SCMP @ IoP PCG PCG @ BCA

Newsletter

Autumn 2013

FROM THE CHAIR

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Autumn 2013 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.

The UK has recently hosted the European Crystallographic Association ECM28 conference. For me personally, this was a very successful meeting, with scientific microsymposia which covered a number of topics of interest to our group, including non-ambient crystallography, magnetism, total scattering and aperiodic crystals, to name just a few. Thanks to Jeppe Christensen for acting as the physical crystallography interest group liaison for this meeting, and for his role in shaping up the programme.

In addition to excellent scientific sessions, ECM28 featured a truly unique tribute to the work of William Henry and William Lawrence Bragg, "The Two Braggs" exhibition. This beautifully laid out exhibition gathered some of the equipment used by the Braggs, their laboratory notebooks, letters and other personal items. We are very grateful to Mike Glazer, who was a major driving force behind the exhibition, for making this possible.

Looking ahead to future events, our Winter Meeting this year will keep 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, 11-12th November 2013. As in previous years, the meeting will be supported by ISIS Crystallography Group and the Institute of Physics. Paul Saines (University for Oxford) is in charge of putting together the scientific programme for the meeting, with local support from Matt Tucker (ISIS). 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/Winter2013. I hope you will be able to join us for what has become a very successful, intensive two-day meeting.

There have been a couple of recent changes on the PCG-SCMP committee. Firstly, I'd like to thank two retiring members, Kirsten Christensen and Helen Maynard-Casely, for their many contributions to the group over the last few years, which included heading the BCA Spring Meeting 2012 programme committee on behalf of the group and editing the group newsletter, respectively. I'd also like to formally welcome two new committee members: Emma McCabe (University of Kent) and Matthias Gutmann (ISIS). Emma has also taken over as the Newsletter Editor.

Finally, I'd like to draw to your attention the two calls for nominations which are being announced in this Newsletter. Owing to the generous support by PANalytical, we are inviting nominations for the PANalytical Thesis Prize 2014. Next year, we will also be awarding the 2014 Physical Crystallography prize. We look forward to a good competition for both awards!

Ivana Evans

PGG-SCMP Chair

ANNOUNCEMENTS

IoP Physical Crystallography Prize 2014

Call for Nominations

IOP Institute of Physics
Structural Condensed Matter Group

This year the Physical Crystallography Prize is being sponsored by the Institute of Physics. The Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field. The award is traditionally presented at the BCA Spring Meeting and the winner gives a Prize Lecture at that meeting.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, Dr. Ivana Evans (ivana.radosavljevic@durham.ac.uk), by 31st January 2014 and the Prize will be awarded at the 2014 BCA Spring Meeting at University of Loughborough, 7-10th April 2014.

PANalytical Thesis Prize 2014

Call for Nominations

PANalytical

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 September 2012 to 31st December 2013.

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).

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. Ivana Evans (ivana.radosavljevic@durham.ac.uk), by 31st January 2014 and the Prize will be awarded at the 2014 BCA Spring Meeting at University of Loughborough, 7-10th April 2014.

EDUCATION

Many of you will be aware of the fantastic work Professor Mike Glazer has been doing as part of his role as education officer. The superb "Two Braggs" exhibition that he organised with Pam Thomas to celebrate the centenary of the work of William Henry and William Lawrence Bragg was enjoyed by ~1040 visitors over 5 days at the Warwick Arts Centre during the ECM28 meeting in August. It was wonderful to be able to see some of the Braggs' equipment (including a number of their ionization spectrometers and crystal samples) as well as their Nobel prizes and lab notes all together. It was a privilege also to admire some of their paintings and other memorabilia lent by the Bragg family, to gain an insight into the lives of these remarkable men. Mike is grateful to many organisations for support and loans of scientific equipment (in particular the Royal Institution, the Cavendish Laboratory, the MRC Cambridge, the Science Museum London, the Diamond Light Source, and the Oxford Museum of History of Science) and for financial support (too numerous to mention here!!). I'd strongly encourage anyone who missed the exhibition to look out for the film being put together by the Diamond Light Source[1] and some items from the exhibit to be displayed at the BCA 2014 Spring Meeting.

[1] A film is being put together by the Diamond Light Source and they hope to have it on their web page and also at the Royal Institution.

"The Two Braggs" exhibition organised by Mike Glazer and Pam Thomas which was enjoyed by ~1040 visitors; the photo must have been taken during one of the very few quiet moments!

On a related note, it was mentioned at the 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).

FUTURE EVENTS

Meeting Calendar

- PCG Winter Meeting and ISIS Crystallography Users Meeting, 11th-12th November 2013, Cosener's House, Abingdon
- BCA Spring Meeting, 7-10th April 2014, University of Loughborough

PCG Winter Meeting, 11th-12th November 2013, 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, 11th-12th November 2013 (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.

The meeting is themed "New Developments in UK Materials Crystallography". We hope that the meeting will be of interest to a wide audience, from experienced researchers to PhD students. This year includes an increased 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 11th November 2013.

The full scientific programme and the timetable will be posted on the PCG-SCMP wiki (http://www.pcg-scmp.org/Meetings/Winter2013). To register for the meeting, please follow the link given on the website, registrations will close in late October.

BCA Spring Meeting, 7-10th April 2014, University of Loughborough

LOOKING TO THE FUTURE
CRYSTALLOGRAPHY@100
LEARNING FROM THE PAST

The BCA Spring Meeting 2014 will take place from Monday 7th April to Thursday 10th April 2014 at University of Loughborough. The PCG plenary will be given by Prof. Malcolm McMahon from University of Edinburgh, UK, and is entitled "Extreme Crystallography in a Flash."

PCG sessions at the meeting will include:

- Non-ambient diffraction
- Magnetic structure determination
- Complementary diffraction and non-diffraction methods

The deadline for abstract submission for oral and poster contributions is 17th January 2014.

The scientific programme and further details about the conference will appear at: http://crystallography.org.uk/spring-meeting-2014/

NEWS

RECENT EVENTS

Functional Inorganic Materials Symposium, 17th September 2013, Liverpool, UK

On the 17th September 2013 the Chemistry Department at the University of Liverpool hosted a one day symposium on Functional Inorganic Materials. After a welcome note from Professor Matt Rosseinsky the day began in earnest. From the first talk delivered by Professor Andrew Bell, on the potential for lead free piezoelectrics to the last given by Professor John Evans on new zero expansion materials, the day powered through talks from some of the UKs (and United States) most highly respected members of the inorganic materials research community including Professors Derek Sinclair, Peter Slater, Ivan Parkin and Ram Seshadri. The symposium showcased a wide range of materials science from thermoelectric to energy materials and multiferroics to intelligent glass coatings and provided an excellent opportunity for networking over the poster session at lunch. After a excellent day of science - the only disappointment was that the day had to come to end!

Donna Arnold (Kent)

ECM28 European Crystallographic Meeting, 25–29th August 2013, Warwick University

The 28th European Crystallography Meeting was held this year at the University of Warwick between the 25th and 29th of August. Preceded by the Software Development for Crystallographers, Olex2, and the inaugural European Young Crystallographers Satellite Meetings, the main event was opened with the 7th Max Perutz Lecture, presented this year by prize winner Prof. Randy Read.

More than 40 microsymposia followed, covering a range of topics such as macromolecular assemblies, cell signalling, aperiodic crystals, total scattering, and art and archaeology. Varied and engaging trade stands distracted conference goers between sessions. This year's conference also celebrated the Bragg Centenary, with a special symposium looking at the life and work of the Braggs, and the highly commended 'The Two Braggs' exhibition which collected together a huge variety of artefacts relating to the Braggs' pioneering work on x-ray crystallography, including equipment, letters, notebooks and artwork.

The Gala Dinner was held on the Wednesday night, and was followed by a hugely successful ceilidh, introducing our European visitors to some of our more esoteric dancing. The highlight of the conference was the plenary lecture given by Nobel laureate Dan Shechtman. Titled 'Quasi-Periodic Materials - Crystals Redefined', it described his discovery of quasicrystals, and the controversy that immediately followed. The meeting was officially concluded with the awarding of the poster prizes and an invitation to ECM 29, to be held in Rovinj, Croatia in two years time. This year's meeting set high standards for future meetings to follow, but we should be confident that 2015 will be just as successful as 2013.

Callum Young (Oxford)

International conference on Neutron scattering (ICNS), 8-12th July 2013, Edinburgh, UK

The International Conference on Neutron Scattering 2013 in Edinburgh was a fascinating and enjoyable festival of neutron science. The organisers really did seem to have thought of everything, supplying each of us with a rucksack which contained not just a comprehensive programme but also an umbrella (and approximately 10^{24} neutrons). In fact, Edinburgh was blessed with temperatures in the high 20s all week, and the umbrella turned out to be entirely unnecessary.

With four parallel sessions running over four days, there were far too many talks for me to describe in detail, so I can only give a few personal highlights. First upon Tuesday morning was Phil Withers' talk on predicting failure in engineering components. He began by showing video footage of collapsed bridges, metal fatigue, and aeroengine explosions. The message, of course, was clear: "They should have used neutrons!" Later in the day, I especially enjoyed Lucy Clark's talk on anion ordering in perovskites. On Wednesday morning, Toby Perring took us on a dizzying tour of spin waves in four-dimensional reciprocal space-time. This was followed by a return to earth for the geosciences session, including Colin Pulham's examination of the phase behaviour and polymorphism of some melt cast explosives. On Thursday, it was time for some quantum physics, with a ground-breaking measurement of excitations in liquid helium-4 reported by Henri Godfrin. On Friday, I enjoyed the frustrated magnetism session; highlights were hard to choose but certainly included Laurent Chapon's masterful talk on multiferroic behaviour in ferroaxial crystals and Tom Fennell's report of magnetoelastic coupling in a spin-liquid pyrochlore. The sheer breadth and scope of the poster session appeared slightly daunting at first, but the simultaneous provision of a whisky-tasting session meant that all were rapidly assimilated.

We shouldn't forget the sponsors, which not only helped to make ICNS2013 possible but also added zest to the proceedings. Chief among these were the neutron facilities themselves, each of which had their own method of advertising their services. The ISIS stall had a collection of snazzy postcards, useful to send to pining friends and family during our "holidays" at Harwell. Large sections of the crowd were seen leafing through the pages of the ESS's comprehensive Technical Report, in testament to its surprising readability, not to mention the rumour that a small but powerful pen drive was concealed somewhere within the document. Meanwhile, J-PARC showed themselves to be best at predicting the weather, providing delegates with elegant handheld fans. All in all, we had an excellent time at ICNS, and already look forward to the next one in Daejeon, 2017!

Joe Paddison and Josh Hill (University of Oxford)

ICNS satellite meeting on Theoretical and Experimental magnetism 4-5th July 2013, Abingdon, UK, and ICNS main meeting 8-12th July 2013, Edinburgh, UK

The ICNS-2013 meeting was held in Edinburgh during the second week of July 2013. Several specialised satellite meetings occurred in parallel including the workshop on Theoretical and Experimental Magnetism hosted in Abingdon on July 4 and 5. This workshop included presentations based upon theory, neutrons, muons, and also thermodynamic measurements and materials characterisation. Talks in this workshop coved a range of scientific topics including quantum magnetism, strongly correlated electron systems, and also oxide multiferroics. Of likely interest to the crystallography community were theoretical and experimental talks discussing skyrmions (a form of topological defect) in MnSi and also spiral magnetic phases in multiferroic oxides. Several talks were given discussing excitations and theory in pyrochlore rare earth oxide materials. Iron based superconductors were also discussed along with talks discussing the current experimental and theoretical status and a comparison with cuprate high temperature superconductors.

The main ICNS meeting in Edinburgh was well attended by neutron groups within Europe and abroad. The conference covered a vast array of neutron based subjects from the application of neutrons to soft matter and biology to hard condensed matter along with neutron instrumentation. Several sessions discussing magnetic and nuclear structures of new oxide multiferroics were given. Many of the plenary talks were heavily focused towards excitations including talks discussing the applications of new chopper instruments (at ISIS) towards understanding the magnetic interactions in three dimensional materials. The combination of new instrumentation to understand the dynamics along with improved software to visualise the data will certainly lead towards understanding new complex problems and materials beyond the traditionally low-dimensional magnets commonly studied in the past with these instruments.

The conference also included several nice social events including trips to Edinburgh castle and the National Museum of Scotland.

Chris Stock (University of Edinburgh)

14th European solid state chemistry conference, 7-10th July 2013, Bordeaux, France

The 14th European Solid State Chemistry Conference was held in Bordeaux from 7 to 10th July. The conference was well attended and covered materials with a range of applications, such as ionic conductors, superconductors and magnetic materials. There were five invited speakers, forty six oral contributions and over two hundred poster contributions.

Colin Greaves gave a very interesting talk about the synthesis and characterisation of $Sr_4Fe_6O_{12}$ for the first time. It was synthesised using a hydride reduction method and exhibits a rare charge ordering in the FeO_4 tetrahedra.

The use of combined precession electron diffraction and electron tomography in structure solution was nicely illustrated by C. Lepoittevin for a Bi-Ca-Fe oxide. This exhibits a complex perovskite superstructure, which retains some disorder on metal sites.

Oliver Mentre gave a talk on the rich crystal chemistry exhibited by bismuth containing oxides and how consideration of the structural building units, such as anion centred tetrahedra, may be helpful in gaining further insights on structure property relationships.

Another enlightening talk was given by Wolfgang Schnick, on nitrides for LED applications. The LEDs have been particularly successful and commercialised through work with Philips.

Two busy poster sessions saw lively discussion between delegates on topics such as electrode materials, nanoparticle synthesis and luminescent materials. There was also plenty of crystallography to be found amongst the posters and talks, with structure solution, magnetic structures and local structure studies using PDF techniques all discussed in posters or in the oral contributions.

Aside from the scientific programme, there was also a welcome event in the Musée d'Aquitaine, where delegates could learn more

about the cultural heritage of Bordeaux, and the conference dinner was held in the magnificent surroundings of Espace Bourse in the Palais de la Bourse, where we were entertained by an excellent Jazz quartet. Here it was announced that the next ESSC conference will be held in Vienna.

As a final piece of food for thought, the conference started with this quote from Winston Churchill, which I think is quite appropriate for researchers: 'Success isn't final, failure isn't fatal, but it is the courage to continue that counts'.

Julia Payne (University of Liverpool)

Workshop on adsorption in compliant solids, 5-7th June 2013, Paris, France

The workshop on adsorption in compliant solids took place during the 5-7th of June 2013 in Chimie ParisTech, Paris. The meeting was well attended by computational as well as experimental scientists. The topics of research ranged from more traditional framework materials such as coal, cement, silica and zeolites to more exotic metal–organic frameworks, whereby adsorption mechanisms and mechanical properties were presented.

Hot topics included the unusual breathing mechanism in MIL metal–organic frameworks using a combination of computational and experimental techniques, presented by several speakers including François-Xavier Courdert (Paris),Tina Düren (Edinburgh), and Guillaume Maurin (Montpellier). The computational modeling of zeolitic imidazolate frameworks presented by Caroline Mellot-Draznieks (Paris) and François-Xavier Courdert (Paris) nicely supplements the experimental work on their mechanical properties, including its known amorphisation, presented by Anthony Cheetham (Cambridge) and gas sorption structural changes by Conchi Ania (Spain). The combination of computational and experimental research was very complementary, and highlights the need for both techniques to achieve a complete understanding. In summary: a great, friendly conference which was matched with sunny weather and delicious food!

Ines Collings (Oxford)

ACKNOWLEDGEMENT

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

Emma McCabe, Kent

PCG-SCMP COMMITTEE

PCG-SCMP Winter Meeting
ISIS Crystallography Users Meeting

"New Developments in UK Materials Crystallography"

11-12th November 2013, Cosener's House, Abingdon

Scientific presentations including:

Phil Lightfoot (St Andrews) "Unusual structural behaviour in multiferroic perovskites"

Mark Senn (Diamond Light Source): 2013 PANalytical Thesis Prize Talk "How much can we learn about a multiferroic mechanism in a material from its crystal structure(s)?"

Serena Corr (University of Glasgow) "Local structure investigations of (nano)materials for energy applications

Jeppe Christiensen (University of Bath) "Time resolved structural science"

Duncan Gregory (University of Glasgow) "Ultrafast microwave processing of nanoceramics: sub-minute synthesis of refractory carbides"

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

http://www.pcg-scmp.org/Meetings/Winter2013