

# PCG Autumn Newsletter

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## From the chair

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Autumn 2016 Newsletter! This issue brings you several meeting reports, information about future events and calls for nominations for awards - I hope you find it enjoyable reading.

It is in fact a year since our last newsletter owing to the committee reshuffle allowing time for our new members to find their feet. In such time there has been a multitude of meetings and events not least the annual BCA spring meeting in Nottingham. This was a very enjoyable meeting with lots of interesting talks, and in particular several high quality student talks during the YCG meeting and during the main meeting.

During the spring meeting we elected some new committee members, so I would like to formally welcome Jonathan Bean (York), Charlottle Kirk (Oxford) [co-opted] as ordinary members of the committee. Furthermore there have been some changes of roles on the committee and now I (Andrew Goodwin) have become chair, Helen Playford taken the role of secretary with Anthony Phillips continuing his role as treasurer. I would like to thank all committee members for their continued contribution during the year.

As usual our winter meeting was held in conjunction with the ISIS Crystallography User Group Meeting, at the Cosener's House, Abingdon, 31st October - 1st November 2016. As in previous years, the meeting was supported by ISIS Crystallography Group and the Institute of Physics. Helen Playford (ISIS) oversaw the scientific programme for the meeting. The meeting was even more oversubscribed than last year and the committee is considering increasing the size of this meeting to meet demand. Details on the meeting can be found on the web at [http://www.pcg-scmp.org/imagesFhj/7/7a/Winter\\_meeting\\_2016\\_program.pdf](http://www.pcg-scmp.org/imagesFhj/7/7a/Winter_meeting_2016_program.pdf) and a full write up appears later in the newsletter. I hope you will be able to join us next year for what has become a very successful, intensive two-day meeting.

There have also been a lot of excellent outreach activities this year, such as the Royal Institution digitising many old films of W.L. Bragg (see more later). Furthermore the committee is considering the idea of creating a PCG school for PhD students to learn topics "de rigueur" of physical crystallography.

Finally, I'd like to draw to your attention to the call for nominations that is being announced in this Newsletter. Owing to the continued generous support by PANalytical, we are inviting nominations for the PANalytical Thesis Prize 2017. Like last year, theses from a two year period are now eligible, so we hope this will help keep the competition as strong if not stronger than last year and also give more great PhD students a chance at the prize.

by ANDREW GOODWIN

## PANalytical 2017 Thesis Prize for Physical Crystallography

The PCG-SCMP 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 January 2016 to 31st December 2016. 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. The candidate must be a member of the Structural Condensed Matter Group of the IoP and/or the Physical Crystallography Group of the BCA. Non-members may enter the competition but will be required to join the IoP/SCMP or the BCA/PCG at the student rate to progress their nomination further. Note that 'roll-over' submissions from the previous year can be considered a second time. Full eligibility criteria and procedures for the PANalytical thesis prize can be found here. [http://www.pcg-scmp.org/imagesFhj/0/0e/The\\_PANalytical\\_Thesis\\_Prize\\_rules\\_v2.pdf](http://www.pcg-scmp.org/imagesFhj/0/0e/The_PANalytical_Thesis_Prize_rules_v2.pdf). To enter the competition, candidates must submit:

- a copy of the thesis in electronic format.
- 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 broadly defined on the website [www.pcg-scmp.org](http://www.pcg-scmp.org)) in the research.
- 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.

Nominations for the prize must be submitted to the PCG-SCMP Chair, Prof. Andrew Goodwin ([andrew.goodwin@chem.ox.ac.uk](mailto:andrew.goodwin@chem.ox.ac.uk)), by 22nd February 2017. The Prize will be awarded at the BCA meeting at University of Lancaster, 10th - 13th April 2017.

### Previous winners

- 2016 Andrew Cairns (Department of Chemistry, University of Oxford) "Mechanical and configurational degeneracy in transition metal cyanide materials"
- 2015 Josh Makepeace (Department of Chemistry, University of Oxford) "Light metal amides for hydrogen storage and ammonia decomposition"
- 2014 Alexander Hearmon (Department of Physics, University of Oxford) "Neutron, X-ray, and Optical Studies of Multiferroic Materials"
- 2013 Mark Senn (Department of Chemistry, University of Edinburgh) "Charge, Orbital and Magnetic Ordering in Transition Metal Oxides"

- 2012 Lucian Pascut (School of Physics, Bristol University) "Neutron and Resonant X-ray Scattering Studies of Low Dimensional Quantum Magnets"
- 2011 Stuart Bland (Department of Physics, Durham University) "X-Ray Scattering Studies of Charge and Orbital Ordering in Transition Metal Oxides"
- 2010 Helen Maynard-Casely (Department of Physics, University of Edinburgh) "The new mineralogy of the outer solar system and the high-pressure behaviour of methane"
- 2009 Aurora Cruz-Cabeza (Department of Chemistry, University of Cambridge) "On the Prediction, Rationalisation and Discovery of New Crystal Forms"
- 2008 Lars Lundegaard (Department of Physics, University of Edinburgh) "High-Pressure Diffraction Studies of Rubidium Phase IV"
- 2007 Lynne Thomas (Department of Chemistry, University of Glasgow) "Disorder in Substituted Benzenes by Combined Diffraction and Computational Studies"
- 2006 Andrew Goodwin (Department of Earth Sciences, University of Cambridge) "Dynamics from Powder Diffraction"
- 2005 Dominic Fortes (UCL) "Crystallisation of Ammonia Hydrates under High Pressure"

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## 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](http://www.pcg-scmp.org)). For further information please contact the PCG-SCMP Secretary Helen Playford ([helen.playford@stfc.ac.uk](mailto:helen.playford@stfc.ac.uk)) or visit the relevant Institute of Physics web page ([http://www.iop.org/about/grants/research\\_student/page\\_38808.html](http://www.iop.org/about/grants/research_student/page_38808.html)).

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## Future Meetings

- 3rd Annual APXPS Workshop, 12-14th Dec 2016,
- Diamond-CCP4 Data Collection and Structure Solution Workshop, 13-20th Dec 2016,
- 36th SSCG Christmas meeting - Loughborough/Keele, 19 - 20 Dec 2016  
<http://www.lboro.ac.uk/departments/chemistry/news-events/sscg-2016/>

The annual Christmas meeting of the Royal Society of Chemistry Solid State Chemistry group will take place at Loughborough University 19th and 20th of December, 2016. This years meeting will be heavily student and early career focussed so please submit abstracts for both posters and oral presentations. Further details about the conference can be found on the website:

### Plenary speakers:

Prof. Matt Rosseinsky, University of Liverpool  
Prof. Olle Eriksson, Uppsala University, Sweden

If you would like any further information, please contact Pooja Panchmatia ([p.panchmatia@lboro.ac.uk](mailto:p.panchmatia@lboro.ac.uk)) or Richard Darton ([r.j.darton@keele.ac.uk](mailto:r.j.darton@keele.ac.uk))

We look forward to welcoming you to Loughborough!

- The BCA Spring Meeting 2017 will take place at Lancaster University on 10-13th April 2017. Please see the conference website for registration and more details <http://www.bcaspringmeetings.org.uk/home>.

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## Outreach and Education

by MIKE GLAZER

Recently the Royal Institution has digitised many old films of W.L. Bragg (and even W.H. Bragg) and made them available on the internet at [www.rigb.org/our-history/bragg-film-archive](http://www.rigb.org/our-history/bragg-film-archive). This is the first tranche of videos with more to follow later on. This was made available through a grant from STFC which a number of us applied for a few years ago. There are many gems in the collection.

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## Recent Events

### PCG Winter Meeting (31st - 1st November 2016)

by SNEHA BAJPE, CARL ROMAO, EMILY REYNOLDS AND HAMISH YEUNG

The first session of scientific talks was opened by Professor Anthony Powell (Reading), who discussed a series of recent structural and electronic studies of layered materials for thermoelectric applications. These materials with 2-D structural motifs have highly structured electronic densities of states, potentially increasing their Seebeck coefficients. By incorporating dopants, the Fermi energy and phonon conductivity could be optimized. Kent Griffith from Prof Clare Grey's group in Cambridge presented results regarding lithium intercalation into several quenchable Nb<sub>2</sub>O<sub>5</sub> polymorphs. The various octahedral tilts in these polymorphs created topologically distinct microporous regions where lithium could be stored. The structure and dynamics of the lithium within Nb<sub>2</sub>O<sub>5</sub> was further elucidated using solid-state NMR. The session concluded with a presentation by Oxford's Professor Simon Clarke, who described soft-chemical modifications of superconductivity in FeSe<sub>2</sub>. The intercalation of lithium-containing layers between the FeSe<sub>2</sub> layers, and subsequent disorder of the iron atoms, was studied in-situ using neutron diffraction.

In the second scientific session, Jacqui Cole (Cambridge/ISIS) presented the first scientific results from recent instrument developments in in-situ neutron reflectometry for solar-cell applications, whereby dye-TiO<sub>2</sub> interfacial structures that comprises the working electrodes of dye-sensitized solar cells are elucidated. The electrolyte is shown to influence the nature of the dye binding to TiO<sub>2</sub>, revealing the importance of studies in the fully assembled photovoltaic device. Jacqui showed how structural studies are providing crucial underpinning information for modelling and interpretation of the reflectometry findings. Nottingham's Stephen Argent spoke about the contrasting CO<sub>2</sub> and CH<sub>4</sub> adsorption behaviours in porous metal-organic molecular solids. While CO<sub>2</sub> was found to adsorb strongly at open metal sites on the inorganic structural building units, CH<sub>4</sub> was found to favour positions where it made multiple long contacts with phenyl rings in the ligands. Next to present was QMUL's Ali Shehu, who presented his doctoral thesis work on defect structure and ionic conductivity of ytterbium-doped neodymium pyrochlore oxides. Yb<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> shows fully disordered fluorite structure while Yb<sub>1.5</sub>Yb<sub>0.5</sub>Zr<sub>2</sub>O<sub>7</sub> shows partial transition to pyrochlore structure. Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> displays almost completely ordered pyrochlore structure. The session concluded with an authoritative talk from Dr Ivana Evans

on the interplay between oxygen order/disorder transitions and ionic conductivity in a range of oxide ceramics.

Session three focussed on the role of neutrons in understanding complex structures and the useful complex properties that arise. Alex Gibbs (ISIS) discussed the role of quantum critical fluctuations in oxides to give low magnetic dimensionality where high resolution neutron diffraction is required to see long range magnetic order. A range of examples were used to demonstrate the variety of multifunctional materials grown and studied at Harwell's crystal growth facility. Finally, neutrons were shown to be ideal in the study of the decomposition of ammonia cracking catalysts in a talk by Oxford's Charlotte Kirk, as well as the microstructural strain due to lattice misfits in multiphase Co and Ti alloys used as aviation components - the appealing work of Cambridge's Dr Howard Stone.

The final session began with the 2016 PCG Thesis Prize lecture by Andrew Cairns (ESRF). Andrew supplemented a presentation of his DPhil studies with recent results demonstrating various interesting parallels between classical and exotic physical systems and the supramolecular frameworks he's studied. A series of short talks followed: hydration of Brownmillerites, new combined imaging + diffraction capabilities currently under commissioning at ISIS, and stacking fault analysis using powder diffraction. In the midst of these, Joe Paddison (Cambridge), gave an energised talk on emergent charge order in  $\text{Dy}_3\text{Mg}_2\text{Sb}_3\text{O}_{14}$ . The meeting concluded with an overview seminar by Prof Bill David FRS (ISIS / Oxford). "10 Decades of Powder Diffraction" traced the origins and key figures - some less well-known than others - of the field as we know it, and gave snippets of useful advice to young researchers. One of them was the daily greeting given by Albert Hull's boss at the General Electric Research Laboratory: not, "Have you solved that problem yet" but, "Are you having fun?" Hull went on to invent Powder X-ray diffraction (independently of Debye and Scherrer) and determined the crystal structures of iron and tens of other metals.

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## Jobs and Studentships

**PhD project:** Understanding the Microscopic Mechanisms in Functional Materials

**Supervisor:** Dr Mark Senn

**Deadline:** 31st January 2017

**Project description:** The project will involve understanding why particular structures and chemistries give rise

to specific physical properties. The successful candidate will gain experience in making novel ceramic materials and characterizing their physical properties and crystal structures. A particular emphasis of the project will be on understanding the microscopic atomic displacements associated with the properties of piezoelectricity, ferroelectricity and magnetoelectricity. In situ and ex situ diffraction experiments will be conducted at synchrotron and neutron facilities by the student to support this work. The insight gained will allow for the design of improved functional materials for use in the electronics industry.

**Requirements:** The studentship provides 3.5 years of funding for UK/EU students, starting October 2017. Applicants should have or be about to receive an honours degree (at least II.1 or equivalent) in Chemistry, Physics or Material Science. Practical experience in the field of ceramic synthesis, crystallography and/or physical property characterization is desirable, and an interest in learning about all of these is essential.

**How to apply:** Please direct informal enquiries and requests for further information to Dr Mark Senn (m.senn@warwick.ac.uk) in the first instance. More details of the research conducted within the group can be found at [www.senngroup.com](http://www.senngroup.com).

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## Acknowledgement

Many thanks to everyone who has contributed to this issue of the PCG-SCMP newsletter. Jonathan Bean (York)

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## PCG - SCMP Committee

**Chair:** Professor Andrew Goodwin

**Address:**

Inorganic Chemistry Laboratory University of Oxford

**Email:** [andrew.goodwin@chem.ox.ac.uk](mailto:andrew.goodwin@chem.ox.ac.uk)

**Treasurer:** Dr Anthony Phillips

**Address:**

Centre for Condensed Matter and Materials School of Physics and Astronomy Queen Mary University of London

**Email:** [a.e.phillips@qmul.ac.uk](mailto:a.e.phillips@qmul.ac.uk)

**Secretary:** Dr Helen Playford

**Address:**

STFC ISIS Facility Rutherford Appleton Laboratory

**Email:** helen.playford@stfc.ac.uk

**Education and Outreach:** Professor Mike Glazer

**Address:**

Clarendon Laboratory Parks Road Oxford OX1 3PU University of Oxford

**Email:** mike.glazer@physics.ox.ac.uk

**Ordinary Committee Members**

Professor Philip Lightfoot, University of St Andrews

Dr John Claridge, University of Liverpool

Dr Nicholas Funnell, University of Oxford

Dr Alexandra Gibbs, STFC ISIS Facility

Dr Emma McCabe, University of Kent

Dr Paul Saines, University of Kent

Dr Mark Senn, University of Oxford

Mr Jonathan Bean, University of York

**Co-opted Members**

Miss Charlotte Kirk, University of Oxford, Young Crystallographer liaison