

SCMP @ IoP PCG @ BCA

Newsletter

Spring 2012

www.pcg-scmp.org

FROM THE CHAIR

Welcome to the Physical Crystallography Group-Structural Condensed Matter Physics Group Spring 2012 Newsletter. By the time you're reading this, the BCA Spring Meeting 2012 will be just over two weeks away. This year, the meeting returns to the University of Warwick, and will take place from 16th – 19th April. Further details of the meeting are available later in this Newsletter and online at www.crystallography-meetings.org.uk, where you can also register for the meeting.

Since the last newsletter, the group have organised, contributed to and supported a number of events.

The PCG-SCMP winter meeting was again held jointly with the ISIS Crystallography User Group Meeting at the Coseners House over a couple of days in early November 2011. It was well-attended and featured a number of high-quality scientific talks and posters. Thanks to Matt Tucker and Dave Keen for being the reliable expert-organisers of this popular meeting!

In December 2011, the group contributed to the Condensed Matter and Materials Physics annual conference. Thanks again to Dave Keen for organizing two symposia: "Local Structures of Functional Materials" and "Structural Studies of Functional Materials".

Finally, my personal thanks go to the IoP for their financial support (via the PCG-SCMP) for the 6th Powder Diffraction & Rietveld Refinement School at Durham University, which has just finished. Literally as I write this, 64 incredibly hard-working students are leaving Durham to return to various places in the UK, and their homes as far away as India, Thailand, USA, Canada, Mexico and Brazil (plus 11 European countries)! Possibly the only people more tired than them at this time are the School teachers, organisers and tutors, each and every one of whom I must thank personally. John Evans (Durham): organiser, lecturer and tutor, and generally the mastermind behind the School; lecturers and tutors Jeremy Cockcroft (UCL) and Andy Fitch (ESRF); tutors Emma McCabe (Durham) and Sarah Tallentire (Durham); our guest tutor Cora Lind (University of Toledo, spending her sabbatical at Durham); and the part-

time tutors Andrew Goodwin (Oxford) and Andrew Tuxworth (Durham). Adjectives "brilliant", "unbelievable" and "awesome" come up again and again in the student questionnaires, which I have just gone through.

The breadth of education and culture amongst the PDRR 2012 School participants is best illustrated by the variety of questions they tackled successfully at the Bar Quiz and Treasure Hunt evenings. They included: "Name the Mexican actor, star of The Motorcycle Diaries, who shares his last name with a British scientist who was a research student of Sir William Bragg and a research supervisor to Dorothy Hodgkin."; "List yttria, ferrocene, pyrochlore and rutile structures in the order of increasing space group serial number." (It was reassuring to see that the tutors' table correctly gave the actual space group numbers and symbols, too!); "Name the city and the building which boasts the largest brick dome ever constructed." (This question created a bit of a debate among our Italian participants!).



Powder Diffraction & Rietveld Refinement School 2012, Durham University

Finally, I would like to say a couple of additional "thank you"s to two people who have contributed generously to the committee and to the group's activities over the last few years: Sarah Tallentire and Andrew Goodwin.

Best wishes,

Ivana Evans
PCG-SCMP Group Chair

ANNOUNCEMENTS

Vacancies on the PCG-SCMP Committee

Call for Nominations

There are two vacancies arising on the PCG-SCMP Committee, one for Treasurer and one for an ordinary member. Nominations for these positions are invited and should be sent to the current Honorary Secretary/Treasurer, Kirsten Christensen (kirsten.christensen@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 Warwick University, 17-19th April 2012.

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).

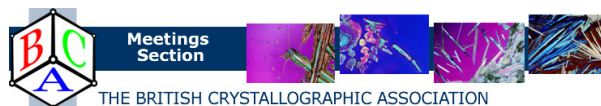
For further information please contact the PCG-SCMP Honorary Secretary/Treasurer (kirsten.christensen@chem.ox.ac.uk) or visit the relevant Institute of Physics web page (http://www.iop.org/about/grants/research_student/page_38808.html).

FUTURE EVENTS

Meeting Calendar

- BCA Spring Meeting, 16-19th April 2012, Warwick University
- UK Neutron and Muon Users Meeting 2012, 17th April, 2012, RAL
- Electron Crystallography School, 16th – 20th June 2012, Stockholm, Sweden
- European Crystallographic Meeting ECM27, 6th – 11th August 2012, Bergen, Norway
- Synchrotron Radiation School, 24th – 28th September 2012, Diamond Light Source, Didcot
- European Powder Diffraction Conference EPDIC13, 28th – 31st October 2012, Grenoble, France

BCA Spring Meeting, 16–19th April 2012, University of Warwick



The BCA Spring Meeting 2012 is themed "Challenges in Crystallography". The meeting begins with the young crystallographers' satellite session on Monday 16th April, and the main meeting will follow the successful format of recent years and runs from 12:15 on Tuesday 17th April to 13:30 on Thursday 19th April.

The PCG Teaching Plenary lecture, entitled "Symmetry Modes: Nature's Favoured Description of Structural Distortions", will be given by Professor Branton Campbell (Brigham Young University, USA) on **Thursday, 19th April**. PCG parallel sessions and speakers include:

Multidimensional Materials (Tuesday 17th April)

Mark Weller (Southampton) *Transition Metal Fluorophosphates: New Structural Motifs and Crystallographic Challenges*

Valeria Nicolosi (Oxford) *Atomic Resolution Imaging of Two-dimensional Nanomaterials*

Paul Saines (Cambridge) *Facile Synthesis and Structural Diversity of Nanosheets of Inorganic-Organic Frameworks*

Elena Marelli (Reading) *The Structure of CuNi(CN)₄: A Simple Cyanide Containing Cu(II) in a Square-Planar Environment*

Piecing Together the Puzzle: Multidimensional Approaches (Tuesday 17th April)

Lynne Thomas (Bath) *Beyond the Structure: Investigating Physical Properties in Molecular Materials*

Andrew Goodwin (Oxford) *Frameworks, Flexibility and Frustration*

Mark Eddleston (Cambridge) *A Novel Approach to Crystal Structure Determination Combining Crystal Structure Prediction and Transmission Electron Microscopy.*

Christopher H. Woodall (Bath) *An Investigation in the Luminescent Behaviour of Gold(I) Trimers at Variable Temperature and Pressure.*

H-bonding: From Water to Supramolecules I (Wednesday 18th April)

Benjamin Murray (Leeds) *The Structure of Ice Crystallised from Supercooled Water*

Angelos Michaelides (UCL) *Ice Nucleation at Surfaces*

Dominic Fortes (UCL) *More Ice than Salt – New Observations of $M^{2+}XO_4$ Cryohydrates*

H-bonding: From Water to Supramolecules II (Wednesday 18th April)

Doris E. Braun (UCL) *Contrasting Organic Hydrate Structures Generated in Silico to in vitro*

Laszlo Fabian (UEA) *Cocrystal Design: Interactions and Properties*

Miren Ramirez (Birmingham) *Hydrogen Bonding and Conformation in Salts of Diclofenac*

Phase Transitions I: Distortion Mode Analysis (Thursday 19th April)

John S. O. Evans (Durham) *Symmetry Mode Analysis of Functional Materials*

Mark Senn (Edinburgh) *The Verwey Structure of Magnetite: Charge Order and Three-Site Distortions*

Philip Lightfoot (St. Andrews) *New Twists on the Perovskite Theme: The Elusive Phases R and S of $NaNbO_3$*

Phase Transitions II: Transformations in the Solid State (Thursday 19th April)

Kenneth Harris (Cardiff) *Structural and Dynamic Aspects of Phase Transitions in Solid Inclusion Compounds*

Spoothi Dharmayat (Pfizer) *Solid Form Transformations of Pharmaceutical Compounds*

Mateusz B. Pitak (Southampton) *Patterns in Aliphatic Amino-acid Phase Transitions*

Full details about the conference and the final scientific programme are available at: www.crystallography-meetings.org.uk

NEWS

Prizes and awards

IoP Physical Crystallography Prize 2012

IOP Institute of Physics
Structural Condensed Matter Group

The winner of the 2012 Physical Crystallography Prize will be announced at the BCA Spring Meeting at Warwick. The Prize Lecture will be delivered on Wednesday 18th April.

PANalytical Thesis Prize 2012



The winner of the PANalytical Thesis Prize in Physical Crystallography 2012 will be announced at the conference dinner, at the BCA Spring Meeting at Warwick.

RECENT EVENTS

PCG-SCMP Winter Meeting, 3rd – 4th November 2011, The Cosener's House, Abingdon

The PCG-SCMP Winter meeting was held jointly with the ISIS Crystallography User Group Meeting in the Coseners House, Abingdon on Thursday 3rd and Friday 4th November 2011. Delegates attended a series of talks around the theme of "Applied Physical Crystallography," as well as hearing about developments within crystallography at ISIS.

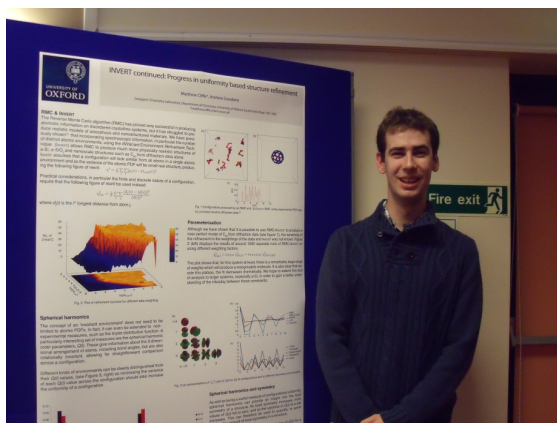
A lovely lunch welcomed weary travellers before the presentations began. The lecture series included talks from Robert Freer (Manchester) on multiferroics, Ian Wood (UCL) on perovskites found in the deep earth, and Alexander Korsunsky (Oxford) discussed materials stress probed by synchrotron techniques. All the talks were very well received.

Younger researchers also had the chance to present some of their work. Ines Collings (Oxford) shared her research on metal-organic frameworks, Sarah Tallentire (Durham) discussed

negative thermal expansion materials, Joe Paddison (Oxford) gave a talk on calculating magnetic structures from powder diffraction and Lewis Downie discussed structure property relations in some multiferroic materials.

The afternoon concluded with an update on the crystallography facilities at ISIS, and the ISIS Crystallography User Group Meeting.

The evening was spent enjoying a drink at the bar and an excellent dinner during which Matthew Cliffe, a PhD student with Andrew Goodwin (Oxford) was presented with a bottled prize for his poster "INVERT continued: Progress in uniformity based structure refinement".



Matthew Cliffe beside his prize-winning poster

The second morning saw another five research talks before the meeting drew to a close and everyone went their separate ways (though not before another delicious lunch!).

Katharina Fucke (Durham) opened the session with her work on water structure in calix{4}arenes, and the importance of OH... π hydrogen bonds. Next we moved on to solid oxide fuel cell materials, as Stefan Norberg (Chalmers) presented his work on vacancy distributions in δ -Bi₂O₃ and doped zirconia, investigated using RMC methods. Panagiota Manti (Cardiff) followed with a discussion of the problems with phase identification encountered when studying tinned archaeological bronzes, for example in Spartan helmets. The session restarted after coffee, and Paul Attfield (Edinburgh) intrigued us with 'The Mystery of Count Perovski's Anions', a look at anion ordering in perovskite oxynitrides. Jon Goff (Royal Holloway) concluded the meeting with his work on the thermoelectric material sodium cobaltate, and the heat recovery possibilities it presents.

Andrew Tuxworth (Durham) and Callum Young (Oxford)

CMMP Meeting, 12th - 15th December 2011, The Cosener's House, Abingdon

The Condensed Matter and Materials Physics annual conference took place 12th-15th December 2011 at the Lancashire County Cricket Ground at Old Trafford in Manchester. The conference was held at The Point, a brand new conference venue overlooking the famous cricket pitch, with some sessions held in the members' areas of the Old Pavilion. Understandably there was a strong cricket theme to the venue and cricket bats, signed by the current LCCC team were raffled during the meeting. Cricket enthusiasts were seen studying and photographing the test honours board in the pavilion at quiet points throughout the meeting!

The meeting was well attended, with around 360 participants and the symposia were grouped in parallel sessions of six symposia. The PCG/SCMP group organised two symposia, one with the title "Local Structures of Functional Materials" and the other "Structural Studies of Functional Materials". Both were reasonably attended with between 20 and 40 attendees throughout. We heard a wide variety of talks from invited experts to young students on topics from thin films to metallic nanoparticles to the dynamics of flexible bulk crystalline frameworks. Our invited speakers were Martin Dove (Queen Mary, London) who gave a talk on local structure with a strong teaching element and Ian Robinson (London Centre for Nanotechnology) who described his exciting recent results on imaging strain in nanocrystals with coherent diffraction. In addition, and amongst other subjects, we heard about the possible stabilisation of a high temperature crystal form of manganese at room temperature within a thin film (from Phil Hasnip, York), how molecular dynamics simulations can help understand the dynamic porosity in nanoporous organic frameworks (from Jelena Jordanovic, Liverpool) and how to grow and characterise InAs nanowires doped with phosphorus (from Ivan Isakov, UCL).

There were also a series of highly appealing plenary lectures throughout the meeting, perhaps highlighted by talks about the behaviour of networks "from the WWW to the cell" by A-L Barabasi (Northeastern, USA), work to replicate biological machinery by A Turberfield (Oxford) and the two prize lectures. The Wolfarth lecturer, C Marrows (Leeds), described artificial spin ice and the Mott lecturer, N Hussey (Bristol), talked about a Catch 22 situation within high-temperature superconductivity. We were very well looked after by Lancashire County Cricket Club, with excellent refreshments throughout and a very enjoyable conference buffet accompanied by a live jazz trio.

David Keen (Rutherford Appleton Laboratory)

Powder Diffraction and Rietveld Refinement Course, 25th - 29th March 2012, Chemistry Department, Durham

The 6th Powder Diffraction and Rietveld Refinement School, generously supported by IUCr, PCG-SCMP, CCP14, Bruker UK, Rigaku UK and Durham University, ran from Sunday 25th to Thursday 29th March. Lectures were given by Prof Andy Fitch (ESRF), Dr Jeremy Cockcroft (UCL), Dr Ivana Evans (Durham) and Prof John Evans (Durham). Tutorial groups were led by the lecturers and Dr Emma McCabe (Durham), Dr Sarah Tallentire (Durham) and Dr Cora Lind (Toledo). Dr Andrew Goodwin (Oxford), Mr Andrew Tuxworth (Durham) also acted as tutors during the morning and afternoon computer practical sessions respectively.

The School was attended by 65 students from 18 UK Universities and disciplines including Chemistry, Physics, Crystallography, Materials, Pharmacy and Engineering, 2 industrial (from Germany and the Netherlands) and 22 international students from Ireland, France, Germany, Belgium, Italy, Spain, Switzerland, Sweden, Denmark, Poland, Slovenia, Thailand, India, Mexico, Brazil, Canada and the USA.

The School combined lectures, small group tutorials and hands-on computer practicals. Lectures were used to introduce the basic concepts of crystallography, powder diffraction and Rietveld refinement. For each hour of lectures there was at least an hour scheduled for small group problems supervised by tutors to help reinforce the concepts. The remaining ~50% of the course was spent with students going through computer practicals at their own pace. Over 50 computer-based problems were available on a range of different topics, with many containing multiple sub-problems.

Based on the student feedback, we believe that the 2012 Durham Powder Diffraction and Rietveld Refinement School was very successful and that it addressed a key training need. The organisers anticipate running the 7th School at Easter 2014.



Students and tutors enjoying the problem sessions at the Powder Diffraction and Rietveld Refinement School, Durham

Sarah Tallentire (Durham)

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 16th April 2012, Warwick University

The YCG Satellite Meeting (16th–17th April) at the BCA Spring meeting has been one of the most subscribed YCG meetings yet, with the highest number of abstract submissions for oral contributions and posters. Presentations will be made mainly by Young Crystallographers, covering all areas of crystallography from proteins and transition metal complexes to modelling and instrumentation. Kenneth Shankland (University of Reading) and Robin Owen (Diamond Light Source) will be giving Plenary lectures and on the 17th April Lynne Thomas (University of Bath) will be giving the Parkin Lecture. A session on Science Outreach has also been included in the programme, highlighting the importance of engaging everyone in science.

Samantha Callear

PCG-SCMP AGM

The 69th PCG-SCMP AMG will take place at the BCA Spring Meeting at Warwick University, on Wednesday, 18th April 2012, 11:45 – 12:30. Elections for the positions of Treasurer and one Ordinary Committee member will be held at the AGM.

The meeting agenda includes the following items:

- Apologies for absence
- Minutes of the 68th PCG-SCMP AGM held in Keele, 13th April 2010
- Matters arising from minutes
- Chair's report
- Secretary/Treasurer's report
- Elections to PCG-SCMP Committee
- Future meetings
- Any other business

ACKNOWLEDGEMENT

Many thanks to everyone who has 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@chem.ox.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