

SCMP @ IOP PCG @ BCA

# Newsletter

Spring 2007

## EDITORIAL

It is my pleasure to present to all Members of the PCG-SCMP Group the first issue of the Group Newsletter, and I would particularly like to thank Ivana Evans for the time and effort invested in this initiative.

In the last few years, the PCG-SCMP Committee has been very active in pursuing the Group objectives. In particular, we regularly organise annual Winter Meetings covering one of the topics in our Portfolio ([http://www.pcg-scmp.org/Topics:PCG\\_Portfolio](http://www.pcg-scmp.org/Topics:PCG_Portfolio)), and over the years we have offered to our Members what we believe is a good array of training workshops and schools. In January, a very successful edition of the PCG Rietveld Refinement School was run in Durham (see report in this issue), whereas next year will see the third edition of the very popular Magnetic Rietveld Workshop, traditionally held in the Coseners' House in Abingdon, Oxfordshire. The Group also sponsors a number of bursaries to attend overseas conferences, and awards two prestigious prizes – the annual PANalytical Thesis Prize for Physical Crystallography (the call for nominations is still open for the 2007 edition), and the Physical Crystallography Award, assigned biennially to recognise early-career achievement in our field.

In addition, we have identified communication with the Membership as the top priority for the Committee. We will endeavour to provide different fora for Members to convey their proposals and ideas to the Committee. Clearly, this Newsletter is an important part of this strategy, but is by no means the only one. Thanks to the effort of Matt Tucker, we launched a new Group web site, (<http://www.pcg-scmp.org>), which takes the form of a "WIKI". This means that each member is free to edit the web pages, add links to related events and contribute to the discussion page.

Finally, I particularly wish to thank two Committee members for their services – Jon

Wright, who served his full term of office, and Mina Golshan, who moved on to a new career. As a result of this, the Committee is seeking nominations to replace two of its members.

A final word and a plea to all our Members: in my view, the PCG-SCMP Group is a resource for the UK Physical Crystallography community, particularly for its youngest members. Please, take full advantage of this resource, and let us know how you want it to change and grow to best serve your needs and interests.

Paolo G. Radaelli  
PGG-SCMP Chairman

## ANNOUNCEMENTS

### PANalytical Thesis Prize in Physical Crystallography

#### Call for Nominations

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 September 1st 2005 to December 31st 2006. The amount of the prize, which will be sponsored by PANalytical Ltd, will be £500. 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 at the student rate (currently £7.00) to progress their nomination further.

To enter the competition, candidates must submit:

- a copy of the Thesis on CD-ROM.
- 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 interpreted below 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 Chair of the Physical Crystallography Group, Prof. Paolo Radaelli ([p.g.radaelli@rl.ac.uk](mailto:p.g.radaelli@rl.ac.uk)), by 10<sup>th</sup> of April 2007 and the prize will be awarded at the 2007 BCA Spring Meeting in Canterbury, 17<sup>th</sup> -19<sup>th</sup> April 2007.

### **Vacancies on the PCG-SCMP Committee**

#### **Call for Nominations**

There are a number of ordinary member vacancies on the PCG-SCMP Committee. Nominations for these positions are invited and should be sent to Matt Tucker ([m.g.tucker@rl.ac.uk](mailto:m.g.tucker@rl.ac.uk)) by 10<sup>th</sup> April 2007. They 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.

### **FUTURE EVENTS**

#### **BCA Spring Meeting, 17th-19th April 2007, Canterbury**

This year's Spring Meeting is hosted by the University of Kent at Canterbury, with "New Methods and Innovation" as its overall theme and sixteen scientific sessions scheduled to take place. In addition, the Young Crystallographers meeting will be held before, and the Sam Motherwell Symposium after the main meeting. One of the three named BCA lectures this year, the Bragg Lecture entitled "Quasi-Crystals and Non-local Assembly: A Quantum-Theory Foundations Issue", will be given by Sir Roger Penrose.

Full scientific programme and the registration details can be found at the meeting website:

[www.crystallography-meetings.org.uk](http://www.crystallography-meetings.org.uk)

### **The full programme of the PCG sessions**

#### ***PCG Keynote lecture: Tuesday 14.00-14.45***

Professor Richard Catlow (UCL) Modelling and Predicting the Structures of Complex Inorganic Materials

#### ***PCG/CCG New science from big facilities: Tuesday 15.15-16.45***

Chair: Jon Wright (ERSF)

Simone Tschert (Max Planck Institute, Göttingen) Time-resolved X-ray Diffraction: Possibilities and Limitations for Studying Light-activated Matter

Simon Brown (ESRF, Grenoble) Science and Instrumentation on the XMaS beamline

Richard Ibberson (ISIS) Recent Highlights and Future Opportunities for Neutron Powder Diffraction at ISIS

#### ***PCG Disordered materials and glasses I: Wednesday 10.15-11.45***

Chair: John Loveday (Edinburgh)

Robert Newport (Kent) The Use of Complementary Probes in the Study of Complex Glasses

Martin Wilding (Aberystwyth) High Energy X-Ray Diffraction Studies of Refractory Oxide Liquids

Adrian Barnes (Bristol) The Structure of Pure Rare Earth Aluminate Glasses, Glass Ceramics and Crystals Produced by Aerodynamic Levitation and Laser Heating.

#### ***PCG Computational methods in crystallography: Thursday 10.15-12.15***

Chair: Dave Allan (Edinburgh)

Carole Morrison (Edinburgh) Finding the Elusive Hydrogen Atoms - how Computational Chemistry can help

Stewart Clark (Durham) Density Functional Methods in Crystallography

Mark Johnson (ILL, Grenoble) The Role of Total Energy Calculations in Structure Determination and Related Problems

Dean Sayle (Cranfield) Ceria Nanosphere Self-assembly into Nanorods and Framework Architectures

**PCG Disordered materials and glasses II:  
Thursday 13.30 – 15.00**

Chair: Robert Newport (Kent)

Eugene Gregoryanz, (Edinburgh) Liquid-like State of Sulphur at Megabar Pressures

Terry Willis (Oxford) Local Disordered Structure in the UO<sub>2</sub>-U<sub>4</sub>O<sub>9</sub> System

Sylvia Mclain, (ISIS) The Structure of Biomolecules in Aqueous Solution

**PCG AGM**

The PCG AGM will be held on Wednesday, 18<sup>th</sup> April at 13:00. Please come to the AGM (feel free to bring in your lunch!) - let your opinions and ideas be heard.

**Developments and directions of powder diffraction on proteins, 22<sup>nd</sup>-23<sup>rd</sup> June 2007, Grenoble, France**

The investigation of protein crystal structures by high-resolution powder X-ray diffraction is being established as a complementary tool to recognized single-crystal techniques. When suitable crystals are not available, a microcrystalline powder can give basic information about the crystal lattice, symmetry and crystallinity.

Recently it has been demonstrated that structure solution of small proteins can be successful using powder data via traditional and/or novel approaches.

The 2-day workshop will cover topics such as sample preparation, data-collection, strategies for data analysis, and structure validation, etc. for powders.

Workshop website can be found at:

<http://www.esrf.eu/events/conferences/PowderDiffraction/>

**European Conference on Neutron Scattering, 25<sup>th</sup>-29<sup>th</sup> June 2007, Lund, Sweden**

Scientific sessions at the 4<sup>th</sup> ECNS will cover:

- Advanced Neutron Sources
- Neutron Instrumentation and Techniques
- Neutron optics and Fundamental physics

- Crystallography, Spectroscopy and Excitations
- Magnetism and Superconductivity
- Earth Sciences
- Thin Films and Interfaces
- Glasses and Liquids
- Soft Condensed Matter – Colloids and Polymers
- Life Sciences
- Archaeology and Heritage
- Industrial and Medical Science Applications e.g. Radiography, Process Studies and Strain

Full programme can be found at the conference website at:

<http://www.ecns2007.org/>

**Condensed Matter and Materials Physics (CMMP) conference, 11<sup>th</sup>-13<sup>th</sup> April 2007, Leicester**

CMMP 2007 starts with the Student Day on Wednesday 11th April. The meeting will feature 16 symposia, with the following themes;

- Computational Physics of Metamaterials
- Quantum Fluids and Solids
- Spintronics
- High Pressure Physics
- Quantum Condensed Matter
- Nano-Magnetism
- Semiconductor Transport and Devices
- Surfaces
- Complexity in Non-Equilibrium Statistical Physics and Beyond
- Symmetries and Novel Fluctuations in Superconductivity
- Semiconductor Optics
- Nano Synchrotron Radiation Science
- Ferroelectrics and Multiferroics
- Vortex Matter and Applications of Superconductivity
- Quantum Magnetism
- Nano Materials

More information about the conference can be found at:

[http://www.iop.org/Conferences/Forthcoming\\_Insitute\\_Conferences/event\\_6582.html](http://www.iop.org/Conferences/Forthcoming_Insitute_Conferences/event_6582.html)

## RECENT EVENTS

### PCG-SCMP Rietveld refinement workshop, 7<sup>th</sup>-10<sup>th</sup> January 2007, Durham

The third PCG-SCMP training course on practical aspects of Rietveld refinement was held in Trevelyan College and Department of Chemistry at Durham University, from 7-11th January 2007. It was attended by 60 students from 23 UK Universities, 6 foreign academic and research institutions and 2 industrial companies. The academic background of the participants was extremely diverse and included students and post-docs from chemistry, physics, materials, crystallography, geology and engineering departments. The international flavour was provided by participants travelling from France, Belgium, Slovenia, Greece, India and the USA.

Lectures on topics including the basics of powder diffraction and data collection, symmetry, peak shape analysis, structure factors, peak intensities and agreement factors in Rietveld refinement, restraints, constraints and rigid bodies were given by Jeremy Cockcroft, John Evans and Ivana Evans. Hands-on problem solving sessions illustrated these topics, but also covered powder pattern indexing and unit cell refinements; Rietveld refinements of extended, molecular and nanomaterials and combined use of X-ray and neutron diffraction data. Examples of structure solution of different types of systems were also provided. During the final morning, students were set the challenge of spotting the mistakes in eight different "badly recorded" data sets. First prize and a bottle of bubbly went to Lee Gerrard and Shirley Fong. With sixty students working on around fifty different problems using four different main software packages, the smooth running of the tutorial sessions was only possible thanks to the hard work of expert tutors: Sarah Lister, Will Bisson, Lars Peters and Graham Stinton. Their help is gratefully acknowledged.

We also thank those who generously supported the course: The Physical Crystallography Group of the BCA, The Structural Condensed Matter Physics Group of the Institute of Physics, The Centre for Molecular Structure and Dynamics, CCP14, AWE and Durham University Chemistry Department.

## PCG-SCMP COMMITTEE

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