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Newsletter

Autumn 2009

FROM THE CHAIRMAN

Welcome to the PCG-SCMP Group Autumn 2009 Newsletter. I hope that you will enjoy the pdf-file equivalent of 'flicking through' these pages and reading what we as a group have been doing in the past six months and are planning for the coming months.

Although we are now no doubt focused on the new academic year or, for those at central facilities, already in the full swing of Autumn programmes of running, many of us perhaps have a general underlying sense of unease, with the uncertain worldwide economic climate felt close to home through possible reductions in funding and rising costs. We all hope that the more alarmist predictions will prove unfounded and I would encourage all of us to continue to be pro-active by taking part in the various funding priority reviews, such as the recent survey for the Neutron Advisory Panel, to ensure that the physical crystallography community is heard strongly. Responding to such consultations is an onerous but increasingly important task!

Against this economic backdrop it is therefore very encouraging to be able to report the formal (and successful!) completion of the ISIS Target Station 2 project (covered in more detail later in this newsletter) and the new opportunities for further experiments at these and other new central facilities. This theme will be enforced at our Winter Meeting this year – again jointly held with the ISIS Crystallography User Group Meeting – at the Cosener's House, Abingdon, 5-6th November. We have an interesting selection of talks focussing on 'New Results from New Facilities'. Our aim is for the talks to focus on the new science whilst posters will be displayed to describe the new facilities. I hope that the meeting will be every bit as enjoyable as our meeting last year. Registration details can be found via a link on www.pcg-scmp.org.

The BCA Spring meeting this year gave me the opportunity to visit Loughborough for the first time. Ignoring the obvious distractions of people playing cricket and football all around the campus, I was very impressed by the standard of work being presented by the various speakers at the PCG-SCMP organised sessions. We have a number of brief articles about the various sessions written by our Young Crystallographers later in this Newsletter. Most of the sessions were also extremely well attended and enthusiastically received, with the exception of the session on multiferroics. Despite the high-quality presentations in this session, particularly from Michel Kenzelmann who gave a very accessible account of his work in this area, the number in the audience was small. We need to assess to what extent we should continue to provide sessions with an exclusive 'Physics' theme in this meeting – please email me if you would like to contribute to our discussions about future meeting content.

It was also a pleasure to present this year's PANalytical PCG Thesis Prize to Dr Aurora Cruz Cabeza at the meeting. She was chosen from a strong group of applicants, all of who could have been worthy winners, but Dr Cruz Cabeza's thesis particularly impressed the judges with its coverage of a wide range of scientific techniques and authoritative writing. I am also delighted to report that PANalytical have agreed to continue sponsoring this award. 2010 is also a year when we present our prestigious biennial Physical Crystallography Prize to a person in the early stage of their career. The calls for nominations for both prizes are detailed later in this newsletter.

Finally I would like to welcome Sarah Lister and Kirsten Christensen to our Committee and Sam Callear as our new Young Crystallographer's representative and to encourage others to consider standing as ordinary Committee members at our next election during the AGM at the BCA Spring Meeting in Warwick, 13-15th April 2010.

David Keen
PGG-SCMP Chairman

ANNOUNCEMENTS

Physical Crystallography Prize 2010

Call for Nominations

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, Prof. Dave Keen (david.keen@stfc.ac.uk), by 31st January 2010 and the Prize will be awarded at the 2010 BCA Spring Meeting at Warwick University, 13-15th April 2010.

PANalytical Thesis Prize 2010

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 1st September 2008 to 31st December 2009. The amount of the prize, which is 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/PCG at the student rate to progress their nomination further (current rate £10 per annum or £27.50 for 3 years of the PhD degree).

To enter the competition, candidates must submit:

(a) a copy of the Thesis on CD-ROM.

(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, Prof. David Keen (david.keen@stfc.ac.uk), by 31st January 2010 and the Prize will be awarded at the 2010 BCA Spring Meeting at Warwick University, 13-15th April 2010.

Vacancies on the PCG-SCMP Committee

Call for Nominations

There are two ordinary member vacancies arising on the PCG-SCMP Committee. Nominations for these positions are invited and should be sent to the current Honorary Secretary/Treasurer, Matt Tucker (matt.tucker@stfc.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 Chairman (david.keen@stfc.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, 13-15th April 2010.

FUTURE EVENTS

Meeting Calendar

- PCG Autumn Meeting and ISIS Crystallography Users Meeting, 5-6th

November 2008, Cosener's House, Abingdon

- Condensed Matter and Materials Physics (CMMP 09), 15-17th December 2009, Warwick University
- BCA Spring Meeting, 13-15th April 2010, Warwick University
- Powder Diffraction & Rietveld Refinement School, 18th-22nd April 2010, Durham

PCG Autumn Meeting, 5-6th November 2008, Cosener's House, Abingdon

Following the success of last year's format, PCG Autumn meeting will take place at the Cosener's House, Abingdon, 5-6th November 2009 (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 "New Results from New Facilities". We have put together a programme of talks which will feature exciting new science and posters which will provide updates on instrument developments. We hope that the meeting will be of interest to a wide audience, from experienced researchers to PhD students, both current and future facility users. Confirmed scientific presentations include:

Martin Jones (Oxford): *Diffraction studies of hydrogen storage materials*

Simon Clarke (Oxford): *Title TBC*

Paul Raithby (Bath): *Photocrystallography - from static to dynamic*

Stephen Moggach (Edinburgh): *Big Squeeze, recent developments in high-pressure single crystal diffraction on I19 at Diamond*

Lucian Pascut (Bristol): *Charge order in the triangular metallic antiferromagnet $AgNiO_2$ probed by single crystal resonant X-ray scattering using I16 at Diamond*

Pascal Manuel (ISIS): *Title TBC*

Aurora Cruz-Cabeza (Cambridge): *Title TBC*

A poster session will take place in the evening of Thursday, 5th November 2009.

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.

Condensed Matter and Materials Physics (CMMP 09), 15-17th, December 2009, Warwick University

Scientific sessions and confirmed invited speakers at CMMP09 include the following:

Plenary lectures

Stephen Blundell (Wohfarth Lecturer) Going organic: the challenges of molecular magnetism

Donal Bradley (Mott Lecturer) - Plastic electronics - The science and application of molecular electronic materials and devices

Colin Carlile - At last the green light for the European Spallation Source

Mike Gillan - Quantum mechanics goes to extremes

Gil Lonzarich - TBA

Gerd Materlik - Diamond: brilliant light for UK sciences

Igor Mazin - General properties of the s+- superconductors

John Pendry (Metamaterials) - Prospects for cloaking at optical frequencies

Energy: Photovoltaics, Solar Cells, Artificial Photosynthesis

Jenny Nelson (Imperial College London)

Nanoscale Physics

Wendy Flavell (University of Manchester)

Nanomagnetism

Dieter Suess (Vienna University of Technology)

Quentin Pankhurst (Royal Institution, London)

Multiferroics

Paolo Radaelli (Oxford University)

Manfred Fiebig (Bonn University)

Spintronics

Will Branford (Imperial College London)

Bartel Van Waeyenberge (Ghent University)

Modern Synchrotron-Based Methods for Surface and Interface Studies

Phil Woodruff (University of Warwick)

Ian Robinson (University College London)

Superconductivity

Harry Jones (Oxford University)

Dimitri Argyriou (Helmholtz, Berlin)

Kosmas Prassides (Durham University)

New Ideas in Condensed Matter Theory

Steven Simon (Oxford University)

Juan Garrahan (University of Nottingham)

Quantum Fluids and Solids

Ian Bradley (Lancaster University)

Nanophysics at Low Temperatures

Miles Blencowe (Dartmouth College)

Matter under Extreme Conditions

Justin Wark (Oxford University)

Metamaterials and Plasmonics

Anatoly Zayats (Queen's University Belfast)

Ortwin Hess (University of Surrey)

Computational Electronic Structure and Transport: from Molecules to Solids

Julie Staunton (University of Warwick)

Chris Pickard (UCL)

Ultracold Atoms

Philipp Treutlein (Max Planck Institute, University of Munich)

BCA Spring Meeting, 13–15th April 2010, Warwick University

The BCA Spring Meeting 2010 is themed "Data matters". The meeting will follow the successful format of recent years and run from 11:30 on Tuesday 13th April to 13:30 on Thursday 15th April. It will feature a total of 19 scientific sessions, including four PCG symposia:

- Electron diffraction (organised by Kirsten Christensen)
- Resonant X-ray diffraction (organised by Peter Hatton)
- New approaches to structure solution (organised by Dave Keen)
- PDF: local structure (organised by Matt Tucker)

Three Plenary lectures will be of special interest to PCG-SCMP membership.

The PCG Plenary lecture will be given by Dr Lynne McCusker (ETH Zurich).

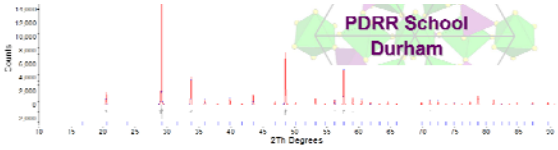
The Teaching Plenary on PDF analysis will be given by Professor Simon Billinge (Columbia University).

Professor Sir John Meurig Thomas FRS (University of Cambridge) will deliver the prestigious Bragg Lecture entitled "The Essence and Promise of 4D Electron Microscopy'.

The deadline for abstract submission for oral contributions is 2nd October 2009, while poster abstracts can be submitted until 5th February 2010. Abstracts must be submitted using the template which will be made available on the meeting website.

The scientific programme, further details about the conference and the form for online abstract submission can be found at: www.crystallography-meetings.org.uk

Powder Diffraction and Rietveld Refinement School, 18th – 22nd April 2010



The EPSRC/IUCr/PCG-SCMP funded biennial Powder Diffraction and Rietveld Refinement School will take place in Durham, 18th – 22nd April 2010. The course will offer a combination of lectures covering the theoretical aspects of powder diffraction and Rietveld refinement, supported by extensive hands-on practical sessions using a variety of modern software packages.

Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Modelling peak shapes
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods

- X-ray and neutron combined Rietveld refinement
- Restrained refinements
- Rigid body refinements

Examples and tutorials will cover both extended and molecular systems. Lectures will be given by Prof. John Evans, Dr. Ivana Evans, Dr. Jeremy Cockroft and Prof. Andy Fitch.

Student bursaries will be available to contribute to local costs and/or travel expenses. We will also offer a small number of IUCr bursaries to overseas students.

For further information and informal inquiries about the School please contact Ivana Evans (ivana.radosavljevic@durham.ac.uk).

Online applications can be submitted until 31st December 2009, at the Powder Diffraction and Rietveld Refinement School 2010 website: http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2010.htm.

NEWS

Prizes and awards

PANalytical Thesis Prize 2009

The PANalytical Thesis Prize in Physical Crystallography 2009 was awarded to Dr Aurora Cruz Cabeza (Cambridge) for her thesis entitled "On the Prediction, Rationalisation and Discovery of New Crystal Forms".

An example of pharmaceutical systems studied is carbamazepine, a well-known drug used in the treatment of epilepsy, and its derivatives. Small flexibility problems (e.g. amide pyramidalisation) were analysed in detail as they were found to greatly influence the results of crystal structure prediction searches. Guided by the poor theoretical prediction of one of the carbamazepine polymorphs (Form II), some interesting experiments were designed to demonstrate the reasons for its observation. The question "How important is the role of molecular shape in crystal structures?" was also addressed and researched in detail for a number of carbamazepine derivatives.

Aurora Cruz Cabeza (Cambridge) receiving the PANalytical Thesis Prize 2009 from the PCG-SCMP Chairman Dave Keen and Dr Paul O'Meara of PANalytical

PCG Poster Prize

There were 20 PCG posters at the BCA Spring Meeting 2009 poster session.

The winner was Dr Jeppe Christensen (Warwick) for his poster entitled "Crystallographic Properties of Ferroelectrics".

Jeppe Christensen (Warwick) receiving the 2009 PCG Poster Prize from Dave Keen

ECM 2013 in the UK

The European Crystallographic Association (ECA) has announced that the 28th European Crystallography Meeting will be held 25 - 29th August 2013 at Warwick University.

RECENT EVENTS

BCA Spring Meeting, 8-10th April 2009, Loughborough

The BCA Spring Meeting 2009 was themed "Dynamic Crystallography". The meeting was opened with an entertaining and informative lecture by David Watkin. This was followed by a joint CCG/PCG session on Computational Crystallography where Frank Leusen presented a significant step forward in crystal structure prediction using a new approach that combines density functional theory simulations and an empirical van der Waals correction. Mustapha Sadki then gave a talk on the development of a data refinement model within an object orientated framework. Philippe Aeberhard then presented some of the results obtained when density functional theory calculations were used in combination with experimental data to gain further understanding of the structure and phase transitions of hydrogen storage materials.

Thursday was the main PCG day, starting with a plenary teaching lecture presented by Martin Dove who gave an insight into how combining the Bragg diffraction with the background of diffuse scattering using reverse Monte Carlo methods provides information regarding the dynamics of atoms. In the following Hydrogen Storage session a range of materials were discussed. Martin Jones demonstrated the utility of the Intelligent Gravimetric Analyzer for Neutrons which, as the name suggests, allows thermogravimetric and neutron diffraction measurements to be performed simultaneously thus enabling full characterisation of the hydrogen and dehydrogenation profile of hydrogen storage materials. Following this, Andrea Baldi talked about thin films comprising multiple layers of Mg and Ti which showed interesting optical and electrical properties depending upon the level of hydrogenation. Neal Skipper concluded the session with a presentation on hydrogen delocalisation in KC_8 and KC_{24} graphite intercalators.

Samantha Callear

In the Dynamics in Framework Structures session, different ways of studying flexible frameworks and their properties were presented with a focus on Metal-Organic Frameworks.

Two of the speakers focussed on the "breathing" properties of MIL-53, where the unit-cell changed with incorporation of different organic guest species. Richard Walton was trying to understand the reactivity of Fe-MIL-53 using time-resolved diffraction. He was able to determine that some of the liquid-phase exchange is taking place via intermediate phases, but overall it is a subtle balance in energetics that gives the change.

Speakers at the Dynamics in Framework Structures session: Ashleigh Fletcher, Richard Walton and Robert Bell, with session organisers Matt Tucker and Andrew Goodwin

Robert Bell presented calculations on Cr-MIL-53 using DFT and forcefield methods in order to understand the CO_2 uptake. Whether the framework is closing or not is highly dependent on guest molecules as there are several minima in configurational energy in the breathing MOF. Ashleigh Fletcher presented a study of adsorption in flexible structures such as the MOFs. This is a way to understand the kinetics in these types of structures. Using the same experimental techniques as for a classic al adsorbent it was possible for Ashleigh Fletcher to show that a structural change can be seen in the isotherms.

Kirsten Christensen, Diamond

In the Crystallography Near the Edge session, Madeline Helliwell showed how fast and reliable wavelength tuning at synchrotron beamlines allow for the collection of multiple wavelength data sets on a given sample. It was demonstrated how tuning the wavelength to the absorption edge of each element present in the sample can resolve the ambiguity of occupancy of a crystallographic site, when the elements present are neighbours in the periodic table. In the following talk by G. Sankar, the anomalous dispersion experiments were combined with EXAFS and entered into a simultaneous refinement. This new method allowed for the

investigations into how catalytically active Co atoms are distributed in a host aluminophosphate lattice.

Speakers at the Crystallography Near the Edge session: Alison Davenport, G. Sankar and Madeline Helliwell, with session organisers Dave Allan and Matt Tucker

The final talk of the session, given by Alison Davenport, was on studies of how corrosion at a metal surface occurs. X-ray diffraction from the salt film formed at the solution – metal interface gave the surprising discovery of sublayers of different hydration states within the salt film.

Jeppe Christensen, Warwick

YOUNG CRYSTALLOGRAPHERS

YC Meeting, 12th April 2010, Warwick University

An early warning for all Young Crystallographers, the deadline for oral abstract submission for the next Young Crystallographers Satellite Meeting (preceding the BCA in 2010) is 15th January 2010. For any new crystallographers that have not attended before, this meeting provides the perfect opportunity to talk about your work in a more relaxed atmosphere.

The YC committee is also pleased to announce that Simon Parsons will be giving the first Parkin Lecture.

Samantha Callear

BEAMLINE NEWS

ISIS Target Station 2 Completed

At its meeting on July 1st, the Second Target Station Project Board formally agreed that the Second Target Station (TS2) has been completed.

The target station and seven neutron instruments are all operational. This is a tremendous achievement - the result of six years of hard work and dedication. All phase 1 instruments are operating with several running scheduled experiments from the user programme. Inter was the first instrument to run user experiments, followed by Offspec and Sans2d. Other instruments are completing their commissioning programmes.

Inter

Professor Jeff Penfold, Chief Scientist for the ISIS Second Target Station, led a team from Oxford University and ISIS for the first scheduled experiment at TS2 on 26 May 2009.

Professor Jeff Penfold and his team carrying out the first scheduled experiment on TS2

The team used Inter to explore the kinetics of formation and dissolution of surfactant and polymer-surfactant mixtures that spontaneously form multilayer structures at interfaces. Using a specially designed trough, the solution sub-phase could be replaced with pure solvent without disturbing the surface. This allowed the dissolution or disassembly of the surface structure to be followed as it progressed in real time. Measurements were made at time intervals as short as 2 minutes (with sub-minute measurement predicted for the future).

"When I first started using neutron scattering for these kind of chemistry studies in the early 1990s, experiments such as these would have been unimaginable," said Jeff. "The new optimized instruments on the second target

station now allow us to see in a minute what used to take a day. It's a real boost for studies in soft matter and biochemistry and will allow us to take a major step forward in our understanding."

The results demonstrate the ability to follow process kinetics opening up exciting new science in areas such as soft lubrication, encapsulation, surface delivery and retention, and in understanding bio-lubrication (lung surfactants, for example).

Offspec

Offspec has successfully demonstrated several of its modes of operation including spin-echo small angle scattering (SESANS) and spin-echo resolved grazing incidence scattering (SERGIS). The complex series of spin manipulation (precession) devices which have developed by our colleagues at TU Delft are working to specification and have allowed Offspec to access length scales that were previously unobtainable in traditional reflectometry. Commissioning of the remaining modes is making strong progress alongside the commencement of the user programme.

Polref

Polref is now into its scientific commissioning phase. In addition to the collimation and sample position equipment common to all three TS2 reflectometers, Polref incorporates a polariser guide field and spin analyser for magnetic studies. This will be complemented by the imminent arrival of a three-dimensional vector cryomagnet with 2 Tesla maximum field.

Wish

Wish has been operating since the end of March with a liquid methane moderator.

Wish sample tank and detector bank

The high count rate produced by the doubly focusing elliptical guide together with the full detector array on one side of the instrument (angular coverage from 10 to 170 degrees) generate 1.6 Gb of data per run. Calibration of the detector linear positions is currently underway and is the final milestone before being able to run the user program.

A first experiment with a single crystal of $BaMnF_4$ has been carried out in collaboration with scientists from Diamond Light Source. The 14 Tesla magnet has been delivered and is soon to be tested on the instrument.

Sans2d

As a first user experiment, Prof Rob Richardson (Bristol) has studied the temperature dependence of liquid crystalline polymer Bragg peaks to obtain order parameters. Data from one 20 minute run (lower Q only) shows the extremely wide simultaneous Q range. The two 1m square detectors were at only modest sideways translation and separation inside the 13 m long vacuum tank: the rear detector at 4 m, front detector offset at 2.5 m, λ = 2 - 14 Å. This experiment is a good test of data reduction using the new Mantid software framework.

Nimrod

The low-angle bank on Nimrod has been installed during the last month. Nimrod has the widest Q-range achievable in a single scan of any diffractometer in the world.

The Q-range is nicely demonstrated by merging low-angle data with data from the wider angle detectors data for different silica samples. Note the nearly 4 orders of magnitude in Q-range and more than four orders of magnitude in intensity.

Further enhancements to the Q-range at low Q are expected after instrument optimisation.

Let

Let is a chopper spectrometer with a massive gap-free detector coverage using 4 m long position sensitive detectors. Currently one 8-pack of detectors has been installed. Let opened its shutter for neutrons for the first time on the 5 August. Results from the detectors are excellent, with a 20 mm vertical position resolution. Over the coming months commissioning of the seven disc chopper system will be carried out and more detectors will be installed.

Martyn Bull, ISIS

Diamond News

As well as supporting an increasing number of users, the small-molecule single-crystal diffraction beamline I19, is deep into its development and commissioning phase. The focussing mirrors are now optimised for both experimental hutches EH1 and EH2 and this work also involved introducing the first light into EH2, which was achieved in May. Work has continued on the development of the large Newport four-circle diffractometer in EH2 and we conducted our first exploratory data collection, using the Oxford Diffraction Atlas CCD detector, at the end of September. The user programme has been supported exclusively so far using the small high-throughput Rigaku diffractometer in EH1 and, as well as allowing conventional small-molecule crystal structure determinations, a number of high-pressure structural studies and excited-states experiments have been successfully performed. The beamline's peripheral laboratory is now equipped to support high-pressure experiments using diamond-anvil cells and a range of techniques will also be supported for handling air-sensitive samples.

The power-diffraction beamline, I11, has been operational since June 2008 when it hosted its first users. Since that time there have been a number of significant developments and one of the most recent is the commissioning the large position sensitive detector which offers rapid data collections in addition to the high-resolution mode. The beamline now offers a range of sample environments including open-flow cryogenic and high-temperature equipment as well as a range of cryostats and furnaces.

The materials and magnetism beamline I16, built in the first tranche of beamlines at Diamond (phase-one), has been supporting users from the first allocation of user time at Diamond, mid-2007. They have been supporting a wide range of experiments, from the determination of the magnetic structures of bulk systems to the study of interfaces in layered materials, and they have been developing a range of techniques and sample environment equipment to both enhance and broaden the scope of the work carried out. One of the key recent developments is the introduction of the Pilatus 2M photon-counting area detector (1475 x 1467 pixels and a total active area of 254 x 252 mm^2) which will allow the extremely rapid, quantitative, mapping of reciprocal space.

The extreme conditions beamline, I15, has also been operational since the first user allocation period. It is a relatively complex beamline offering monochromatic or white beam modes for both powder-diffraction and single-crystal diffraction techniques. Both of these techniques have been supported on the Newport diffractometer which has been equipped with detectors appropriate to the users' requirements. To cater for more permanent and dedicated experimental setups, the main experimental hutch has been equipped with a large motorised optical table which is placed down-stream of the Newport diffractometer. The table and the ancillary equipment are currently being commissioned.

The deadline for direct access to Diamond, duringAP7, is Thursday 15th October 2009.

Kirsten Christensen, Diamond

PCG-SCMP AGM

The PCG-SCMP Annual General Meeting was held during the BCA Spring Meeting in Loughborough, on Wednesday, 22nd April 2009. The AGM minutes are posted on the PCG-SCMP wiki (www.pcg-scmp.org).

The next AGM will take place at the BCA Spring Meeting at Warwick University, on Wednesday, 14th April 2010. The meeting agenda will be circulated in due course.

ACKNOWLEDGEMENT

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

Ivana Evans, Durham

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PCG-SCMP Autumn Meeting
ISIS Crystallography Users Meeting

"New Results from New Facilities"

5-6th November 2009, Cosener's House, Abingdon

ISIS Facility Update

Crystallography Instrument and Software Update

Open Discussion

Scientific Presentations:

Martin Jones (Oxford): *Diffraction studies of hydrogen storage materials*

Simon Clarke (Oxford): *Title TBC*

Paul Raithby (Bath): *Photocrystallography - from static to dynamic*

Stephen Moggach (Edinburgh): *Big Squeeze, recent developments in high-pressure single crystal diffraction on I19 at Diamond*

Lucian Pascut (Bristol): *Charge order in the triangular metallic antiferromagnet $AgNiO_2$ probed by single crystal resonant X-ray scattering using I16 at Diamond*

Pascal Manuel (ISIS): *Title TBC*

Aurora Cruz-Cabeza (Cambridge): *Title TBC*

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

www.pcg-scmp.org

Powder Diffraction and Rietveld Refinement School

18th – 22nd April 2010, Durham

The PCG-SCMP (Physical Crystallography Group of the British Crystallographic Association and Structural Condensed Matter Physics Group of the Institute of Physics) will be holding the 2010 Powder Diffraction and Rietveld Refinement School at Durham University. Lectures will be given by Jeremy Cockcroft, Andy Fitch, John Evans and Ivana Evans. There will also be small group tutorials and a large number of practical hands-on computer sessions.

Topics to be covered will include:

- Data collection strategies for X-ray and neutron diffraction
- Constant wavelength and time of flight diffraction
- Modelling peak shapes
- Indexing powder patterns
- Rietveld, Le Bail and Pawley fitting methods
- X-ray and neutron combined Rietveld refinement
- Extended solids and molecular systems
- Restrained refinements
- Rigid body refinements

Accommodation will be at a Durham College and lectures/computer workshops will be held in the Chemistry Department.

We have managed to raise significant sponsorship and will be able to offer a number of bursaries. Thanks to our sponsors: EPSRC, IUCr and PCG-SCMP.

For more information please email Ivana Evans (ivana.radosavljevic@durham.ac.uk). Applications for the School can be submitted online, via the school website: http://www.dur.ac.uk/john.evans/webpages/pcg_rietveld_school_2010.htm.