SCMP @ IoP PCG PCG @ BCA

Newsletter

Autumn 2011

FROM THE CHAIR

Welcome to the Physical Crystallography Group-Structural Condensed Matter Physics Group Autumn 2011 Newsletter!

Firstly, I'd like to take this opportunity to say that I look forward to acting as the group Chair over the next few years, and working with the other two new officers (Matt Tucker, Vice-Chair and Kirsten Christensen, Secretary / Treasurer) and the rest of the Committee. I would also like to thank Dave Keen for his three years of excellent service as the Group Chair, and I'm happy to say that Dave will continue to contribute to the PCG-SCMP leadership as a Committee member. Last but not least, I would like to thank Sarah Tallentire for taking over as the PCG-SCMP Newsletter Editor.

Since the last Newsletter issue, there have been several interesting conferences, details of future meetings have been announced and a few general notable issues have arisen. I hope you will enjoy reading about these in this Newsletter.

For me personally, the highlight of recent conferences was the PCG Plenary Lecture entitled "Crystallography in cultural heritage", given by Gilberto Artioli (Università di Padova) at the BCA Spring Meeting 2011. I thought Gilberto offered a perfect mix of high-quality rigorous scientific content and a fascinating wider story.

As you may know, at the AGM at Keele there was a discussion on the possible group name change, which was followed by an online consultation. This discussion, initiated by the Committee, was inspired by occurrences of low attendances of the BCA meeting sessions with a "pure physics" focus. We were keen to learn the reasons for this, and whether any group "rebranding" could boost the involvement of our physics-based colleagues in the BCA Spring Meetings. While different views were heard at the AGM, there were very few responses to the online consultation. On balance, there hasn't been sufficient support to the name change in general, nor clear agreement on possible alternative names.

Looking at future events, our Winter Meeting will follow 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, on Thursday and Friday 3rd/4th November. As in previous years, the meeting will be supported by ISIS Crystallography Group and the Institute of Physics. The meeting theme will be "Applied Physical Crystallography". The programme is currently being developed, but will be updated regularly at: http://www.pcgscmp.org/Meetings/Winter2011, where you can also find a link to the online registration form. I hope you will be able to join us for what has become a very successful, intensive two-day meeting.

I'm pleased to say that plans are underway to hold the Durham Powder Diffraction & Rietveld Refinement School next spring, 25-29th March 2012. Further details will be circulated by the organisers later this autumn.

Slightly further down the line, we are the lead group for the BCA Spring Meeting 2012, which will take place in April next year. You can find the titles of the planned symposia in this Newsletter, and I would like to invite members to submit abstracts for contributed talks, for which there should be slots available in each session.

In another recent development, the BCA have decided to recruit representatives from each group to lead education and outreach activities. I'm delighted to announce that the PCG-SCMP education representative will be Professor Mike Glazer.

This year, we again had high-quality PANalytical Thesis Prize competition. The prize was awarded to Dr. Stewart Bland (Department of Physics, Durham University) for his thesis entitled "X-ray Scattering Studies of Charge and Orbital Ordering in Transition Metal Oxides". We are very grateful to PANalytical for continuing to sponsor the Thesis Prize. In addition, in 2012 we will be awarding the prestigious IoP-sponsored Physical Crystallography prize. The calls for nominations for both prizes can be found in this Newsletter.

Ivana Evans
PGG-SCMP Chair

ANNOUNCEMENTS

IoP Physical Crystallography Prize 2012

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. The Physical Crystallography Prize currently consists of a cash award plus expenses for attending the Spring Meeting to deliver the Prize Lecture.

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 2012 and the Prize will be awarded at the 2012 BCA Spring Meeting at Warwick University, 16-19th April 2012.

PANalytical Thesis Prize 2012

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 2010 to 31st December 2011.

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 2012 and the Prize will be awarded at the 2012 BCA Spring Meeting at Warwick University, 16-19th April 2012.

Vacancies on the PCG-SCMP Committee

Call for Nominations

A vacancy for the position of General Member is arising on the PCG-SCMP Committee. Nominations for this position are invited and should be sent to the current Secretary/Treasurer, Kirsten Christensen (kirsten.christensen@diamond.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 take on the leadership responsibilities for the group, and to contribute to the Committee efforts by actively participating in BCA and PCG-SCMP meetings and meeting organisation. Informal enquiries about the committee members' roles should be directed to the current Chair (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 Warwick University, 16-19th April 2012.

EDUCATION

Professor Mike Glazer has started acting as the PCG-SCMP education coordinator. There is a new Education section on our web pages (http://www.pcg-scmp.org/Education), which already contains a number of useful educational resources and links.

It would be useful if PCG-SCMP members could suggest any changes or additions to this site. Please send your suggestions to Mike Glazer at: glazer@physics.ox.ac.uk.

FUTURE EVENTS

Meeting Calendar

- PCG Autumn Meeting and ISIS Crystallography Users Meeting, 3rd-4th November 2011, Cosener's House, Abingdon
- Condensed Matter and Materials Physics (CMMP 11), 13-15th December 2011, Lancashire County Cricket Club, Manchester
- BCA Spring Meeting, 16-19th April 2012, Warwick University

PCG Autumn Meeting, 3rd-4th November 2011, Cosener's House, Abingdon

Following the success of the format used the last couple of years, the PCG Autumn meeting will take place at the Cosener's House, Abingdon, 3rd-4th November 2011 (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 "Applied Physical Crystallography". We hope that the meeting will be of interest to a wide audience, from experienced researchers to PhD students. Confirmed scientific presentations include:

Paul Attfield (Edinburgh) Title TBC

Katharina Fucke (Durham) "*Water structure is important - OH...pi hydrogen bonds in p-sulfonatocalix[4]arene"*

Jon Goff (Royal Holloway) Title TBC

Alexander Korsunsky (Oxford) "*Synchrotron X-ray micro-beam methods"*

Panagiota Manti (Cardiff) "*The Cu_6Sn_5 phase 'problem' of tinned archaeological bronzes*"

Stefan Norberg (Chalmers, Sweden) "*Neutron scattering studies of SOFC oxides"*

Ian Wood (UCL) "*Post-perovskites and the deep earth"*

A poster session will take place in the evening of 3rd November 2011.

The full scientific programme and the timetable will be posted on the PCG-SCMP wiki (www.pcg-scmp.org).

To register for the meeting, please follow the link given at www.pcg-scmp.org. The closing date for registration is 24th October, 2011.

CMMP, 13-15th December 2011, Lancashire County Cricket Club, Manchester

CMMP 2011 will take place from Tuesday 13th December to Thursday 15th December 2011 at Lancashire County Cricket Club. Scientific sessions and confirmed invited speakers include the following:

Plenary lectures

Prof. C Bechinger (University of Stuttgart)

Prof. Y M Gupta (Washington State)

Prof. A Mackenzie (University of St Andrews)

Local structures of functional materials

Prof. M Dove (Queen Mary, London)

Structural studies of nanomaterials

Prof. I Robinson (UCL)

BCA Spring Meeting, 16-19th April 2012, Warwick University

The BCA Spring Meeting 2012 will take place from Tuesday 16th April to Thursday 19th April 2012 at Warwick University. The PCG plenary will be given by Prof. Branton Campbell from Brigham Young University, Utah, USA, and is entitled "Symmetry modes: Nature's favoured description of structural distortions."

PCG sessions at the meeting will include:

- Multidimensional materials
- Hydrogen bonding: from water to supermolecules

- Phase transitions: distortion mode analysis

The deadline for abstract submission for oral and poster contributions is 16th January 2012.

The scientific programme and further details about the conference will appear at: http://crystallography.org.uk/spring-meeting-2012.

NEWS

Prizes and awards

PANalytical Thesis Prize 2011

The PANalytical Thesis Prize in Physical Crystallography 2011 was awarded to Dr. Stewart Bland (Department of Physics, Durham, and now Elsevier) for his thesis entitled "X-ray Scattering Studies of Charge and Orbital Ordering in Transition Metal Oxides".

Stewart has used both hard and soft X-ray resonant diffraction to investigate charge and orbital ordering in a number of systems. Notably he has shown that the resonant scattering signal from magnetite can be fully described by a simplified charge ordered structure without the need to invoke complicated orbital configuration. Also a successful soft X-ray scattering experiment was performed on lutetium ferrate, which was previously believed to be an orbital glass system. Stewart has shown that lutetium ferrate is actually ordered in contrast to previous conclusions.

Stewart Bland (Department of Physics, Durham University) receiving the PANalytical Thesis Prize 2011 from Dr Paul O'Meara of PANalytical

PCG Poster Prize

The PCG Poster Prize was this year given to Jonathan Coome (Durham) for his poster entitled: "Masquerade: Improving Data Quality with Masks for Beryllium Rings".

Jonathan Coome (Department of Chemistry, Durham University) receiving the PCG Poster Prize from Dave Keen (ISIS)

RECENT EVENTS

BCA Spring Meeting, 13–15th April 2011, Warwick University

The BCA Spring Meeting 2011 featured 25 scientific sessions, including five PCG symposia:

- New Developments at Diamond
- Local Structure
- High Pressure and Energetic Materials
- Time Resolved Structural Science
- Cultural Heritage

The PCG Plenary lecture was given by Gilberto Artoli (Università di Padova) and chaired by Ivana Evans. Gilberto applied modern analytical techniques to (literally) age old problems in his talk "Crystallography in the Cultural Heritage: Personal Experiences".

Ivana Evans with the PCG Plenary speaker, Gilberto Artoli (Università di Padova)

From the designs of early Greek astronomical measuring devices extracted from 3D tomography

to the determination of whether some ancient objects had been hammered into shape or slow cooled to form (large) single crystals, Gilberto has used scientific techniques to open up and answer questions from the past. He has also cast light on the necessary precautions when storing ancient flint tools as cushions designed to protect these artefacts can in turn react with them to form dyes and change the colours of the tools. Overall this was a fascinating tour through the world of applied crystallography in cultural studies.

Helen Maynard-Casely has reviewed several of the PCG sessions at the Spring Meeting:

New developments at Diamond

This session focused on techniques that are perhaps new directions and used for 3rd generation synchrotron light, such as that delivered by the Diamond Light Source. The first speaker was Professor Ian Robinson from University College London. His work on beamline I13L at Diamond Light Source centres on developing imaging with coherent X-ray diffraction. Professor Robinson's group are now able to obtain quantitative three-dimensional maps, which show the nanometre scaled strain on their single crystals of gold and silver.

Dr Steve Baker, from University of Leicester, presented how magnetic properties in nano-particles can be tailored with detailed knowledge of their crystal structure. Using EXAFS on beamline I18 at Diamond Light Source, Dr Baker is able to observe that the magnetic moment of his nano-particles increases with the increase in lattice parameter, which was achieved by heating the sample.

The last talk in the session, given by Jawaard Darr of UCL, detailed advances in high throughput analysis. As a synthetic chemist he has used a hydrothermal synthesis method to automate much of the synthesis process, allowing wider and more controlled mixing across the input materials. As an example he presented a thorough mapping of the ternary CeO_2-ZrO_2-$YO_{1.5}$ system. Collecting data on the high resolution powder diffractometer I11 at Diamond Light Source allowed Dr Darr to obtain detailed results on molecular volume, crystallite size and phase behaviour across the ternary system.

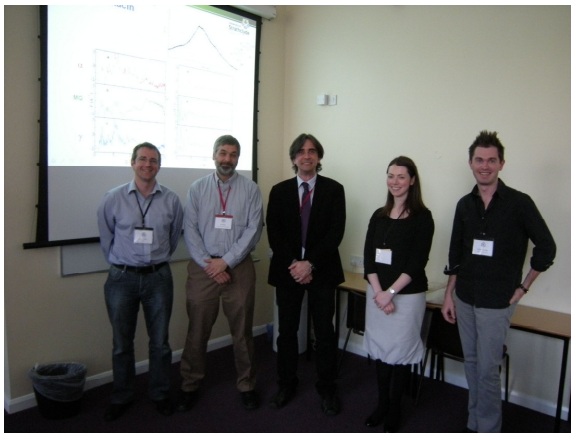
Speakers at the New Developments at Diamond Session: Jawwad A. Darr (UCL), Ian Robinson (London Centre for Nanotechnology), Session Organiser Dave Keen (ISIS) and Steve Baker (Leicester).

Local structure

Dr Serena Corr from the University of Kent presented her work with pair distribution functions to probe the insulator transition in nano-scale rutile-type VO_2. The transition which occurs at 340 K (changing symmetry from monoclinic to triclinic), was investigated by charting the change in V-V distances. Dr Corr was able to show that there was no intermediate phase as had been previously speculated.

The second speaker, Dr Joe Hriljac from University of Birmingham, discussed the use of pair distribution functions in studying amorphous zeolites that form under pressure. Dr Hriljac presented work both on samples that had been recovered from high-pressure treatment and data that had been collected *in-situ* within a diamond anvil cell. Previous studies on amorphous zeolites had suggested that the amorphisation occurs leaving the individual sodalite cages intact. However, Dr Hriljac's results indicate that this view is incorrect and that the local structure of amorphous zeolites is likely to be much more complex.

The last speaker in this session was Dr Alistair Florence from the Institute of Pharmacy at the University of Strathclyde. He discussed the often-overlooked and discarded amorphous 'polymorphs' of pharmaceutical compounds. Dr Florence pointed out that amorphous materials can show some enhanced properties in view of drug delivery, particularly in solubility. He presented a pair distribution function study of Carbanazepine that showed that a particular amorphous phase of this compound was in fact a nano-crystalline sample of its monoclinic form.



Speakers at the Local Structure Session: Session Organiser Matt Tucker (ISIS), Joe Hriljac (Birmingham), Alistair Florence (Strathclyde), Serena Corr (Kent) and co-chair Andrew Goodwin (Oxford).

High pressure and energetic materials

Professor Colin Pulham of Edinburgh University presented his work on high-pressure polymorphs of high-energy materials. In particular he discussed his group's work on azide compounds and the compound FOX-7, which, under ambient conditions, has a layered structure that is stabilised by hydrogen bonding. Prof Pulham's aim was to investigate if this hydrogen bonding could be modified, with the eventual aim to be able enhance the desired properties of these types of materials.

The second speaker was Dr Martin Davis, from University of Sheffield who presented work on attempting to synthesise nitrogen rich polyazides. He described some of the difficulties working with samples of this type, and the structural trends in the compounds that have been synthesised to date. One of the biggest issues in his field was that DFT calculations are not able to adequately predict the sensitivity of a given compound. As sensitivity is a key physical property in the usability and safety of working with energetic compounds, this remains quite a challenge to the community.

Helen Maynard-Casely (Australian Synchrotron)

Time-resolved structural science

Dave Allen chaired a joint session across the PCG, CCG and BSG entitled Time-Resolved Structural Science. Speakers included Jacqui Cole (Cambridge), Simon Kimber (ESRF) and Thomas Penfold (Lausanne).

Speakers at the Time Resolved Structural Science Session: Session Organiser Dave Allen (Diamond), Jacqui Cole (Cambridge), Simon Kimber (ESRF) and Tom Penfold.

Cultural Heritage

Our final PCG session followed on from the PCG Plenary Session given by Gilberto Artoli. Talks were given by Liana Vella-Zarb (Heritage Malta), Andy Smith (STFC, Daresbury) and Margaret West (West X-ray Solutions Ltd). The session was chaired by David Taylor and Winfried Kockelmann (ISIS).

Speakers at the Cultural Heritage Session Liana Vella-Zarb (Heritage Malta), Andy Smith (STFC - Daresbury), Margaret West (West X-ray Solutions Ltd) and Organiser David Taylor.

IUCr Meeting, 22nd-29th August 2011, Palacio Municipal de Congresos Madrid

The 22nd International Union of Crystallography (IUCr) conference was held in the Palacio Municipal de Congresos in Madrid, Spain. The venue covered four floors with state-of-the-art facilities and easily catered for the almost 3000 participants at the largest and most comprehensive crystallography conference held every three years. The topics up for presentation reflected the breadth and diversity of

crystallography. There were large plenary lectures on the macromolecular structure and dynamics of the ribosome given by four Nobel laureates, along with associated protein crystallography microsymposia. Futhermore, the range of topics included microsymposia on X-ray absorption spectroscopy, energy related materials and structure property relationships of graphene and its derivatives. There was even a whole afternoon session on different ways to educate current undergraduate students about crystallography through using some of the currently existing crystallographic software. One of the major topics of the conference that I enjoyed was the latest results and progress of X-ray free electron lasers (XFEL). These are the newest machines to be built and have a brightness of X-ray pulse many orders of magnitude above that of synchrotrons (which were previously the best X-ray sources in the world). Furthermore due to extremely short X-ray pluses from the XFEL, time-resolved pump probe diffraction studies down to the femtosecond time scale can be investigated. This current up and coming research is directly related to my current research into the excited state structures of dyes for dye sensitized solar cells. The sessions on XFEL progress have given me ideas for future experiments and possible research avenues. I also found the microsymposia of solid state photochemistry and quantitative real space electron imaging very helpful as many of the leading figures in the field of time-resolved X-ray diffraction gave enlightening talks.

Kian Sing Low (University of Cambridge)

The International Union of Crystallography (IUCr) was held in Madrid during late August. I very much enjoyed this conference, and will be sharing with you some of the most memorable moments and scientific highlights.

Professor Omar M. Yaghi, sparked the interest and curiosity of many scientists as the full lecture theatre awaited his plenary talk. Yaghi shared with us his enthusiasm for metal-organic frameworks (MOFs) and their promising future as functional materials. To my surprise, he announced that MOF-74 had been used as a hydrogen store within a car for a tour around the world. There were many talks on MOFs throughout the week, and a particularly stimulating talk about guest/host reversible interactions from Alessia Bacchi. Her examples showed that, by tuning the local control of the framework interactions, a desired collective behaviour could be achieved. Diffuse scattering was well introduced by Richard Welberry, captivating and amusing the audience with his introductory slide: “diffuse rings to rule them all”. The work he described involved diffuse scattering observed in a protein crystal.

Nobel Prize laureate Thomas Steitz was allocated the first lecture of the conference to show his work on the ribosome. Many animations were shown to convey the mechanisms involved. One in particular was very memorable, and involved the ribosome carrying out translation with the Star Wars theme tune as background music.

The scale of the MOF research impressed me, and as a PhD student also working in this field, it allowed me to contextualise my research. I found the poster sessions very useful, in particular, discussing my work with different specialists and getting new ideas for further work. I would like to thank the structural condensed matter group for their help in funding this conference.

Ines Collings (University of Oxford)

ACKNOWLEDGEMENT

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

Sarah Tallentire, Durham

PCG-SCMP COMMITTEE

Dr. Ivana Evans, Chair
Department of Chemistry
Durham University
ivana.radosavljevic@durham.ac.uk

Dr. Matt Tucker, Vice-chair
Rutherford Appleton Laboratory
matt.tucker@stfc.ac.uk

Dr. Kirsten Christensen, Secretary/Treasurer
Diamond Light Source
kirsten.christensen@diamond.ac.uk

Dr. Dave Allan
Diamond Light Source

Dr. Andrew Goodwin
Department of Chemistry
University of Oxford

Prof. David Keen
Rutherford Appleton Laboratory

Dr. Helen Maynard-Casely
Australian Synchrotron

Dr. Christoph Salzmann
Department of Chemistry
UCL

Dr. Sarah Tallentire
Department of Chemistry
Durham University

PCG-SCMP Autumn Meeting
ISIS Crystallography Users Meeting

"Applied Physical Crystallography"

3rd-4th November 2011, Cosener's House, Abingdon

ISIS Facility Update

Crystallography Instrument and Software Update

Open Discussion

Scientific Presentations:

Paul Attfield (Edinburgh) Title TBC

Katharina Fucke (Durham) "*Water structure is important - OH...pi hydrogen bonds in p-sulfonatocalix[4]arene*"

Jon Goff (Royal Holloway) Title TBC

Alexander Korsunsky (Oxford) "*Synchrotron X-ray micro-beam methods*"

Panagiota Manti (Cardiff) "*The Cu_6Sn_5 phase 'problem' of tinned archaeological bronzes*"

Stefan Norberg (Chalmers, Sweden) "*Neutron scattering studies of SOFC oxides*"

Ian Wood (UCL) "*Post-perovskites and the deep earth*"

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

www.pcg-scmp.org