SCMP @ IoP PCG PCG @ BCA

Newsletter

Spring 2014

FROM THE CHAIR

Welcome to the PCG-SCMP Spring 2014 Newsletter. For me, this issue is special for a couple of reasons. Firstly and most importantly, it is our first newsletter in the International Year of Crystallography. Secondly, and on a more personal note, it is the last Newsletter to which I am contributing as the PCG-SCMP Group Chair, having served on the committee for a total of 8 years, as an ordinary member/Newsletter Editor, Vice-Chair and Chair.

The International Year of Crystallography 2014 is a global event, much written about world-wide. I will therefore devote my final "From the Chair" article to things closer to home. I will use it as an opportunity to share some of my thoughts about the way in which the Group has evolved over this time, highlighting what I feel have been our key achievements.

The PCG-SCMP Group Newsletter was revived with the Spring 2007 issue. Since then, it has been regularly distributed to our members via the IoP and the BCA admin offices, and posted online at our Wiki site bringing UK and international conference previews and reports, news stories of developments at central facilities, calls for nominations and announcements of prizes. I'd like to thank the Newsletter Editors who have made this possible: Sarah Lister-Tallentire Helen Maynard-Casely and now Emma McCabe, as well as everyone who has contributed to the Newsletters over the years.

I have already mentioned the group Wiki and I'd like to thank our webmaster, Matt Tucker, for setting the Wiki up in 2007 and maintaining it ever since then.

One big success has been the group Winter Meetings, which since 2008 have been held jointly with the ISIS Crystallography Users Group, over two days at Cosener's House. I understand the same format had been tried some years before without taking root, but it was a conversation between Richard Ibberson and John Evans during an HRPD experiment in early 2008 that rekindled the idea to try to merge these two event again and create a meeting with stronger science and stronger numbers. Thanks to Richard and John for the initiative (and to the slowly-cooling HRPD furnace for making this conversation happen in the first place). In this format, the meeting has gone from strength to strength and this will hopefully continue to be the case in the future.

As the final landmark, I will mention the update of the Group Constitution, previously revised in 1985. At the 2012 AGM, we announced the plan to update the group Constitution. This was carried out in consultations with the IoP and the BCA, and the new Constitution was approved by both institutions. At the Winter Meeting 2012, we held an Extraordinary General Meeting at which the new PCG-SCMP group Constitution was formally adopted.

Over the last several years, specifically since 2008, the group has strengthened its links to the solid state chemistry and materials chemistry community. This was done principally though the interactions between the PCG-SCMP Group committee and the Royal Society of Chemistry Solid State Group committee, by cross-advertising meeting announcements and reports, organising conference sessions on topics of mutual interest and exchanging sponsorship of poster prizes at meetings. Of course, the natural overlap between this community and the ISIS Crystallography Users Group has been another significant factor in strengthening these links.

One area where I feel there is still room for improvement is finding effective ways to make the PCG-SCMP Group the natural home for the structural condensed matter physics community. With the current committee comprising a number of physicists and more physicists having been nominated for the vacancies arising on the committee, this task will hopefully be more readily achievable.

Finally, I would like to close by thanking all my fellow committee members and Group officers with whom I've served in the past 8 years. It has been a great pleasure, and I hope the future committees find their work equally rewarding.

Ivana Evans

PGG-SCMP Chair

ANNOUNCEMENTS

Vacancies on the PCG-SCMP committee

Call for Nominations

Three are two vacancies arising on the PCG-SCMP committee, one for Chair and one for an ordinary member. 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, Ivana Evans (Ivana.radosavljevic@durham.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 Loughborough, 7-10th April 2014.

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, 7-10th April, The University of Loughborough, UK, http://crystallography.org.uk/spring-meeting-2014/
- IOP's "Magnetism 2014", 7-8th April, The University of Manchester, UK, www.magnetism2014.og
- UK neutron and muon user meeting, 10th-11th April, Warwick University, UK, http://wwwisis2.isis.rl.ac.uk/useroffice/NMUM2014/Register.asp
- RSC Solid State Group Easter Meeting 2014: Solid state chemistry and renewable energy, 14th-1th April, The Kavli Royal Society International Centre, UK, http://ssg-eastermeeting.moonfruit.com/
- International summer school of crystallography 2014, 11-17th May, DESY, Hamburg, Germany, http://conferences.cfel.de/issc14/
- EPDIC 14 (The European powder diffraction conference), 15-18th June, Aarhus University, Denmark, http://epdic14.au.dk/
- EURODIM 2014 (12th Europhysical Conference on Defects in Insulating Materials), 13-19th July, University of Kent, http://www.kent.ac.uk/physical-sciences/eurodim/index.html
- IUCr-UNESCO OpenFactory training on theoretical and practical training on X-ray diffraction, 10th-19th September 2014, Darmstadt, Germany (Stoë) and Grenoble, France (ESRF), http://www.iycr2014.org/openfactory

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

The BCA Spring Meeting 2014 has the theme "Crystallography@100: Looking to the future, learning from the past". The conference begins with the Young Crystallographers' Meeting on Monday 7th April, with the main meeting following the successful format of recent years,

running from late morning on Tuesday 8th April until 1:30pm on Thursday 10th April.

The PCG-SCMP plenary lecture, entitled "Extreme crystallography in a flash" will be given by Malcolm McMahon (University of Edinburgh) on Tuesday 8th April.

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

Non-ambient diffraction (Tuesday 8th April)

- Bill David (ISIS, University of Oxford), *In operando diffraction studies of reversible hydrogen storage materials*
- Stephen Hull (ISIS), *In situ studies of batteries and fuel cell materials*
- Andrzej Katrusiak (Adam Mickiewicz University, Poland), *Pressure-induced changes in the heirarchy of intermolecular interations*
- Simon Parsons (University of Edinburgh), *Elucidating structure-property relationships with high pressure crystallography*

Magnetic structure determination (Wednesday 9th April)

- Andrew Wills (UCL), *Magnetic structures: representations, space groups and other relatives*
- Paolo Radaelli (University of Oxford), *Can complex magnetic structures be used to store and retrieve information?*

Complementary non-diffraction methods (Thursday 10th April)

- Yaroslav Khimyak (University of East Anglia), *Probing intermolecular interactions and dynamics in porous host-guest systems using solid-state NMR*
- Joke Hadermann (University of Antwerp), *Mapping of chemical order in inorganic compounds*
- Martin Dove (Queen Mary University), *Reverse Monte Carlo method: coupling scattering data with computer simulation*

In addition to the parallel session, three plenary lectures and prize lectures, delegates will also be treated to the Lonsdale lecture given by Harry Chapman (DESY, Hamburg) on Tuesday 8th April, and the Bragg lecture given by Judith Howard (Durham University) on Thursday 10th 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.

NEWS

Prizes and awards

IoP Physical Crystallography Prize 2014

IOP Institute of Physics
Structural Condensed Matter Group

The winner of the 2014 Physical Crystallography Prize will be announced at the BCA Spring Meeting in Loughborough. The prize lecture will be delivered on Wednesday 9th April.

RECENT EVENTS

PCG-SCMP winter meeting, 11 – 12th November 2013, The Cosener's House, Abingdon

From the point of view of a first-timer with few preconceptions, this annual joint meeting between the ISIS crystallography user group and the PCG/SCMP was an exciting blend of information, ideas and inspiration. The unprecedentedly large turnout over the two days was evidence of the value of such a meeting to the various scientific communities present, as well as the breadth of expertise and quality of science on display. Of course, it would not have been possible without generous support from ISIS and the effort of the organising committee, so hearty thanks must go to them.

The afternoon session began with a trio of talks by early career researchers. Steven Pramana (Imperial College) was first up, talking about the structure of apatite, including a discussion of oxygen conduction pathways. Tom Bennet (University of Cambridge) followed, engaging us with amorphous MOFs and how they might be used as 'intelligent safes'. Next came Craig Hiley (University of Warwick) with an interesting look at magnetic ruthenium oxides.

The session concluded with a foray into the heartlands of physical crystallography, with Phil Lightfoot (University of St Andrews) talking about multiferroic perovskites. Subtleties of diffraction pattern fitting, tilt systems and phase transitions were all covered, and we even received a comparison of 'Perovski's cube' with 'Rubik's triclinic pseudocube'! All in all, a most entertaining and informative session which paved the way for an excellent poster session and dinner.

The second day began with Jeppe Christensen outlining recent progress in time resolved structural science at the Dynamic Structural Sciences consortium in Harwell, and was a real eye-opener into the challenges of experiment design at a major facility. Four short presentations by young scientists then followed on diverse topics covering

polymorphism, diffuse scattering and order-disorder transitions, illustrating a delightful mixture of different experimental methods and theory. After more fruitful discussions and a coffee break, the 2013 PANalytical Thesis Prize winner, Mark Senn, gave a thoughtfully-constructed talk on his work on multiferroic materials, giving every indication that he will thrive in his new position on the Materials and Magnetism Beamline I16 at Diamond. In the last talk of the meeting, Donna Arnold graciously stepped up at late notice to describe her interesting work on relaxor effects in tetragonal tungsten bronzes. Before that, a change in direction towards metallurgy came with Howard Stone, who brought the harsh realities of crystal- and microstructure control in jet turbine blades to light: perhaps now the difficult choice of in-flight entertainment won't be the only thought on our minds when we board a trans-Atlantic aeroplane. Overall, with so many opportunities to foster ideas, friendships and collaborations, the meeting was a resounding success for new students and old-timers alike.

Hamish Yeung, Callum Young

11th and 12 of November saw the return of the ISIS crystallography user group meeting, held in conjunction with the BCA's PCG and IoP's SCMP (few letters of the alphabet went unused) group winter meeting at Cosener's House, Abingdon. The event began with a state of the union address from ISIS director Professor Robert McGreevy, followed by updates on instrumentation and capabilities at ISIS.

Topics up for discussion in the afternoon included solid oxide fuel cells, and metal-organic frameworks, with the final talk from Professor Phil Lightfoot (St. Andrews) about unusual structural behaviour in multiferroic perovskites. Dinner was preceded by a busy poster with over 20 entries.

The first session on the 12th was well attended despite the early hour, with delegates apparently well caffeinated. A personal highlight of this session was "Explosives at extreme conditions" (Mr Paul Coster – Edinburgh) detailing some of the many difficulties in procurement and production of reliable explosives. The talk did not cover how to stay off NSA watchlists.

After a short tea break, 2013 PANalytical thesis prize winner Dr Mark Senn (Edinburgh) asked: how much can we learn about a materials multiferroic mechanism from its crystal structure? The final talk of the day was – in a change to the schedule – by Dr Donna Arnold (Kent) where she discussed the advances in her work on tetragonal tungsten bronzes.

The 2012 meeting was the first meeting I attended as a PhD student. I found it a fantastic introduction to ISIS and the crystallography community. 2013's meeting with an increased focus on early career researchers gave me an idea of my place in this community. I am very much looking forward to the 2014 meeting and the revelations that it will bring.

Helen Duncan (Queen Mary, University of London)

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

On 18th-19th December 2013, members of the solid state chemistry community from all over the UK and beyond gathered at the University of Bath for the 33rd RSC Solid State Chemistry Group Christmas Meeting. The meeting was opened with the John Goodenough Prize winning lecture by Anthony West of University of Sheffield, who spoke about unusual oxygen oxidation states in defect materials. The two further plenary lectures were given by Christian Masquelier of Picardie, who gave us an insight into his investigations into the use of phosphates as positive electrodes in Li ion batteries, using a variety of experimental techniques, and Graeme Watson of Trinity College Dublin explained his work on modelling ionic conduction in doped ceria. As ever, the highlight of the meeting was the range of talks by PhD students and young researchers covering both computational and experimental work in fields as diverse as battery materials, magnetism, waste containment and nanoparticles. A particular mention should be made of Ruth Downie of Heriot Watt University who spoke excellently about the control of thermoelectric properties of half-Heusler phases. The evening of the first day kicked off with a very lively poster session, with around fifty presenters (and conversations well lubricated with plenty of beer and wine), before we were bussed to the Hilton hotel for a Christmas dinner. In a break from recent tradition, the second day of the meeting was started off with three excellent invited talks by newly established researchers spanning the topics of photocatalysis, multiferroicity and magnetic structure. All in all it was a lively and diverse meeting, and I am sure that we are all looking forward to meeting again in Glasgow in December 2014.

Fiona Coomer (ISIS)

The 33rd RSC Solid State Chemistry Group (S_2CG) annual Christmas meeting was held at the University of Bath from 18th – 19th December 2013. The conference commenced with an excellent plenary talk given by Professor Anthony West, recent winner of the RSC John Goodenough Prize. Our view that oxygen in oxides is always present as O^{2-} was

challenged in his talk which was certainly captivating and a great start to the meeting.
In session 2 Professor Christian Masquelier (Amiens) delivered an engaging talk on his research regarding the use of phosphates as positive electrodes for Li batteries, covering areas such as synthesis and results obtained from X-ray and *in situ* neutron diffraction. The session was concluded by Jennifer Kennedy presenting her research regarding the use of microwave synthesis instead of conventional solid state methods as a synthetic route to p-block carbides. Such materials are very important with a variety of applications.
A poster session followed and I believe 2 hours was just enough time to get round and see all 50 posters. The poster session was great and gave a chance to network with students (over a free beer or two) and to discuss their work illustrated in their poster. There were many great posters spanning a wide range of interesting research areas.
The conference dinner was taken at the Hilton in Bath and consisted of a delicious turkey roast and plenty of wine. The dinner provided another chance to network with students and academics. I and my group sat with students from Cambridge and discussed many things, often going off on a tangent from solid-state chemistry.
We started the next day full of vigour with talks in session 3 given by the invited speakers (Dr Robert Palgrave from UCL, Dr Christopher Knee from Chalmers and Dr Emma McCabe from Kent). These talks covered interesting areas of their current and recent research: 'the designing of visible light photocatalysts,' 'neutron diffraction of high pressure phase transitions in multiferroic $Bi_{0.9}La_{0.1}FeO_3$ and 'the structural chemistry and magnetic behaviour of iron oxyselenides' respectively.
The plenary talk of final session of the meeting was given by Professor Graeme Watson, Trinity College and discussed multiscale modelling of the doped ceria. We were told that ceria, a hugely important material in catalysis, was lacking in a detailed study of how dopants affect its electronic structure. His study focussed on how DFT can be used to model the modified electronic structure of ceria containing dopants. Dr Paul Saines from the Goodwin group at Oxford finished the session with a talk on his detailed study of wüstite. Previous literature regarding this mineral is rather conflicted owing to its non-stoichiometry.

The conference was a great success with really great talks from students and from highly respected academics of the materials chemistry community. A poster prize session ended the conference around lunchtime leaving plenty of time to do some last minute Christmas shopping in the beautiful city centre of Bath.

Daniel Cook (University of Warwick)

PCG-SCMP COMMITTEE

ACKNOWLEDGEMENT

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

Emma McCabe, Kent