



Newsletter

Spring 2015

FROM THE CHAIR

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Spring 2015 Newsletter. This issue brings you a number of meeting reports, information about future events and calls for nominations for the PCG-SCMP committee – I hope you enjoy browsing through it.

Since our last newsletter the International Year of Crystallography has come to an end, with two very enjoyable meetings (reviewed later in this newsletter) and now we have entered the International Year of light. This gives us the opportunity to build on a very successful year for Crystallography and since many of us use Synchrotron light in our research, to keep up the momentum on raising the importance of our research in the minds of the public and decision makers.

Thanks to our members the 2014 PCG-SCMP winter meeting was a great success. As with the previous meeting, we reached maximum capacity and had to close registration slightly early, so we are looking into how we can add a few more places. A review of the meeting can be found later in this newsletter and I would like to thank Peter Thygesen for writing this for us. Our current thoughts are to increase the structural condensed matter physics content of the next meeting, so if you have any suggestion of topics and or speakers you would like to hear from please let us know.

For me the scientific year ended with The Solid State Group (of the Royal Society of Chemistry) Christmas Meeting. I had the pleasure of being invited to give a talk and this was the first of these meetings I have attended. I thought the meeting was excellent and the standard of the plenaries and contributed talks extremely high (I did my best not to let the standards drop). Again there is a review of this meeting later on and I would like to thank Daniel Jackson for contributing this.

The deadline to enter this year's PANalytical Thesis Prize for Physical Crystallography was the 9th of February and I am very pleased to say that we have had some very strong entries. So the entrants have already

succeeding in making the job of deciding a winner very tricky. The winning thesis will be announced at the BCA spring meeting 2015 and on our website.

This brings me very nicely to the next big event in our calendar the BCA spring meeting 2015. This year it is being held at the University of York, March 30 – April 2. The PCG have organised or jointly-organised five of the parallel sessions and of course the PCG plenary. Key highlights of the meeting are given later in this newsletter and full details can be found on the Spring meeting website <http://york2015.crystallography.org.uk/>.

The PCG-SCMP AGM will as usual also be held at the Spring Meeting this year at 12:15 pm Wednesday 1st April 2015. More details are given below. Please come along if you have any ideas on things you would like the PCG-SCMP to do for its members and/or if you just want to take the opportunity to provide feedback. Registration for the BCA Spring meeting is still open and I look forward to seeing many of you there.

Matt Tucker
PCG-SCMP Chair

ANNOUNCEMENTS

Vacancies on the PCG-SCMP committee

Call for Nominations

There are three vacancies arising on the PCG-SCMP committee for ordinary members. Nominations for these positions are invited and should be sent to the current Secretary Paul Saines (paul.saines@chem.ox.ac.uk).

Nominations should include the name of the proposer, the name of the seconder and the nomination acceptance by the nominee, confirming his/her willingness to contribute to the Committee efforts by actively participating in BCA and PCG-SCMP meetings, meeting organisation and our educational activities.

Informal enquiries about the Committee members' roles should be directed to the current Chair, Matt Tucker (matt.tucker@stfc.ac.uk).

Elections for these positions will be held at the Annual General Meeting of the PCG-SCMP, which will be held during the BCA Spring Meeting at University of York, 12:15 pm Wednesday 1st April 2015. Details of the current agenda are given at the end of this newsletter

PCG-SCMP Bursaries

Student bursary applications are welcome from the IoP members affiliated to the PCG-SCMP group. Bursaries are intended to help research students to attend meetings, conferences and training schools relevant to PCG-SCMP areas of interest. Students may apply for up to a total amount of £250 during the course of their PhD.

Applications can be submitted to the IoP throughout the year, but will be considered by the Group Committee on a quarterly basis (and therefore should reach the IoP by 1st March, 1st June, 1st September and 1st December).

Successful bursary applicants are expected to produce a short written report on the meeting, which may be published in this Newsletter (see section Recent Events in this issue), in Crystallography News or on the PCG-SCMP website (www.pcg-scmp.org).

For further information please contact the PCG-SCMP Secretary Paul Saines (paul.saines@chem.ox.ac.uk) or visit the relevant Institute of Physics web page (http://www.iop.org/about/grants/research_student/page_38808.html).

FUTURE EVENTS

Meeting calendar

- BCA Spring meeting, 30th March – 2nd April, The University of York, UK, <http://york2015.crystallography.org.uk/>
- IOP's "Magnetism 2015", 30 – 31st March 2015, The University of Leeds, UK, <http://magnetism2015.iopconfs.org/home>
- Advances in Li-battery research, 9 – 10th April, The University of Loughborough, UK, <http://www.esrn.co.uk/events/advances-in-li-battery-research-uk-9-10-apr-2015/>

- European Materials Research Society Spring Meeting, 11th – 15th May 2015, Lille, France, http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=800&Itemid=1652
- UK neutron and muon science user meeting, 19th – 21st May 2015, Hinckley Island Hotel, Leicestershire, UK, http://www.wis2.isis.rl.ac.uk/useroffice/NMU_M2015/Register.asp
- Gordon Research Conference: Neutron scattering, 21st – 26th June 2015, The Chinese University of Hong Kong, Hong Kong, China, <http://www.grc.org/programs.aspx?year=2015&program=neutron>
- 12th International Conference on Materials Chemistry, MC12, 20 – 23rd July 2015, University of York, York, UK, <http://www.rsc.org/ConferencesAndEvents/RSCConferences/MC12/index.asp?gclid=C MH5ob6p-MMCFWfJtAodbiUAUw>
- ECSSC15: 15th European conference on solid state chemistry, 23rd – 26th August 2015, Vienna, Austria, <https://ecssc15.univie.ac.at/>
- ECM29: 29th European crystallographic meeting, 23rd – 28th August 2015, Rovinj, Croatia, <http://ecm29.ecanews.org/>
- ECNS 2015: 6th European conference on neutron scattering, 30th August – 4th September 2015, Zaragoza, Spain, <http://ecns2015.unizar.es/>

Training calendar

- 7th Annual school on neutron diffraction and data treatment using the Fullprof suite, 2nd – 6th March 2015, ILL, Grenoble, France, <http://www.ill.eu/FPSchool2015/>
- ISIS neutron training course, 16 – 25th June 2015, ISIS, UK, <http://www.isis.stfc.ac.uk/learning/neutron-training-course/isis-neutron-training-course9135.html>
- 14th Oxford school of neutron scattering, 6 – 18th September 2015, Oxford University, UK, <http://www.oxfordneutronschool.org/>

**BCA Spring meeting, 30th March – 2nd April
2015, University of York**



The BCA Spring Meeting 2015 begins with the Young Crystallographers' Meeting on Monday 30th March, featuring "Space groups – the final frontier" from Profs. Bill Clegg and Mike Glazer. The main meeting will follow this, running from late morning on Tuesday 31st March until 1:30pm on Thursday 2nd April.

The PCG-SCMP plenary lecture, entitled "Phase transitions in metal organic frameworks" will be given by Prof. Anthony Cheetham FRS (University of Cambridge) on Tuesday 31st March.

Parallel sessions and invited talks likely to be of particular interest to the PCG-SCMP community include:

Beyond the elastic line: resonant and inelastic diffraction (Tuesday 31st March)

- Keynote: Steve Collins (Diamond), *Resonant X-ray Diffraction and the elusive sign of the DM interaction in weak ferromagnets*
- Matthias Gutmann (ISIS), *Combining ab-initio phonons and diffraction to study thermal diffuse scattering*
- Chris Stock (University of Edinburgh), *Helical and multiparticle fluctuations in chiral magnets*

Challenges and technical advances in powder diffraction (Tuesday 31st March)

- Keynote: Pascal Manuel (ISIS), *Extreme Conditions and Magnetic Neutron Diffraction: how far can we push it?*
- Claire Murray (Diamond), *New Facility for Long Duration Experiments at Diamond Light Source*
- Yue Wu (University of Oxford), *Observing MOF crystallization using in-situ diffraction*

Structural insights into ferroic materials (Wednesday 1st April)

- Keynote: Pam Thomas (University of Warwick), *Structures and Properties of Lead-Free Piezoelectrics – Domains, Disorder and Disagreements*
- Mark Senn (University of Oxford), *Hybrid multiferroics and novel negative thermal expansion mechanisms*
- Semën Gorfman (University of Siegen), *Understanding high electromechanical activity in uniaxial ferroelectric by using single crystal time-resolved X-ray diffraction*

Complementary calculations (Wednesday 1st April)

- Keynote: Keith Refson (STFC, RAL), *Structures and Properties of Lead-Free Piezoelectrics – Domains, Disorder and Disagreements*
- Dr CL Hobday (University of Edinburgh), *Combining high-pressure gas loading and GCMC simulations to elucidate 'breathing' mechanism of Zeolitic Imidazolate Frameworks*

Amorphous materials, nanomaterials and liquids (Thursday 2nd April)

- Keynote: Sam Callear (ISIS), *No Bragg Peaks? No Problem! – Amorphous and Nanomaterials Research at ISIS*
- Keynote: Fiona C. Meldrum (Leeds), *Structure and Crystallization of Amorphous Calcium Carbonate*
- Nicholas Funnell (University of Oxford), *Reverse Monte Carlo modelling of low-dimensional materials*
- Sylvia McLain (University of Oxford), *The essential role of water in the structure of biomolecules in solution*
- Neal Skipper (University College London), *Neutron diffraction studies of aromatic interactions in liquids*

Workshop: Diffractometer software, Agilent and Bruker (Tuesday 31st March)

Workshop: Symmetry modes, Branton Campbell (Wednesday 1st April)

In addition to the parallel session, three plenary lectures and prize lectures, delegates will also be treated to the Dorothy Hodgkin lecture given by Prof. Sir Tom Blundell FRS on Tuesday 31st March, and the Lonsdale lecture given by Prof. Simon Parsons (University of Edinburgh) on Wednesday 1st April.

The Solid State Group of the Royal Society of Chemistry have kindly agreed to sponsor a prize for the best poster in the field of solid state chemistry/physical crystallography presented at the BCA spring meeting.



PCG-SCMP AGM

The 72nd Annual General Meeting of the Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Group of the Institute of Physics will take place at:

12:15 pm Wednesday 1st April 2015, York

The meeting agenda includes the following items:

1. Apologies for absence
2. Minutes from the 71st AGM held at Loughborough, 9th April 2014 (<http://www.pcg-scmp.org/2014>)
3. Matters arising from minutes
4. Chair's report
5. Treasurer's report
6. Elections to PCG/SCMP committee
7. Future Meetings
8. Any other business

Please email 'any other business' items to the PCG/SCMP secretary Paul Saines (paul.saines@chem.ox.ac.uk).

NEWS

Prizes and awards

PANalytical Thesis Prize 2015



The PANalytical thesis prize has now closed and the 2015 winner will be announced at the BCA spring meeting, University of York, 30th March – 2nd April 2015.

RECENT EVENTS

Illuminating Atoms exhibition, 4th November – 7th December 2014, The Royal Albert Hall

Wandering around the *Illuminating Atoms* exhibition, Royal Albert Hall 4Nov2014-7Dec2014, was inspiring. Max Alexander's portrait photography and reportage shots are visually stunning and pairs the science with the human story. They artistically allude to the diverse role that crystallography plays in modern life – be it in evaluating the origins of our solar system, determining improvements in pharmaceutical drugs, identifying new quasicrystals, studying viruses or characterising composite ceramics/magnetic oxides for use in computer memory and hard discs.

Refreshingly the collection of 21 portraits faithfully reflects the gender balance equality present today – a legacy from the earliest days when in the 1920s the Braggs taught and encouraged many female students. The 16 documentary images meanwhile juxtapose the huge scientific facilities with the often minute, fragile or transient crystals being studied. All

together these images illustrate how, since its birth 100 years ago, crystallography has had such a profound impact upon our scientific knowledge and how it continues to make a real contribution to society.

The photographs are still available to view online (<http://www.stfc.ac.uk/3395.aspx>) however if you would like this celebration of crystallography to be exhibited in your institution then please do get in touch (contact newsletter secretary, e.e.mccabe@kent.ac.uk who will forward your email on).

Hazel Hunter (ISIS Facility)

PCG-SCMP winter meeting, 10-11th November 2014, The Cosener's House, Abingdon

The PCG-SMP winter meeting is the annual meeting of the PCG/SMP group and, as is now tradition, is jointly held with the ISIS crystallography user group. Again this year there was a large turnout over the two days with vibrant discussion, sharing of ideas and collaboration providing ample value of the meeting. This would not be possible without support from ISIS and the organising committee, which all the participants appreciate, so great thanks must go to them. The afternoon session was split into two sessions. The first featured updates on the ISIS facility with a particular focus on recent developments on the WISH diffractometer and the muon spectroscopy suite. This session concluded with Paz Vaqueiro (University of Reading) talking about investigation of thermoelectric materials using neutron diffraction. The second session began with three presentations given by young scientists covering a wide range of topics from Matt Dunstan (University of Cambridge) discussing materials development for CO₂ capture to Jerome Wicker (University of Oxford) regarding predicting what drug like molecules will crystallise and Gabriele Sala (Royal Holloway University of London) who talked about the importance of impurities in spin ice. The session ended with a talk given by Serena Corr (University of Glasgow), on the structure and dynamics of Li-ion battery electrode materials and paved the way for an excellent poster session and dinner.

The second day started with a talk about Bragg coherent diffraction imaging and dynamics with an XFEL given by Marcus Newton (University of Southampton) followed

by Phil Chater (Diamond) who talked about properties of the upcoming beamline XPDF. Talks after coffee included an enlightening talk by Antonella Scherillo (ISIS) regarding recent archeometry results from INES, Sihai Yang (University of Nottingham) who discussed the development of an interesting new family of metal-organic frameworks and finally, but definitely not least, Mike Pitcher (University of Liverpool) who discussed the rational, and successful design, of a new multiferroic layered perovskite. Andrew Goodwin (University of Oxford) then gave a fascinating talk about frustration, hidden order, and emergence in non-magnetic inorganic salts. To end the two day meeting, Mike Glazer (University of Oxford) showed how crystallographic studies could explain piezoelectricity. Overall, the two days gave friendships, collaborations and inspiration to new ideas for new and returning students.

Peter Thygesen (Oxford)

The Solid State Group (of the Royal Society of Chemistry) Christmas Meeting, 18 – 19th December 2014, University of Glasgow

On 18th-19th December 2014, members of the solid state chemistry community gathered in Glasgow for the RSC Solid State Chemistry Group Christmas Meeting, hosted by the Universities of Glasgow and Strathclyde.

The meeting was opened with a plenary lecture from Martin Jansen (Max Planck Institute for Solid State Research) speaking about the discovery of new materials and adding a degree of control and predictability to their synthesis. Further plenary lectures were given by: Ivana Evans (Durham University) on oxide ion conductors for energy applications and their characterisation using a combination of techniques to understand the complexity of novel functional materials; Matt Tucker (ISIS Neutron and Muon Facility), who spoke about RMCProfile and its capability for complex modelling; and Nicola Spaldin (ETH Zürich), who gave a fascinating talk on an overlap between materials chemistry and cosmology, whereby materials can be used to test Kibble-Zurek scaling laws. Accompanying these plenary lectures was a great range of talks by PhD students and posters showcasing new and developing research. The conference itself was a wonderful event and so thanks must go to the conference organisers Serena Corr, Eddie Cussen and colleagues.

Daniel Jackson (University of Kent)

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Many thanks to everyone who has contributed to this issue of the PCG-SCMP newsletter.
Emma McCabe (Kent)

