SCMP @ IoP PCG PCG @ BCA

# Newsletter

Autumn 2015

## FROM THE CHAIR

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Autumn 2015 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.

Since our last newsletter there have been several meetings, not least the annual BCA Spring meeting in York. This was a very enjoyable meeting with lots of interesting talks, and in particular several high quality student talks during the YCG meeting and during the main meeting. There have also been a lot of excellent outreach activities this year, such as the Big Bang Fair and Cheltenham Science festival, where we have had a presence.

One of my personal high points this year was the very enjoyable and impressive Harwell Open day, where thousands of people came to see and learn about the science carried out on the campus. There we crystallography stands at Diamond and ISIS and once again many sweet crystals were consumed. Overall it was a great day, a view echoed by Julia Payne later in this issue.

On another personal note, I had the honour of organising a PDF workshop to launch the new XPDF beamline at Diamond as part of this year's synchrotron user meeting. The workshop was very well attended and we received some good feedback saying it was a useful meeting. There is a full write-up authored by two PhD students later in this issue.

This year our winter meeting was earlier than usual and it once again kept the successful and popular format of the last few years, and was held in conjunction with the ISIS Crystallography User Group Meeting, at the Cosener's House, Abingdon, 19-20th October 2015. As in previous years, the meeting was supported by ISIS Crystallography Group and the Institute of Physics. Mark Senn (Oxford) and Silvia Capelli (ISIS Facility) were in charge of putting together the scientific programme for the meeting. The meeting was oversubscribed again and everyone who could attend seemed to enjoy the event. If you were there I hope you did have fun and if you couldn't make it I hope you can come next year. Some details can still be found on the web at http://www.pcg-scmp.org/Meetings/Winter2015 and a full write up will appear in our next newsletter. I hope you will be able to join us for what has become a very successful, intensive two-day meeting.

During the spring meeting we elected some new committee members, so I would like to formally welcome Nicholas Funnel (Oxford), Helen Playford (ISIS) and Mike Glazer (Oxford) as ordinary members of the committee. Mike, as you may know, has been co-opted on to the committee as our excellent education rep for the past few years and he has kindly agreed to carry on that role as an ordinary member of the committee.

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 2016. Like last year, theses from a two year period are now eligible, so we hope this will help keep the competition as strong if not stronger than last year and also give more great PhD students a chance at the prize.

Matt Tucker

PCG-SCMP Chair

## ANNOUNCEMENTS

**PANalytical Thesis Prize 2016**

**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 1st January 2014 to 31st December 2015.

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/imagesFhj/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 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), by 31st January 2016 and the Prize will be awarded at the 2015 BCA Spring Meeting at University of Nottingham, 4th – 7th April 2016.

## EDUCATION AND OUTREACH

There have been a number of educational and training events that members of the PCG-SCMP community have been involved, but our members have also enjoyed attending events such as the recent Harwell open day:

After years of telling my Dad about doing experiments at ISIS and Diamond, I could not let the Harwell Open Day pass by without bringing my Dad to RAL. After an early morning train journey, our knowledgeable Taxi driver from Didcot informed us that he had been bringing staff to RAL since 4:30 am that morning. This was clearly an early indication of all the hard work and effort that had gone in to organising the event.

The open day saw thousands of visitors of all ages and scientific backgrounds descend onto the sun-soaked campus. The top priorities for our day were to visit ISIS and Diamond. Never before had such queues of eager visitors been witnessed to get into both facilities! The queues to get into Diamond went around the block, but nobody minded, as everyone was curious to find out what goes on in this 'spaceship' like building! Once inside we were greeted by Diamond staff, with Andrew Harrison giving a perfectly pitched explanation of how Diamond actually works. Next stop was ISIS TS2, where a huge range of different sample environments and synchrotron parts were on display. This was followed by a visit to the ISIS marquee, which was a hub of activity, with live science demonstrations and enthusiastic instrument scientists on hand to help with a range of different activities from growing your own crystals to making models of crystal structures with sweets and cocktail sticks!

Finally, we managed to also take in the excellent and imaginative 'Illuminating Atoms' photography exhibition of crystallographers, along with the CLF, RAL Space and RCaH, which are usually hidden behind closed doors when I visit RAL! Enthusiastic, keen and helpful staff were again on hand to help us learn more about the science they do. The attention to detail that went into organising extra on-site facilities (from coffee booths to hot dog stalls to water fountains) should also not go unmentioned and was greatly appreciated.

Everyone who organised the event deserves massive congratulations, as a great day was had by all and I know people are already looking forward to the next open day, whenever that may be!

Julia Payne (St Andrews)

## FUTURE MEETINGS

### Meeting Calendar

- PCG Winter Meeting and ISIS Crystallography Users Meeting, 19th – 20th October 2015, Cosener's House, Abingdon (http://www.pcg-scmp.org/Meetings/Winter2015)
- Electronic properties of modern materials, 17th – 19th November 2015, Diamond Light Source (RAL), (http://www.diamond.ac.uk/Home/Events/2015/Electronic-Properties-of-Modern-Materials.html)
- Solid State Group (of the Royal Society of Chemistry) Christmas meeting, 21st – 22nd December 2015, University of Kent (http://www.kent.ac.uk/physical-sciences/s2cg/index.html)
- BCA Spring Meeting, 4th – 7th April 2016, University of Nottingham (http://bca2016.crystallography.org.uk)
- Powder Diffraction & Rietveld Refinement School, 10th – 14th April 2016, Durham University (http://community.dur.ac.uk/john.evans/webpages/pdrr_school_2016.htm)
- ISIS neutron training course 12th – 21st April 2016, ISIS Neutron Source (RAL), (http://www.isis.stfc.ac.uk/learning/neutron-training-course/isis-neutron-training-course9135.html)

### Electronic properties of modern materials meeting, 17 – 19th November 2015, Diamond, Rutherford-Appleton Laboratory

Advanced electronic materials are one of the most exciting research frontiers in the physical sciences. Electron-electron correlations generate ever more surprising collective states with novel symmetries, novel topologies and new types of excitations. Many of these materials interact with electric an magnetic fields in new ways, offering the prospect of disruptive technologies. Understanding and controlling such complex forms of quantum matter requires cutting-edge facilities and ground-breaking ideas.

This meeting will be a focal point for the community of physicists, chemists and materials scientists using synchrotron, neutron, and muon sources as well as low-temperature, computational and theoretical techniques to investigate magnets, superconductors, multiferroics and other advanced materials. Specifically it aims to: foster links between the Diamond and ISIS user communities in the fields of strongly correlated electrons/magnetism/superconductivity (both physics and chemistry); showcase Diamond's capabilities in these areas; and foster links between the theory and experimental communities.

Topics:

- Quantum Magnetism
- Frustrated Magnetism
- Unconventional pairing in superconductors
- Multiferroic order
- Topological defects and excitations
- Topological order and quantum phase transitions

**Keynote Speakers (confirmed)**

- James Annett (University of Bristol)
- Felix Baumberger (PSI, Switzerland)
- Steve Bramwell (University College, London)
- Laurent Chapon (Institut Laue Langeving)
- Radu Coldea (University of Oxford)
- Andrew Goodwin (University of Oxford)
- Andrew Harrison (CEO, Diamond Light Source)
- George Jackeli (MPI for Solid State Research, Stuttgart)
- Stephen Lovesey (Diamond Light Source)
- Des McMorrow (University College, London)
- Matt Rosseinsky (University of Liverpool)
- Nicola Spaldin (ETH Zurich)
- James Dracott (EPSRC)
- Steven Lovesey (STFC)

For more information, please visit http://www.diamond.ac.uk/Home/Events/2015/Electronic-Properties-of-Modern-Materials.html

### Solid State Group Christmas meeting, 21st – 22nd December 2015, University of Kent

The annual Christmas meeting of the Royal Society of Chemistry's "Solid State Group" will take place in Canterbury on the 21st and 22nd of December 2015, organised by the School of Physical Sciences at the University of Kent.

Confirmed plenary speakers include:
Professor Sharon Ashbrook (University of St Andrews)
Professor Andrew Harrison (CEO of Diamond Light Source)
Professor Jean-Marie Tarascon (Collège de France)

Confirmed invited speakers include:
Dr Sian Dutton (University of Cambridge)
Dr Julian Dean (University of Sheffield)
Dr Houria Kabbour (Ecole Nationale Supérieure de Chimie de Lille, France)

Abstract submission (http://www.kent.ac.uk/physical-

sciences/s2cg/abstracts.html) will close on 13th November and registration (http://www.kent.ac.uk/physical-sciences/s2cg/registration.html) will close on 1st December 2015.

For more details, please visit the website: http://www.kent.ac.uk/physical-sciences/s2cg/index.html .

**BCA Spring Meeting, 4th – 7th April 2016, University of Nottingham**

The BCA Spring Meeting 2015 will take place from 4th – 7th April 2016 at University of Nottingham. The PCG plenary will be given by **Prof. Bill David** from the ISIS neutron source and University of Oxford, UK, and is entitled "*120 Years of Powder Diffraction*".

PCG sessions at the meeting will include:

- Advanced functional materials
  (Chair: Matthias Gutmann)
  Keynote: Paolo Radaelli (University of Oxford)

- Modelling crystals and crystallographic data
  (Chair: Anthony Philips)
  Keynote: Carole Morrison (University of Edinburgh)

- Future of structural science (two sessions organized by BSG and PCG)
  (Chairs: Mike Glazer and Xiaodong Zhang)
  Keynote: John Spence FRS (Arizona State University) and Xiaodong Zhang (Imperial College)

- Phase transitions
  (Chair: Christoph Salzmann
  Keynote: John S. O. Evans (Durham University)

- Local structure – property relationships
  (Chair: Matt Tucker)

The deadline for abstract submission for oral and poster contributions is 9am on 22nd January 2015.

The scientific programme and further details about the conference will appear at: http://bca2016.crystallography.org.uk/.

**Powder diffraction and Rietveld refinement school, 10th – 14th April 2016, Durham University, UK**

The biennial Powder Diffraction & Rietveld Refinement School will take place at Durham University, 10-14th April 2016.
As in previous years, it will offer a combination of lectures covering the theoretical aspects of powder diffraction and Rietveld refinement, classroom-based "by-hand" problem sessions/tutorials and extensive hands-on practical sessions using a variety of modern software packages.
Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Modelling peak shapes (including microstructure analysis)
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods
- X-ray and neutron combined Rietveld refinements
- Restrained refinements
- Rigid body refinements
- A number of more specialised and advanced optional topics (ab-initio structure solution, parametric and symmetry-mode refinements)

Lectures will be given by Prof. John Evans, Dr. Ivana Evans, Dr. Jeremy Cockcroft and Prof. Andy Fitch.
Online applications can be submitted until 22nd January 2016, at the Powder Diffraction & Rietveld Refinement School 2014 website: http://community.dur.ac.uk/john.evans/webpages/pdrr_school_2016.htm

## NEWS

## RECENT EVENTS

**British Crystallographic Association Spring Meeting, 30th March – 2nd April 2015, York,**

The PCG program kicked-off after lunch on Tuesday by challenging the very boundaries of Crystallography, with a session entitled "Beyond the elastic line". In the first talk, " Resonant X-ray Diffraction and the elusive sign of the DM interaction in weak ferromagnets", Steve Collins (Diamond Light Source) demonstrated how resonant x-ray diffraction can be used to elucidate coupling interactions between magnetic and ferroelectric order in multiferroic materials. This was followed by a talk given by Matthias Gutmann (ISIS) on modelling beautiful thermal diffuse scattering observed on SXD using ab initio methods to calculate both quasi-elastic and inelastic contributions to the diffraction patterns. The session was concluded by Chris Stock (University of Edinburgh) who demonstrated how triple axis neutron spectroscopy can be used to probe the magnetic excited states of the chiral mineral Langasite.

The next PCG symposium 'Challenges and technical advances in powder diffraction' focussed on recent instrumental developments, particularly at the ISIS and Diamond central facilities. The first talk (Pascal Manuel, ISIS) showed a number of developments for the WISH diffractometer, including capabilities for measurements under high magnetic field and enhancements for small quantities of sample, such as those synthesised under high pressure. This was followed by Claire Murray (Diamond) talking about the newly operational 'Long Duration' hutch at I11, allowing for synchrotron diffraction experiments to be conducted at intervals over many months, or even years. The automated robotics allows a wide range of possible sample environments, and provides an exciting opportunity for long-term, in-situ studies. The final talk of the session (Yue Wu, University of Oxford) revealed the use of the newly developed 'Oxford-Diamond in-situ cell' (ODISC) to study the formation of pillared-paddle-wheel MOFs under time- and temperature-resolved diffraction conditions. His results shed light on the formation pathways of some of these materials, as well as highlighting the advantages of this new in-situ cell. Overall, the session showed the exciting new possibilities available to users at UK facilities.

A particular highlights of the PCG program was the plenary lecture by Tony Cheetham (Cambridge) entitled "Phase transitions in metal-organic frameworks" delivered on Wednesday morning. Tony showed that MOFs can undergo pretty much every imaginable kind of phase transition – and even hinted at some intriguing magnetoelectric coupling in a MOF!

Phil Lightfoot (St Andrews) chaired an excellent session on "Structural insights into ferroic materials": talks from Pam Thomas (Warwick), Mark Senn (Oxford) and Semën Gorfman (Siegen, Germany) covered mechanisms for piezo- and ferroelectricity in perovskite and perovskite-related systems as well as the latest techniques for characterising these materials. The PCG is also grateful to Branton Campbell (Brigham Young University, USA) for making time during his Fulbright Scholarship (hosted in Durham) to give a workshop on "Introduction to ISODISTORT and the exploration of symmetry-lowering phase transitions" that was very instructive, again covering a range of phase transitions.

A busy Wednesday scientific programme concluded with the presentation of the Lonsdale Lecture, this year given by Professor Simon Parsons from the University of Edinburgh. Professor Parsons gave a fascinating description of Kathleen Lonsdale's life and work as an introduction to his lecture on "High Pressure and the Molecular Crystalline State". After a lively BCA AGM, the day concluded with a delicious conference dinner, during which we celebrated this year's prize winners and danced the customary crystallography Ceilidh!

Thursday saw the PCG program draw to a close shared symposium with the industrial group on amorphous materials, nanomaterials and liquids included presentations by Fiona Meldrum (University of Leeds), Sylvia McLain (University of Oxford) and Neal Skipper (UCL). Fiona Meldrum spoke about the complex crystallisation kinetics of calcium carbonate and introduced some methods for forming calcium carbonate based nanomaterials. Sylvia McLain's talk beautifully demonstrated the role water might play in the structure of biomolecules in solution. In his talk, Neal Skipper gave structural details of the aromatic interactions present in liquid benzene and highlighted the value of diffraction data to studies of liquids in general.

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 Josh Hill (Oxford) for his work on dicyanometallates including studies of phase transitions in super-perovskites.

Overall, the meeting was an excellent opportunity to learn about recent developments in many areas of crystallography and for fruitful discussions with other researchers. We look forward to the BCA2016 spring meeting to be

held at the University of Nottingham (http://www.crystallography.org.uk/bca-spring-meeting-2016/)!

Report assembled from various contributions!

**Advances in Li battery research: UK 2015, 9-10 April 2015, Loughborough**

The Advances in Li Battery Conference: UK 2015 recently organised by Dr. Pooja Panchmatia hosted 70 participants at Burleigh Court 09-10 April 2015. Sponsored by STFCbatteries (STFCbatteries.org), CCP5 and SSCG - RSC division, the meeting was over 2 days with all expenses covered. It boasted prominent speakers including, Prof. Peter R. Slater (Birmingham), Dr. Mark Copley (Johnson Matthey), Dr. Edmund Cussen (Strathclyde), Dr. Peter Baker (STFC), Dr. Jawwad Darr (UCL), Prof. Jon Goff (RHUL) and Dr. Alodia Orera (Zaragoza) among many others covering a wide range materials research as well as advanced characterization techniques that could be used in optimising Li battery materials. Jaguar Landrover, Alstom, Johnson Matthey, Renishaw and Qinetiq were among the industrial representatives at the meeting.

Pooja Panchmatia (Loughborough)

**ISIS neutron training course, 16th – 25th June 2015, RAL, UK**

This year the ISIS Neutron Training School began with a poster presentation session, giving us the opportunity to practice presenting our research in a less formal environment to that of a conference. This was also a good chance for us all to get to know each other right at the start of the course.

The course itself provided a good background on the history and basics of experimenting using neutrons, as well as a refresher on useful mathematical techniques. Each group was able to gain invaluable hands on experience on beamlines such as ALF, MARI and MERLIN learning different types of techniques such as single crystal alignment, inelastic neutron scattering and single crystal spectroscopy. We were also introduced to and given tutorials on Mantid, including how to plot and manipulate data, how to use instrument view and how to fit models to our data.

Overall I found this course to interesting and engaging, having been led by good teachers. I also found it to be an excellent way to meet other postgraduate researchers socially as well as academically, many of whom I'm sure I will see again at future conferences.

Ben Coles (Kent)

**PDF Analysis: The Local Point of View of Materials Development, 2nd – 3rd September 2015**

As part of the annual synchrotron radiation user meeting at Diamond, on 2nd-3rd September, a pair distribution function (PDF) workshop was organised to coincide with the launch of the new X-PDF beamline on I15-1. The session was opened by **Andrew Goodwin**, chair of the User working group, who outlined the ethos behind the creation of the XPDF beamline; one of bringing PDF analysis to a wider interest group and maintaining strong working relationships with ISIS while setting new high standards for data quality and speed of data collections. These points were nicely complimented by **Phil Chater** and **Dean Keeble,** X-PDF instruments scientist and support scientist, who addressed the technical specifications and user interface aspects of the beamline respectively. **Simon Billinge** subsequently spoke in greater detail about the information that can be obtained from a PDF, with a particular focus on the use of small box modelling. The use of large-box modelling was discussed by **Nick Funnel**, whose talk highlighted the capabilities of large box reverse Monte Carlo (RMC) modelling in the analysis of nanostructured materials (e.g. nanoparticles or layered materials). **Helen Blade** then gave an overview into the use of PDF analysis in the pharmaceutical industry, outlining some of the difficulties in producing amorphous drug preparations, with regards to stability and distinguishing between amorphous and nano-crystalline samples. **Emma Barney** concluded the session with the first talk exclusively about non-crystalline materials, exploring the interesting absorption properties and the challenges inherent in modelling chalcogenide glasses with EPSR (Empirical Potential Structure Refinement). Before the conference dinner, **Professor Justin Wark** gave the keynote speech on the life and work of Henry Moseley, a much-overlooked founder of spectroscopy, sadly killed during the First World War.

The Thursday morning session was opened by **Pete Chupas,** who introduced the topic of energy materials, expounding the virtues of PDF analysis for the type of material due to the interest in their nanoscale structure. **Phoebe Allan** spoke about her work in replacing Lithium used in battery cathodes with sodium in order to reduce cost, using a combination of X-ray and neutron diffraction studies. The importance of a PDF for the complete understanding of some complex systems was stressed by **Gopinathan Sankar,** who highlighted the use of PDF as a probe for mid-range structure, inaccessible to most other conventional analysis techniques. **Helen Playford** gave an interesting account of the structural nuances of γ-$Ga_2O_3$ demonstrating the necessity for large-box modelling in the complete understanding of the material. The intuitive nature of the PDF was highlighted by **Emil Bozin,** tracking changes in structural properties of superconductors with compositional and thermal variation. **Anthony Phillips** then spoke about his group's work using RMCProfile to model carbon nanotubes

filled with ferromagnetic nanowires, along with the not insignificant difficulties encountered in such modelling. The complexities of collecting a PDF under high-pressure conditions where explored by **Joseph Hriljac**, and emphasised as a key area for future development, for the extension of the technique to a host of interesting systems. **Julia Parker**, who demonstrated the use of in-situ PDF experiments for the understanding of bio-mineralization, brought the workshop to a close. The workshop was extremely well attended, with the largest number of delegates out of the workshops run during the main synchrotron radiation user meeting at Diamond. After a variety of talks from an excellent list of speakers, it is clear to see that the broad scope of the XPDF beamline will help to advance and extend the use of the technique to a wide range of fields in the future.
Further details of the meeting may still be available at
http://www.diamond.ac.uk/Home/Events/2015/SR-User-Meeting-2015/Pair-Distribution-Function-.html

Lewis Owen & Giles Flowitt-Hill

**PCG Winter Meeting, 19 – 20th October 2015, Cosener's House, Abingdon**

PCG Winter meeting took place at the Cosener's House, Abingdon, 10-11th November 2014 (lunchtime-to-lunchtime), in conjunction with the ISIS Crystallography Users Meeting following the format of previous years.

Registration for the meeting was 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 were 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.

The meeting was of interest to a wide audience, from experienced researchers to PhD students. Following last year's success, the meeting included a focus on the work of early career researchers A poster session took place in the evening of 19th October 2015.

The full scientific programme and the timetable are available on the PCG-SCMP wiki (http://www.pcg-scmp.org/Meetings/Winter2015).


## ACKNOWLEDGEMENT

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

Emma McCabe (Kent)

Solid state group Christmas meeting 2015

S2CG

21 – 22nd December 2015, Canterbury, Kent

The annual Christmas meeting of the Royal Society of Chemistry's "Solid State Group" will take place in Canterbury on the 21st and 22nd of December 2015, organised by the School of Physical Sciences at the University of Kent.

**Confirmed plenary speakers include:**

**Professor Sharon Ashbrook (University of St Andrews)**

**Professor Andrew Harrison (Diamond Light Source)**

**Professor Jean-Marie Tarascon (Collège de France)**

**Confirmed invited speakers include:**

**Dr Julian Dean (University of Sheffield)**

**Dr Sian Dutton (University of Cambridge)**

**Dr Houria Kabbour (Ecole Nationale Supérieure de Chimie de Lille, France)**

Further details will be publicised nearer the time on the conference website: http://www.kent.ac.uk/physical-sciences/s2cg/index.html.

Please contact Emma McCabe (e.e.mccabe@kent.ac.uk) or Mark Green (mark.green@kent.ac.uk) for any other information.

We look forward to welcoming you to Canterbury!