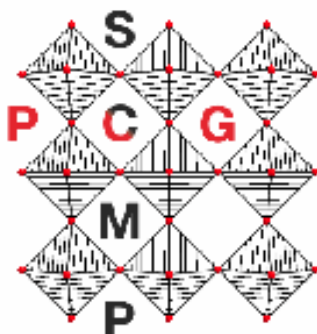


PCG Winter Newsletter



From the chair

Welcome to the Physical Crystallography Group - Structural Condensed Matter Physics Group Winter 2017 Newsletter! This issue brings you some exciting events coming up in the new year along with interesting initiatives which the committee has embarked upon.

Since last year there has been a committee reshuffle with me Anthony Phillips becoming chair and Dr Alexandra Gibbs taking on the role of treasurer. There has also been a multitude of meetings and events including the annual BCA spring meeting at Lancaster University.

As usual our winter meeting was held in conjunction with the ISIS Crystallography User Group Meeting, at the Barn/Cosener's House, Abingdon on Monday 6th and Tuesday 7th November 2017. As in previous years, the meeting was supported by ISIS Crystallography Group and the Institute of Physics. Peter Slater, Emma McCabe, Steve Hull & Helen Playford oversaw the scientific programme for the meeting. The change of venue was to accommodate 100 people rather than 80.

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 2018. 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. There is also the lecture prize for the best (2 - 3) papers published by an early stage researcher over the last couple of years and the PCG school to give a tour de force of modern crystallography for PhD students.

I would like to thank all committee members for their continued contribution during the year.

by ANTHONY PHILLIPS

PANalytical 2018 Thesis Prize for Physical Crystallography

The PCG-SCMP invites 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 2017. 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/Prizes>.

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 broadly defined on the website

www.pcg-scmp.org) 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.

Nominations for the prize must be submitted to the PCG-SCMP Chair, Dr Anthony Phillips (a.e.phillips@qmul.ac.uk), by 20th April 2018. The prize will be awarded at the winter meeting.

I am delighted to announce Pu Zhou as the winner of this years prize announced at the winter meeting.

This years winner

- 2017 Pu Zhou (Department of Earth Sciences, University of Cambridge) "The structure-property relations of zeolitic imidazolate framework 7 for carbon dioxide capture"

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"

Physical Crystallography Prize

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 IoP definition of early career is up to 12 years following the award of a first degree. The award is traditionally presented at the BCA spring meeting and the winner gives a prize lecture at that meeting. The prize will next be awarded in 2018.

History of the Prize

For many years, Philips Analytical have sponsored a prize lecture in physical crystallography. Since the purchase of Philips Analytical by Spectris PLC in September 2002 the company is trading under the name of PANalytical Limited. PANalytical agreed to continue to sponsor the annual award for Physical Crystallography, which was renamed the "PANalytical Physical Crystallography Award". Since the 2006 edition, the prize has been sponsored by the Institute of Physics, and has been again renamed the "Physical Crystallography Award". The award is presented for the best recently published work (say 2 - 3 papers in

the last few years) by a person in the early stages of their career in the field of physical crystallography. It is to be expected that his or her research has or is expected to make a significant impact in this field. The award is traditionally made at the annual BCA spring meeting and the recipient is expected to give an oral presentation of his or her work at that meeting. The PCG-SCMP committee decide on the awardee and award the prize, which currently consists of a cash award of £500.

Nominations for the prize must be submitted to Dr Andrew Wills (a.s.wills@ucl.ac.uk), by 19th January 2018.

Previous winners

- 2016 Dr Paul Saines (Kent)
- 2014 Dr Roger Johnson (Oxford)

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 PCG 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 Secretary Helen Playford (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).

Future Meetings

- The 37th annual Christmas Meeting of the Royal Society of Chemistry Solid State Chemistry Group is hosted by the University of Reading and will run from lunchtime on Monday 18th December to lunchtime on Tuesday 19th December. Further details about the venue and how to get there can be found [here](#).

Plenary speakers:

Prof. Peter Bruce (University of Oxford)
Prof. Nora de Leeuw (University of Cardiff)
Prof. Antoine Maignan (CRISMAT, Caen, France)
Prof. Paul Wright (University of St Andrews)

If you would like any further information, please contact Paz Vaqueiro or (p.vaqueiro@reading.ac.uk) or Dr Livia Bartok-Partay (l.bartokpartay@reading.ac.uk).

- The annual N8 HPC / CCP5 / UKCP one-day network meeting will be held at the Bar Convent in York on January 5th 2018. This meeting will consist of invited and contributed talks, and a poster session. This year there will be three sessions (Functional materials, Interfaces and multiscale modelling and Ab initio spectroscopy), with invited speakers who will introduce the three main topic areas chosen for this meeting:

Plenary speakers:

Dr Andrew Morris (University of Birmingham)
Prof Steve Parker (University of Bath)
Dr Dominik Jochym and Dr Peter Byrne (Rutherford Appleton Laboratory)

For more information and registration see here.

- The Total Energy and Force Methods Workshop will take place in Cambridge, UK, from 9th January - 11th January 2018. It will focus on the most recent developments in the field of electronic structure methods from the first-principles perspective, their diverse applications and mathematical foundations. See here for more information.
- 2018 Joint meeting of the DPG and EPS Condensed Matter Divisions, Berlin, 11th - 16th March 2018, Link
- American Chemical Society - Spring meeting, 18th - 22nd March 2018, Link
- The BCA Spring Meeting 2018 will take place at the University of Warwick, 26th - 29th March 2018.

Plenary speakers:

Prof. Eleanor Dodson (University of York)
Prof. Bill Clegg (Newcastle University)
Prof. Ilme Schlichting (MPI Heidelberg)
Prof. Jonathan Nitschke (University of Cambridge)
Prof. Susan Reutzler-Edens (Eli Lilly)
Prof. Nicola Spaldin (ETH Zurich)

Please see the conference website for reg-

istration and more details <http://www.bcaspringmeetings.org.uk/home>.

- 50 years of Synchrotron Radiation in the UK, 29th June 2018, Link.
- EPDIC16 (2018), Edinburgh, 1st - 4th July 2018, please contact j.p.attfield@ed.ac.uk (Paul Attfield) or go here for more detail.
- The American Crystallographic Association - 68th Annual Meeting, 20th July 2018. For more info see here
- 31st European Crystallographic Meeting (Spain), 22th August 2018, Link
- The 10th International Workshop on Nanoscale Spectroscopy and Nanotechnology, 10th - 12th September 2018, Link

Training Events

- Training sessions for users of the Macromolecular Crystallography (MX) beamlines. 13th - 14th December 2017, Link
- Approaches to dealing with twinned crystals, 5th January 2018, 10:00 - 17:00, Link
- 1st LACA School: Small Molecule Crystallography, 19th - 25th February 2018, Link
- International School of Crystallography, 1st - 10th June 2018, Link
- Over the past year the PCG has been organising a "PCG summer school" designed to teach PhD students essential crystallography at research level. The first PCG school entitled "PCG Intensive School in Physical Crystallography: From Phonons to Phase Transitions" and is going to be held at Cosener's House, Abingdon, Oxfordshire on 18th - 21th June 2018.

Please see the following link <http://pcgschool2018.wordpress.com/> or contact m.senn@warwick.ac.uk for more details.

- Following the success of the Summer School on Nanoscience@surfaces in 2016 the Thin Films and Surfaces Group, Structural Condensed Matter Physics Group, Vacuum Group and Nanoscale Physics and Technology Group is organising a second meeting from 30 July - 2 August 2018. Aimed at PhD students and early-career researchers, this

summer school will cover key aspects of surface analysis and surface science including spectroscopy, microscopy and theoretical approaches to understanding fundamental processes occurring at surfaces on the nanoscale.

The summer school will be held in Cambridge again with accommodation at Murray Edwards College and meals both included in the registration fee. Although the fee has not yet been finalised we aim to keep it as low as possible. Further details on registration will be circulated by the Institute of Physics early in the New Year. Please contact Dr Andrew Thomas for more information andrew.g.thomas@manchester.ac.uk.

Confirmed speakers:

Phil Woodruff (Warwick)
Bill Allison (Cambridge)
Wendy Flavell (Manchester)
Rob Jones (Nottingham).

Acknowledgement

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

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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