and structural disorder in [M(CN)<sub>2</sub>] coordination polymers*. It was a great pleasure for me to present some of my PhD work at the most important crystallographic meeting and formed, I think, an important milestone in my career.

Joshua Hill (Oxford)

**Euophysical conference on defects in insulating materials (EURODIM), 13-19th July, Canterbury, UK**

The 12th Euophysical Conference on Defects in Materials (Eurodim), held at the University of

Kent in Canterbury, began on the day of the World Cup 2014 final in Brazil, and set the tone for the entire week, with very interesting talks and an enjoyable social atmosphere, with great weather for the week. The conference showed the continuing importance of defects in materials, with talks ranging from the development of phosphors, to quantum dots, from functional ferroelectrics to solar cells, and from detectors to nuclear fuel. All of these topics showed a vibrant and expansive community with great opportunities for future collaborations. Of particular note was the excursion to Whitstable where we learned all about the history and brewing of ale, of course this did lead to a few headaches the following day! The next meeting in this series (ICDIM 2016) will be held in Lyon, France in July 2016 and has a lot to beat.

Karl Whittle (Sheffield)

**British Crystallographic Association Spring Meeting, 7 – 10<sup>th</sup> April 2014, Loughborough, UK**

The British Crystallographic Association spring meeting was held at the University of Loughborough in April 2014 and showcased some of the highest quality research from within the UK and internationally. Details of some of the PCG-related sessions are given below.

The meeting began with a series of excellent talks from both invited and contributed speakers on non-ambient diffraction. Steve Hull started off the session with a talk on in-situ neutron diffraction studies of battery and fuel cell materials, providing examples of analyses performed on both electrolytes for SOFCs and rechargeable batteries, and even entire fuel cells. This was followed by Jorge Sotelo who talked about an in-situ gas adsorption X-ray diffraction study of single crystals of a Sc-based MOF. This study using high-pressure gas cells has allowed for the different gas adsorption sites in the frameworks to be determined. Gas sorption was also the theme of the third talk presented by Inigo Vitorica, this time focussing on a non-porous, crystalline silver coordination polymer. As in Jorge's talk, in-situ X-ray diffraction has allowed the adsorption properties to be studied, illustrating how adsorption can occur in spite of the presence of pore channels. Bringing the session to a close, Bill David spoke about in-situ diffraction of reversible hydrogen storage systems. These studies were performed using a combination of neutron and X-ray diffraction, and provided insight into the storage mechanisms for different types of systems, and their use in real world applications. The high quality of these talks set a good standard for the rest of the meeting, shining light on a range of different tools available to scientists for non-ambient



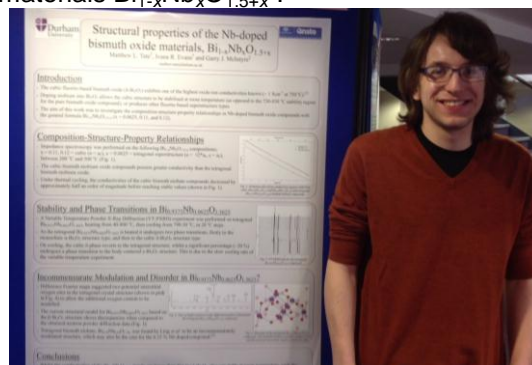
diffraction, and illustrating their potential to provide answers to some of the problems we currently face in the field.

The second session on non-ambient diffraction began with two excellent talks highlighting the different effects high pressure has on organic and inorganic materials. Andrzej Katrusiak (Adam Mickiewicz University, Poland) gave a detailed lecture on the effects of high pressure on hydrogen bonding in organic compounds. He discussed the energetics of these, including unusual results on these lengthening under compression. This was followed by a talk from Simon Parsons (University of Edinburgh) presenting some insightful research into how great the changes in bonding in coordination complexes under pressure can be; cases where either the coordination geometry or number change significantly with temperature were highlighted, as was the role of intermolecular interactions on their compressibility. The final talk in the session was given by Nick Funnell (University of Oxford) about the ferroelectric ordering of ice in an organic host with one dimensional channels, HHTP. This presented the first case of a host material in which the interactions of water molecules within a channel and between channels is balanced so that three dimensional ferroelectric order is achieved but at a temperature well below the melting point of water in the host.

This year one of the PCG group sessions was given over to a very successful and informative microsposium on magnetic structure determination. There is little consensus over the best way to describe the symmetry of a magnetic structure. Andrew Wills started the session trying to unite the two main approaches for classifying magnetic structures in the solid state, that of irreducible representation and that of magnetic space groups. He highlighted the complementarity between the two approaches and called for a unification of these “dysfunctional family members”. This was followed by two talks on systems exhibiting novel magnetic behaviour. Alex Gibbs presented work on the hexagonal perovskites  $Ba_2MTeO_6$  ( $M = Ni, Cu, Zn$ ) which have both rich magnetic and structural phase diagrams. Paul Saines presented his results on unusual dipolar mediated long range magnetic ordering in metal organic frame work materials. Paolo Radaelli brought the session to a close with a look at how practically complex magnetic structures might be used to store and retrieve information with particular emphasis on the magnetoelectric effect. He highlighted the need not just to determine a magnetic structure but also to understand the polarity of that magnetic structure with respect to the polarity of a given structural domain.

The PCG is very grateful to the Solid State Group (of the Royal Society of Chemistry) for

kindly sponsoring a poster prize which the judges were pleased to award to Matthew Tate (Durham) for his poster entitled “Structural properties of the Nb-doped bismuth oxide materials  $Bi_{1-x}Nb_xO_{1.5+x}$ ”.



The BCA meeting was not only interesting and enlightening, but provided many opportunities for networking and socialising. Aside from the tasty buffet dinners which accompanied the poster sessions (a great way to round off each day of talks), Loughborough's excellent student bar came in handy to wind down. The conference dinner was a highlight: a fantastic 3 course dinner with wine which was followed by a ceilidh, where even those who are least inclined to dance were persuaded to join in and ended up having a great time! All in all the conference was a huge success, helped by the excellent facilities and accommodation at Loughborough University and the diligent organisation of the planning committee. We look forward to the BCA2015 spring meeting to be held at the University of York!

E. E. McCabe (Kent), P. J. Saines (Oxford), M. L. Tate (Durham), J. Wicker (Oxford)

### **Powder diffraction & Rietveld refinement school, 30<sup>th</sup> March – 3<sup>rd</sup> April 2014, Durham, UK**

The Powder Diffraction and Rietveld Refinement School was held at Durham University from 30<sup>th</sup> March to 3<sup>rd</sup> April. Sixty four people from all around the world met in Durham for this renowned biennial crystallographic training led by Professor John Evans, Dr Ivana Evans, Dr Jeremy Cockcroft and Professor Andy Fitch. In addition, Dr Emma McCabe and Dr Chun-Hai Wang were tutors for the helpful practical sessions.

The school began with lectures covering the basics of symmetry, crystallography and powder diffraction, interspersed with hand-written tutorial work, which promoted discussion within smaller groups, and plenty of well-received coffee breaks. Once the basics were covered some practical sessions were held in the computer rooms covering the use of several software packages: Microsoft Excel, Topas Academic, GSAS and Fullprof, with plenty of opportunity to ask questions. The interesting lectures were very useful and varied. Dr Jeremy Cockcroft introduced the

fundamentals of symmetry and diffraction, with Dr Ivana Evans covering powder diffraction and the practical considerations of X-ray analysis and Professor John Evans addressing the finer details of Rietveld refinement in the context of the statistical reasoning behind the method and relating it to the software we used. Also particularly interesting was the lecture given by Professor Andy Fitch regarding synchrotron radiation and the comparison to the use of laboratory diffractometers.

The evenings allowed ample opportunity for networking, including a rather competitive pub quiz, a mysteriously named “fun” tutorial (all scientifically relevant, of course) and a pleasant course dinner during which prizes were awarded, all of which made this meeting, if possible, an even more exciting and enjoyable event.

Leopoldo Enciso-Maldonado and Zoe Taylor (University of Liverpool)

### **ISIS neutron training course, 26<sup>th</sup> February – 6<sup>th</sup> March 2014, RAL, UK**

The ISIS neutron Training course was held from 26<sup>th</sup> February to 6<sup>th</sup> March 2014 at the ISIS facility. The course was mainly targeted at students who are new to neutron scattering and who wanted to gain experience working with neutron scattering instruments.

Accommodation was provided at Ridgeway house and at the Premier Inn. The first few days involved lectures covering the theory of neutron scattering and introduction to ISIS target stations and instruments, Fourier transforms etc. The following days were a mixture of lectures and practical sessions, for which we were assigned groups.

My group consisted of 5 members, with whom I developed a good rapport and working relationship. For this part of the course, our group was based at Pearl (a high pressure station) with Dr Craig Bull and at SXD with Dr Matthias Gutmann. Both Dr Gutmann and Dr Bull were excellent mentors throughout the course, teaching us how to use the instruments, how to collect diffraction patterns from various samples such as SiO<sub>2</sub> and how to do a Fourier transform of the data. We used OpenGenie and the Mantid software to analyse the data we collected. I found the mathematical calculations involved in this course, such as deriving an equation relating time of flight and wavelength and working with structure factors to explain the selection rules for systematic absences, interesting and enjoyable.

This course was informative and stimulating. I'd recommend it to anyone interested in gaining experience in neutron scattering.

Reeya Oogarah (Kent)

## **ACKNOWLEDGEMENT**

Many thanks to everyone who has contributed to this issue of the PCG-SCMP newsletter.

Emma McCabe (Kent)

## **PCG-SCMP COMMITTEE**

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# PCG-SCMP Winter Meeting ISIS Crystallography Users Meeting

10<sup>th</sup> – 11<sup>th</sup> November 2014, Cosener's House, Abingdon

ISIS Facility Update

Crystallography Instrument and Software Update

Open Discussion

Scientific presentations

*For further information and the link to registration please go to:*

<http://www.pcg-scmp.org/Meetings/Winter2014>



RSC Solid State Chemistry Group

Annual Christmas Meeting

WestCHEM 2014



The annual Christmas meeting of the Royal Society of Chemistry Solid State Chemistry group will take place at the University of Glasgow on the 18<sup>th</sup> and 19<sup>th</sup> of December, 2014. Further details about the conference can be found on the website:  
<https://ssc2014.wordpress.com/>

Further information regarding registration and travel will be regularly updated on the website. The meeting will start at 1pm on Thursday 18<sup>th</sup> December and finish at lunchtime on Friday 19<sup>th</sup> December, with a banquet dinner at the Hilton Hotel on Thursday evening.

**Plenary speakers:**

Dr Ivana Evans, University of Durham  
Professor Martin Jansen, Max Planck Institute for Solid State Research  
Professor Nicola Spaldin, ETH Zürich  
Dr Matt Tucker, ISIS Neutron and Muon source

If you would like any further information, please contact Serena Corr ([serena.corr@glasgow.ac.uk](mailto:serena.corr@glasgow.ac.uk)) or Eddie Cussen ([edmund.cussen@strath.ac.uk](mailto:edmund.cussen@strath.ac.uk))  
We look forward to welcoming you to Glasgow!