

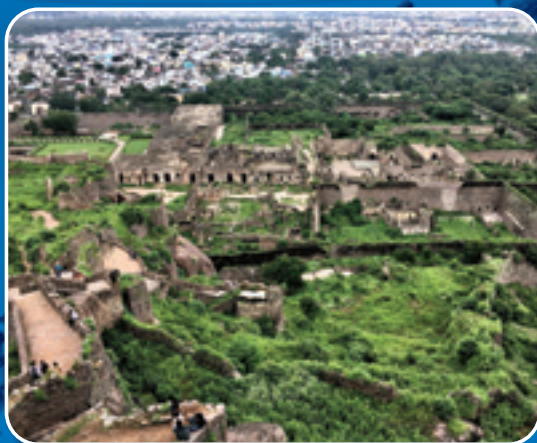
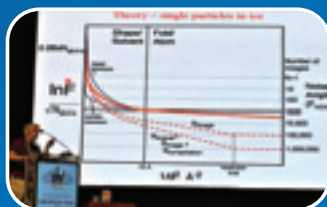
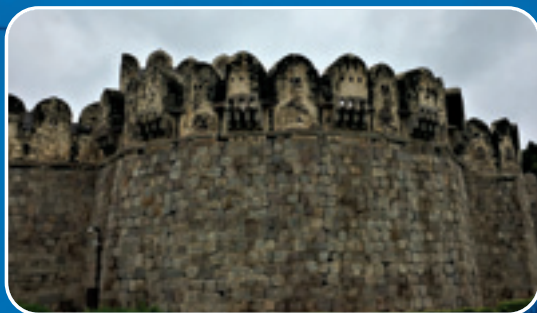
Crystallography News

British Crystallographic Association



Issue No. 143 December 2017

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24th IUCr Congress in Hyderabad, India

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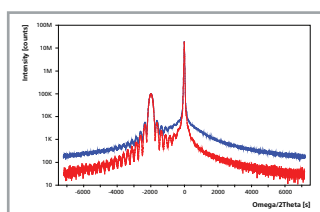
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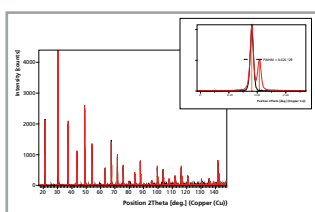
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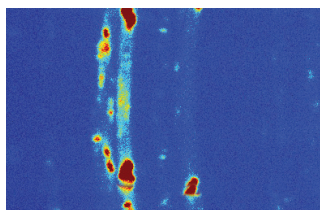
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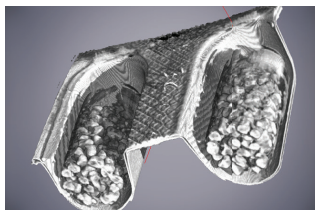
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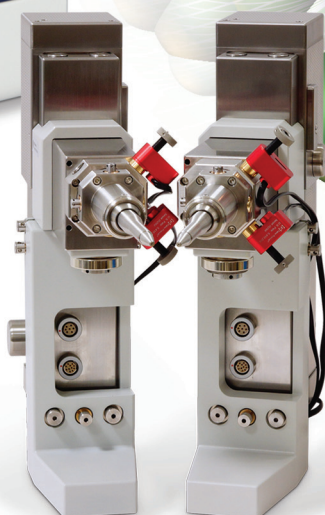
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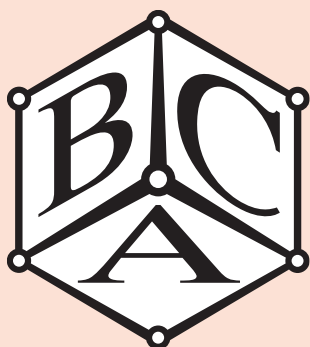
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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration.

These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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Erratum

Erratum on page 16 of the September issue, right column, paragraph 2, line 7: It was stated that "the R enantiomer of carvone smells like spearmint, the S like spearmint." Actually, only R-(+)-carvone smells like spearmint leaves. Its mirror image, S-(-)-carvone, smells like caraway seeds. This error was probably the result of a moment's distraction, but you may have attributed it to your Editor's increasing age. According to J M Boyce and G R Shone (2006) "Effects of ageing on smell and taste", *Postgrad Med J.* 82: 239-241, we lose our sense of smell as we get older, and also our ability to discriminate between smells.

This month's cover:

*IUCr Congress scenes, the
Charminar and Golkonda
Fort photographed by
Helena Taberman*



From the President



AS I write we are once again in the midst of the autumn/winter meetings of the BCA groups, but can also look forward to the 2018 BCA meeting at University of Warwick, the programme for which is in place and summarised in this issue of *Crystallography News* (<http://www.bcaspringmeetings.org.uk/home>). The

deadline for abstract submission is Friday 26th January, 2018.

We have also begun the 2018 election cycle for positions on the BCA Council. This is the first year of our new election procedures, following the changes in Statutes and Bylaws approved at the BCA AGM in April this year. Thus, the newly established Nominating Committee has been active in identifying candidates for the open positions. Candidates for President, Education & Outreach Officer and Ordinary Member are presented in this issue of the newsletter. Each has provided some background and a candidate statement. Voting will be by electronic ballot via the BCA website and open to all BCA members. Further details regarding voting will be circulated to the membership via email. You will recall also that in the last election cycle no candidate for Treasurer was nominated. We were fortunate to be able to co-opt outgoing Treasurer **Pamela Williams** to continue in the role on an interim basis until a new treasurer could be found. At the most recent meeting of the BCA Council, held on September 19th at University of Oxford, the Council co-opted **Elizabeth Shotton** (Diamond Light Source) as Treasurer. An extended handover period will give Elizabeth the opportunity to ease into the role and Pamela has kindly agreed to continue in an advisory role to ensure a smooth transition. The next scheduled election for Treasurer is in 2020.

I am very pleased to announce that the BCA Council has decided to award BCA Honorary Life Membership to two highly respected and distinguished members of the UK crystallographic community. Honorary Life Membership is the BCA's highest membership accolade, awarded to a small and select band of colleagues who have contributed significantly to crystallographic science and to the work of the BCA. Prof. **Elsbeth Garman** has previously delivered the BCA Lonsdale Lecture and received the ACA Fankuchen Award for her research and teaching in crystallography. She has long been active in the BCA, serving as President (2012-15) and helping to bring the ECM to the UK in 2012 as its co-chair. Prof. **Carl Schwalbe** is recognised not only for his research contributions in crystallography but as a longstanding contributor to the BCA, in particular in his role as editor of *Crystallography News* over the past decade and for his tireless activity in gathering information from so many sources. A full list of Honorary Life Members can be found on the BCA website.

Since writing my previous President's column I attended the IUCr Meeting in Hyderabad in August. The meeting contained a full programme of excellent science. I was also part of the

UK delegation at the IUCr General Assembly along with **Richard Cooper**, **Simon Coles**, **Elsbeth Garman**, **Georgina Rosair**, **Alex Stanley** and **Andrew Maloney**, who ensured that we were always able to cast the 5 votes allocated to us as a Category 5 IUCr member. The General Assembly voted to admit 4 new member countries (Albania/Kosovo, Tunisia, Singapore and Bangladesh) and after two very good presentations voted to hold the 2023 IUCr Congress in Melbourne, Australia (2020 Congress will be in Prague). Prof. **Sven Lidin** (Sweden) was elected from 5 candidates for President in a closely fought election (full details of the Executive Committee can be found at <http://www.iucr.org/iucr/governance/ec>). Of 14 UK nominations for IUCr Commission membership that I made on behalf of the BCA, three were elected as Commission members: **Stephen Moggach** (High-pressure Crystallography), **Andrew Wills** (Magnetic Structures) and **Ivana Evans** (Powder Diffraction), along with **Yaroslav Khymyak** (NMR Crystallography) and Sandy Blake (Crystallographic Teaching) who were appointed as Commission consultants. UK-based scientists were also retained on three other Commissions: **Uwe Grimm** (Aperiodic Crystals), **Paolo Radielli** (Neutron Scattering) and **Sofia Diaz-Moreno** (XAFS), along with consultants appointed to or retained on 5 further Commissions.

Richard Cooper and I shared duties in attending (as UK delegates) the ECM Council meetings held during the IUCr Congress. Upcoming ECMs will be held in: Oviedo, Spain (2018), Vienna, Austria (2019) and Versailles, France (2021). Future European Crystallography Schools are scheduled: ECS4 Stellenbosch, South Africa (2018) and ECS5 Poland. The 2nd PanAfrican Crystallographic Meeting (PCCR2) will be held in 2019 at The University of Ghana. There will be a crystallography school held in Senegal (Nov 20–Dec 2, 2017), for which the BCA Council have agreed to provide modest financial support along with similar support from the French and Italian Crystallographic Associations.

It was also noted that the most recent IUCr Congress had a rather low proportion of female speakers, and programme committee members, and on reflection this has been the case at some past IUCr meetings. Prior to the Congress a letter was written to the IUCr Executive Committee, seeking a response on this matter. This initiative was led by **Elsbeth Garman** in conjunction with a number of colleagues from around the world. I signed the letter among many others. This initiative led to a statement from the IUCr Executive Committee on policy for future meetings, which was approved by the General Assembly (almost) unanimously. The statement could have been stronger, but it's a start and there is reason to think that the new Executive Committee will be more pro-active. I would like to point BCA members to a document written by Prof. **Jenny Martin** (Griffiths University, Australia), who was elected to the IUCr Executive Committee, which provides a sensible guide to more organising inclusive and gender-balanced conferences (published in PLOS Computational Biology <http://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1003903>). This is a matter that we had already begun to discuss within the BCA Council. Guidance to BCA Programme Committees

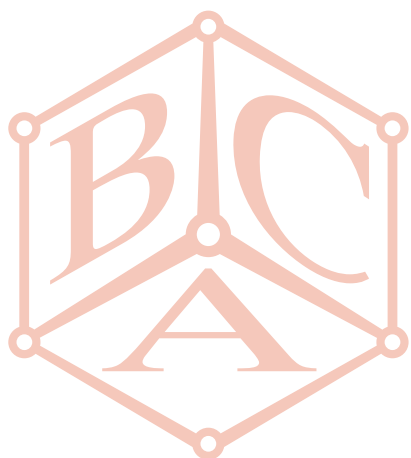
has always been rather informal, but the BCA has no formal gender and diversity policy. BCA Officers have begun collecting statistical data in order that the Council (and membership) can be informed. The BCA Council have also taken the decision to draft a formal gender and diversity policy, which can be discussed and considered for approval at the next BCA Council Meeting in April 2018.

Elsewhere in this issue, **Simon Coles**, the BCA E&O Officer, reports on recent activities, particularly in regard to the Education and Outreach Programme launched last year to develop resources that can be used by the crystallographic community, teachers and community leaders for educational and outreach events. The BCA invites applications for funding to develop new projects and to establish internships to develop new resources. See the full announcement on page 19 of this issue.

We will also need to soon start thinking ahead to the planning of the 2019 Spring Meeting, planning for which will begin at the end of the 2018 meeting. With that in mind, I'd like to remind BCA members of the opportunity to make nominations for the 2019 BCA Prize Lecture and 2019 Lonsdale Lecture. Full details can be found on the BCA web site and on page 18 of this issue.

I'll close my column by recounting an interesting crystallographic link that I was unaware of until a recent museum visit. A few weeks ago, I visited The Hepworth Wakefield (<https://hepworthwakefield.org/>), which opened in 2011 in Wakefield, West Yorkshire, the home town of the sculptor Dame **Barbara Hepworth** (1903-75). The museum resides in a very pleasant setting on the River Calder, and contains a number of Hepworth's works. In one section, which focuses on Hepworth's developing interest in geometric forms, it is noted that she had an interest in science and a friendship with crystallographer **J. D. Bernal**. The museum also hold a copy of Bernal's 1967 book *The Origin of Life* which includes a short dedication to Hepworth signed by Bernal.

Lee Brammer



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The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
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- Influence on the development of crystallography and the BCA

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From the Editor



THIS summer's Big Event was the 24th Congress of the International Union of Crystallography in India. While excited participants were gathering in Hyderabad to await the start of the meeting, I was back in England having two non-melanoma skin cancers removed from my scalp. Therefore I am most grateful to the people who actually were there for the

coverage in this issue. The BCA provided 4 bursaries, and the recipients summarise the high points of the Congress. I thank **Helena Taberman** for the cover pictures, which show ceremonial events, important participants, the iconic Charminar in its bustling surroundings and the Golkonda Fort. Helena also provided the pictures in a comprehensive photo spread. The IUCr commissioned a blog from **Clare Sansom** for each day of the Congress. Because Clare's blog for Day 1 sets the scene so vividly, I reproduce it here. The rest of the blogs can be accessed at <http://blogs.iucr.org/crystallites/> (entries from August 22 to the end of the month, and then September 6).

You will see how well next year's BCA Spring Meeting at the University of Warwick is taking shape. The range of topics will interest every crystallographer, and some very distinguished crystallographers will be giving presentations. From our experience of previous BCA Spring Meetings and even a European Crystallographic Meeting at Warwick we know that this site is easily reachable from just about everywhere in the UK, and it provides congenial and comfortable surroundings. Last year I promised you that you would see ducks at our venue, Lancaster University; and I was glad to find ducks just outside our main hall. Since Warwick has lakes and lakeside paths, waterfowl "twitchers" should be happy once again.

Until recently, details of this year's Biological Structures Group meeting were opaque. The venue and date, exactly a week before Christmas, have now been fixed, and the spectacular line-up of speakers will be an early Christmas present for participants! According to the BSG website "the BSG Winter Meeting will be held at the Cavendish Laboratory, Cambridge on Monday 18th December. Confirmed speakers include the 2017 Nobel Prize winner Richard Henderson, Sir Tom Blundell, Judith Howard, Malcolm Longair, Randy Read, Janet Thornton and Ben Bax." Keep consulting the BSG website for further details. Always a matter of great interest to macromolecular crystallographers, the CCP4 Study Weekend will take place at the East Midlands Conference Centre, University of Nottingham, early in the New Year from 10-12 January. This year's absolutely indispensable topic is "Multi and Serial Crystal Data Collection and Processing". Where would we be without data? More information can be obtained from ccp4@stfc.ac.uk. For crystallographers of a more physical inclination, there will be a PCG Intensive School in Physical Crystallography: From Phonons to Phase Transitions. The dates are 18-21 June 2018; and the venue, Cosener's House, Abingdon, Oxfordshire, will be familiar to PCG members. The website <http://pcgschool2018.wordpress.com/> will provide up-to-date information when it goes live.

The showy splendour of the International Year of Crystallography 2014 remains a vivid memory. The year just finishing, 2017,

has been the International Year of Sustainable Tourism for Development. Participation by BCA members as instructors in various international crystallography schools seems to fit the objectives of this International Year exactly. However, according to the UN website at the time I write this, 2018 isn't a year of anything! Evidently there is nothing else that can match the significance of crystallography.

Closer to home, BCA outreach activities continue apace, led by our enthusiastic Education and Outreach Coordinator, Prof. **Simon Coles**, and vigorously supported by our Young Crystallographers and our not-quite-so-young-but-still-young-at-heart crystallographer Prof. **Mike Glazer**. Simon's latest report appears in this issue.

This issue contains the draft minutes of the 2017 AGM. These minutes merit your careful attention since important decisions were made about nomination and election procedures which are now being implemented. In line with the new procedure, candidate statements are provided. **The BCA AGM 2018 will be held at 6pm on Wednesday 28th March at the University of Warwick.**

It has become increasingly obvious that the information content of a crystal structure determination is not adequately represented by atomic coordinates alone; and although the additional storage of structure factors is better, the ultimate resource is the raw data. The International Union of Crystallography appointed a Diffraction Data Deposition Working Group (DDDWG) led by **John Helliwell** and **Brian McMahon** to chart the way forward. Since the first meeting of this group in Madrid in 2011, significant technical improvements have taken place that facilitate such deposition. The final report of the DDDWG has been released and appears at <http://forums.iucr.org/viewtopic.php?f=21&t=396>.

Lee's announcement of my BCA Honorary Life Membership came as a delightful surprise. Just like the winner of an Oscar, I have to thank lots of people whose help was indispensable. Much of my research has been on correlating structural systematics and pharmaceutical properties of related series of compounds. For this to work, we needed data both on the compounds that crystallized easily and on those that only yielded tiny crystals of low quality. Thanks to the efforts of the National Crystallography Service in Southampton, we got all the data we needed. My colleagues at CCDC gave me the software and advice that made it possible to rationalise the structural systematics. As for *Crystallography News*, just look at all the different by-lines for articles in recent issues. Your contributions make this magazine possible; and in many cases my contribution is limited to gentle reminders about deadlines and the addition of a few semicolons, for which I seem to have a greater fondness than many other people. Finally I must thank my wife **Joan** for providing so many photographs and for enhancing the beauty and impact of other pictures with judicious editing.

In many ways 2017 has been a year of anxiety, ranging from future support for science to the peace of the world itself. I hope that the gentle spirit of Christmas will bring peace to our readers and to those in positions of power everywhere, and 2018 will be a year of peace and progress.

Carl Schwalbe

BCA Council 2017

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(The dates in parentheses indicate the end of the term of office).

Full committee details on the
 BCA website

www.crystallography.org.uk

BCA Spring Meeting

Monday 26th – Thursday 29th March 2018



PREPARATIONS for the 2018 BCA Spring Meeting, which will take place at the University of Warwick from 26th until the 29th March 2018, are continuing. Further details are available from the programme website (www.bcaspringmeetings.org.uk). The site is now open for the submission of abstracts for consideration for both poster and oral presentations. Abstracts must be submitted online before the deadline of **Friday 26th January 2018**. We particularly encourage early career researchers to consider submitting an abstract, this traditionally being an especially friendly and supportive meeting. The submission form will allow you to opt for poster presentation only, or to also have your abstract considered for an oral presentation. Session chairs will select the oral presentations based on fit to the session topic and quality of the science, in addition to ensuring a diverse mix of presentations and presenters. This is an excellent opportunity for early career researchers to gain experience and exposure of your work.

The programme for BCA18 is now available on the website and promises highly relevant, interesting and prescient talks in every session. Session themes cover many of the most topical areas in crystallography today. Coupled with a readily accessible venue for all, this meeting is a great opportunity to catch up with the latest crystallographic science, and of course with your fellow crystallographers.

We are very pleased to announce an eminent list of prize and plenary lecturers as follows:

Hodgkin Lecture:

Prof. **Eleanor Dodson** (University of York).

Lonsdale Lecture:

Prof. **Bill Clegg** (Newcastle University).

BSG Plenary:

Prof. **Ilme Schlichting** (MPI Heidelberg).

CCG Plenary:

Prof. **Jonathan Nitschke** (University of Cambridge).

IG Plenary:

Prof. **Susan Reutzel-Edens** (Eli Lilly).

PCG Plenary:

Prof. **Nicola Spaldin** (ETH Zurich).

The traditional early-career prize session will be held on the afternoon of Wednesday 28th March. Throughout the rest of the program there will often be three sessions running in parallel in addition to a range of workshops. Brief details of the planned sessions are below, along with some practical information concerning deadlines and abstract submission. Further details and updates are available from the BCA Spring Meetings site: <http://www.bcaspringmeetings.org.uk>.

We very much look forward to seeing you at Warwick University in Coventry.

Leo Brady

Programme Committee Chair

Biological Structures Group (BSG)

BSG Session (1): Membrane and multi protein complexes

Chair: Alex Cameron (University of Warwick) & *Kostas Beis* (Imperial)

Keynote: Simon Newstead (Oxford)

Protein assemblies, particularly those embedded within membranes, are crucial to our understanding of cellular function. They are also frequently the targets of many drugs. This session will focus on the latest advances in this very challenging area of crystallography.

BSG Session (2): Crystallisation of macromolecules

Chair: Naomi Chayen (Imperial College)

Keynote: Terese Bergfors (Uppsala University)

The past two decades have seen remarkable advances in the miniaturisation, automation and analysis of crystallization experiments. However, production of high quality crystals of proteins and other bio macromolecules persistently remains a major hurdle to structure determination. The focus of this session is on strategies, techniques and tools for obtaining useful crystals for x-ray crystallography.

BSG Session (3): Structural dynamics and time-resolved crystallography

Chair: Mike Hough (University of Essex)

Keynote: Dr. Jörg Standfuss (Paul Scherrer Institut)

Macromolecular crystallography typically provides structures that are averaged over many molecules and over the time taken to measure the diffraction data. However, proteins are dynamic, sample many functionally-relevant conformations, and undergo time-dependent structural change, e.g. through an enzymatic cycle or signalling pathway. This session will focus on the exciting science made possible by developments in structural dynamics and time-resolved X-ray crystallography using synchrotron and free-electron laser sources. Contributions describing these and other structural time-resolved methods or computational simulations are welcomed.

BSG Session (4): New instrumentation

Chairs: Pierre Aller & Anna Warren (Diamond Light Source)

Keynote: Tim Grüne (Paul Scherrer Institute)

Crystallisation is often the bottleneck when it comes to obtaining a crystallographic structure, due to the difficulties in obtaining crystals of suitable size for diffraction experiments. To overcome issues of getting decent sized crystals or crystals in the first instance, new instrumentation and techniques are being developed to help the user community get the most out of their samples. New beamlines at synchrotrons are maturing to accommodate smaller and smaller crystals for either regular crystallography or serial crystallography. XFEL instruments, cryoEM and microED are becoming more popular as either an alternative to regular crystallography or to obtain complementary data. This session will focus on the scientific opportunities offered by the development of new instrumentation, and how these are aiding the crystallographic community.

BSG Session (5): Protein structure and human disease

Chair: Svetlana Antonyuk (University of Liverpool)

Keynote: Ravi Acharya (Bath)

Changes in protein structure are associated with many human diseases. Whether studying familial disease, viral invasion or drug resistance, proteins are at the centre of nearly all therapeutic strategies. The focus of this session is on recent discoveries in targeting proteins to alter neurodegeneration in ALS, Alzheimer's and Parkinson's diseases, to understand disease mechanisms, to prevent adverse drug reactions, and recover from viral and parasitic invasion or antibiotic resistant bacteria.

BSG Session (6): Ligand binding

Chair: Atlanta Cook (University of Edinburgh)

Keynote: Richard Bayliss (University of Leeds)

The binding of ligands (peptides, nucleic acids, small molecules) to proteins is essential for the formation of protein complexes, allostery, enzyme catalysis and signalling. In turn, the ability of proteins to bind other molecules very specifically is exploited in drug discovery. Structural studies of ligand bound complexes are essential to understanding the rules of recognition and specificity, which will be the focus of this session.



Chemical Crystallography Group (CCG)

CCG Session (1): Chemistry in action (time resolved crystallography)

Chair: Claire Murray (Diamond Light Source)

Keynote: Sam Chong (University of Liverpool)

The inherently active nature of chemical reactions means crystallography is perfectly placed to (quite literally) shed light on how molecules move, bonds break and structures stretch or shrink. This session will explore cutting edge experiments being explored in labs and at central facilities as well as advances in *in situ* insight.

CCG Session (2): Molecular Machines & Rotaxanes

Chair: Stephen Moggach (University of Edinburgh)

Keynote: TBC

Following the Nobel Prize awarded to Feringa, Sauvage and Stoddart in 2016, this session will highlight recent advances in the area of molecular machines. These fascinating materials and their properties will be the cornerstone of the session, highlighting the role of crystallography in the analysis and development of this research area.

CCG Session (3): Surfaces and polymorph selection

Chairs: Iain Oswald (University of Strathclyde) & *Cheryl Doherty* (Pfizer)

Keynote: Jerry Heng (Imperial College)

Surfaces play a significant role in phase transformations and isolation of new polymorphic forms of materials. Whether it is through nucleation of pharmaceuticals on heterogeneous surfaces, or through the use of seeds to isolate new polymorphic forms, surfaces and their interaction with the molecule of interest pose key questions that are fundamental for us to manipulate the solid state. This session will explore the advances in our understanding of the role of surfaces on the isolation of particular polymorphs.

CCG Session (4): Electron diffraction

Chair: Andrew Stewart (University of Limerick)

Keynote: Xiadong Zou (Stockholm)

This session will explore the application of electron diffraction techniques to solving a broad range of crystallographic problems for small molecule crystallographers. Electron diffraction is a very versatile tool, with multiple modes which can be utilised to explore the nano world. Electron diffraction tomography (EDT) mimics X-ray crystallography at the nanoscale for *ab initio* structure solution of unknown crystals. Nano beam diffraction (NBD) can be used to identify individually nano scale crystals, whereas convergent beam electron diffraction (CBED) enables the study of crystal defects and accurate determination of crystal symmetries. While scanning electron diffraction (SED) facilitates the study of polycrystalline materials, via mapping of grain orientations, identification of multiple phases in a specimen, as well as stress and strain measurements within crystalline materials.

CCG Session (5): Service crystallography forum

Chair: William Lewis (University of Nottingham)

Keynote: Amber Thompson (University of Oxford)

A large proportion of published crystal structures are collected by service crystallographers. This session will offer an opportunity to share and discuss common issues and best practices encountered in a modern crystallography laboratory.



Industrial Group (IG)

IG Session: Hydrates and solvates in pharmaceuticals

Chair: **Helen Blade** (AstraZeneca), **Spoorthy Dharmayat** (GSK)

Keynote: **Amy Robertson** (AstraZeneca)

Crystalline solvates or hydrates are frequently encountered within the pharmaceutical field and the development of functional medicines requires the need for a thorough understanding of their structural aspects along with the mechanisms of their formation and desolvation. The aim of this session is to link the critical factors important in building an understanding of solvated systems to mitigate the problems encountered when developing a solvate or a material that readily solvates. Such an understanding can be used to devise control strategies during handling, processing and storage to ensure that the desired functionality of the medicine can be achieved and maintained.



Physical Crystallography Group (PCG)

PCG Session (1): Computational crystallography

Chair: **John Claridge** (University of Liverpool)

Keynote: TBC

Computational techniques are important in both materials discovery and the understanding of the origin of their physical properties, particularly when combined with crystallographic studies. This session is devoted to computational structure prediction and materials “design” as well as the combination of computational techniques with experimental studies.

PCG Session (2): Ferroics and multiferroics

Chair: **Mark Senn** (University of Oxford)

Keynote: **Phillipe Ghosez** (University of Liege)

Ferroics are a technologically important class of materials that include ferromagnets, ferroelectrics, and ferroelastics. This session is devoted to experimental and theoretical studies that explore the relationship between structure and ferroic properties. Abstracts for talks exploring the coupling between different ferroic orderings in multiferroic materials are particularly encouraged.

PCG Session (3): Perovskites

Chair: **Mike Glazer** (University of Oxford)

Keynote: **Patrick Woodward** (Ohio State University)

The study of perovskites has been of increasing interest in the last 30-40 years, since they show such a large range of useful physical properties. The number of publications has been growing exponentially (approximately 22400 in 2016!). The latest discoveries centre around the discovery that so-called hybrid perovskites show a highly efficient photovoltaic effect, thus making them candidates as inexpensive solar cells. This session is devoted to the structures and properties of perovskites and perovskite-related materials.

PCG Session (4): Functional materials

Chair: **Helen Playford** (Warwick/ISIS)

Keynote: **Richard Walton** (University of Warwick)

Much of current research effort in materials science is targeted towards improving functional materials to meet the increasingly complex demands of modern society. However, this can only be done in a rational manner if the structural origins of desirable properties are understood. The focus of this session is on the use of state-of-the-art crystallography to determine structure/property relationships in functional materials, including catalysts, batteries, fuel cells, etc.

PCG Session (5): Neutron and synchrotron techniques

Chair: **Anthony Phillips** (QMUL)

Keynote: **John Duffy** (University of Warwick)

The range of experiments available at central facilities goes far beyond traditional diffraction measurements. This session will focus on techniques that take advantage of modern instruments and enhance or complement our understanding of crystallographic data. Such techniques might include magnetic X-ray scattering, anomalous scattering, small-angle scattering, total scattering, and X-ray and neutron spectroscopy.

PCG Session (6): Hot topics

Chair: **Jan-Willem Bos** (Heriot-Watt University)

Keynote: TBC

Session covering hot topics in physical crystallography not covered by the other session themes. This could for example focus on new developments in instrumentation and data analysis or studies of “hot” materials.



Young Crystallographers Group (YCG)

YCG Sessions 1-3 will showcase the work of the next generation of crystallographers from across the BSG, CCG, PCG and IG. We aim to provide new researchers (undergraduate to postdoctoral level) with the opportunity to present their work in a relaxed, friendly environment and to encourage discussion of their work.

YCG Session (1): YCG Presentations

Chair: **Matthew Dunstan** (University of Cambridge)

Plenary: **Serena Corr** (University of Glasgow)

YCG Session (2): YCG Presentations: Failing badly – of all the things that can go wrong in macromolecular crystallography

Chair: **Sam Horrell** (University of Hamburg)

Plenary: **Ivo Tews** (University of Southampton)

YCG Session (3): Flash poster presentations

Chair: **Alex Cousen** (University of Bath)

YCG Session (4): When crystals go wrong

Chair: **Claire Hobday** (University of Bath)

Plenaries: Prof. **Elspeth Garman** (Oxford) '*The good, the bad and the ugly: macromolecular crystals in all their glory*' & Dr. **John Claridge** (Liverpool) '*Interesting problems: aperiodicity, homometry and twinning in materials*'

Crystals, the cause of and solution to all of the problems in your PhD. Whether your crystals consist of great big molecules, great small molecules or something in-between we have all experienced problems with our crystals at some point. This session aims to unite the worlds of macromolecular and small molecule crystallography against a common enemy, misbehaving crystals, and give you some tips and tricks to help make them behave.

Parkin Lecture: Will be announced in January 2018.



Registration and Abstracts

Registration and abstract submission will open in October 2017. The deadline for early-bird registration is Friday 23rd February 2018, and the final registration deadline is Tuesday 20th April 2018. The deadline for abstract submission is Friday 26th January 2018.

Programme Committee

Chair: **Leo Brady** (University of Bristol)

BCA: **Lee Brammer** (University of Sheffield), **Richard Cooper** (University of Oxford)

BSG: **Mike Hough** (University of Essex), **Mark Roe** (University of Sussex)

CCG: **Iain Oswald** (Strathclyde University), **William Lewis** (University of Nottingham)

IG: **Helen Blade** (AstraZeneca), **Spoorthy Dharmayat** (GSK)

PCG: **John Claridge** (University of Liverpool), **Jan-Willem Bos** (Heriot-Watt University)

YCG: **Sam Horrell** (DESY), **Matt Dunstan** (University of Cambridge)

Organisers: **Joanne McBratney**, **Nicola Hardaker** (Hg3 Conferences)

Draft minutes of the British Crystallographic Association Annual General Meeting 2017

6pm April 12th 2017, Faraday lecture theatre, University of Lancaster

- 1. Approval of the Agenda** – proposed by Simon Parsons and seconded by Mike Glazer and approved by the meeting
- 2. Apologies for absence** – from Bill Clegg
- 3. Minutes of the 2016 AGM**
The minutes had been circulated previously, published in *Crystallography News* and are available in the members area of the BCA website. Proposer Moreton Moore and seconded by Pamela Williams and accepted without any changes.
- 4. President's report**
The President, Lee Brammer, started with the sad but important note of crystallographers who had passed away in the last year: Stanley Nyburg and Howard Flack and noted that they would both be missed by the community. He thanked all those involved in producing a very successful Spring meeting, in particular, Andrew Bond for accepting and carrying out the role of Programme Chair, Nicola Hardaker and her staff at Hg3. The President highlighted that next year's Spring meeting will be held in Warwick 26-29th March 2018 and Leo Brady, Bristol is the Programme Chair for next year's meeting. There would be a short planning meeting for the Programme committee at 1.30 the following day. Once the members of the Programme Committee are in place their names will

be circulated to the members and everyone was encouraged to give input and ideas for sessions and speakers to them.

Congratulations were given to Sir Tom Blundell who will be awarded the 11th Ewald Prize at the IUCr congress in Hyderabad.

The President provided an update on Education and Outreach Activities through information from the Education and Outreach Coordinator, Simon Coles. The focus has shifted from the big events the BCA recently participated in, particularly during the IYCr, to trying to develop resources, both physical and electronic available to members to use for outreach activities with information housed on the learn-crystallography website. Support for this is being provided through bursaries, the first call for which was a few weeks earlier. These bursaries are intended for 8 week internships or for funds to develop resources by the applicant themselves and the finances of the BCA are such that we can continue to support these. From the first round there were 3 successful applicants from Newcastle University and the Universities of Southampton and Sheffield. The President concluded with information on Project M where 1000 samples, from 100 schools for one great experiment will have the samples analysed by PXRD on Diamond Light Source beamline I11 in a single 24 hour period.

5. Secretary's report

There was nothing to report.

6. Hg3 report

Lee Brammer presented the information from Hg3 with Nicola Hardaker, Hg3, present to answer any questions. It was reported that the number of registrations for the Spring meeting on April 5th was 188 (258 in 2016) with 139 as full residential package, 37 as day delegates and

11 exhibitors. There were 76 delegates for the YCG satellite meeting. A list of Corporate members and current advertisers in Crystallography News was also provided. Jeremy Cockcroft asked whether there was an increase or decrease in the membership figures over recent years and the reply was deferred to later in the meeting under item 12.

7. Treasurer's report

The Treasurer, Pamela Williams, started with a reminder of the reporting period from January 1st to December 31st 2016. A full breakdown of the accounts is included in the BCA annual accounts available via email or online at the Charity Commission website. This is the first year that the BCA has presented its financial statements under SORP 2015 and FRS 102 which has not impacted on the funds or net income and expenditure but has changed the presentation a little. Slides presenting income and outgoings for governance and charitable expenditure and a summary of spring meetings were all presented. The Spring meeting showed a small surplus in 2016 which was very good. Crystallography News expenditure was lower with more use of pdf over hard copies that are posted out. Bursary requests were down in 2016 and members were reminded to apply.

In summary the Treasurer stated that the BCA continues to try and reduce governance costs and maintain a cautious, balanced investment of funds. Overall the total BCA income rose over the year to £265,835 (2016) compared to £248,720 (2015). The BCA continues to award student bursaries and the funds are sufficient to permit increased and sustained sponsorship of educational outreach activities. The Treasurer concluded with thanks to Hg3, Council members, BCA group treasurers, Charles Stanley Bank and the Young Company accountants.

8. Acceptance of the Accounts for 2016. Proposer Jeremy Cockcroft, seconded by Sandy Blake and accepted.

9. Appointment of examining accountant The Young Company were appointed as the examining accountant for 2017, fee £5100, proposed by Paul Raithby and seconded by Mike Glazer.

10. Elections to Council

Two positions on BCA Council were open this year: one Ordinary Member, as Amber Thomson completed her term, and Treasurer. The President thanked Amber for her contribution to Council and Stephen Moggach, Edinburgh was elected unopposed (nominated by Simon Parsons and seconded by Pete Wood). Gareth Lloyd enquired whether there was any problem given that Stephen had been elected Chair of the CCG earlier that day. It was clarified that there is a difference between Ordinary Members elected to Council and group reps who are chosen by the groups and need not necessarily be Chair of the group. It was also noted that an officer of one of the groups would not normally be eligible to be an officer of the BCA but it is not a restriction for an Ordinary Member.

There were no nominations for the Treasurer despite Council trying to identify candidates. With the deadline passed for nominations a new Treasurer cannot be elected but can be co-opted onto Council until the next AGM. We are required to have a Treasurer and the President expressed that he was very grateful to Pamela Williams for agreeing to be co-opted back onto Council

as Treasurer in the short term. Members were encouraged to think about and give suggestions of people that might be co-opted to replace Pamela. It was noted that Pamela has agreed to help the new Treasurer with transition through the first year.

Looking ahead there will be elections for the President and one Ordinary Member when Lee Brammer completes his term as President and Mark Senn will complete a first 3-year term and will be eligible to stand again.

11. Honorary members

There were no new Honorary members this year. Members were reminded that the process and timing for nominations for Honorary members has been formalised and is given on the BCA website. The next deadline will be August 31st 2017 for 2018 to allow any nominations to be considered at the September Council meeting.

12. Membership

BCA membership numbers at December 31st were presented for 2016 and 2015 and were as follows: Total membership 733 in 2016 (666 in 2015) with the following breakdown (2015 figures in parentheses): BSG 177 (200), CCG 225 (202), IG 62 (57), PCG 97 (92), YCG 163 (128), Corporate 9 (10), unknown/not verified 172 (97 + 18 with none given).

There is an increase in membership for 2016 over 2015 and numbers close to historical high of 800 and far from low of around 400. The President checked that this had answered Jeremy Cockcroft's earlier question.

Membership fees unchanged for 2018 at £35 for full membership, £17.50 for concessions, student (four years) £58.50 and overseas member (5 years) £175.

13. Election and Nominating Committee proposals

Two proposals, approved by BCA Council, were sent by email to all BCA members on 10th March 2017 with a supporting document and details of the changes to the Statutes and By-laws that both these proposals require. These proposals were made following consultation with the BCA membership where 91 responses were received, 89% of which supported elections taking place in advance of the AGM and 98% supported electronic voting for BCA councils.

Proposal 1: BCA Council elections will be held ahead of the AGM with voting by electronic ballot

The aim is to maximise the participation of BCA membership in the elections, ensure sufficient time at the AGM for discussion of reports and other matters and to allow a smoother transition of Council members at the Spring meeting. If approved the implementation involves a change of the deadline for nominations to September 30th and candidates would provide a written statement, a brief CV and photograph to be published in the December issue of *Crystallography News*. The Electronic ballot would open upon publication and remain open until January 31st.

The following proposed revised versions of Statutes E4, D4 and E2, an additional new Statute F5, By-laws D3, E1 and E2 and an new By-law E3 are required if approved.

Statute E4 Elections shall take place as follows:

(a) *Elections of Officers, Ordinary Members and the Education and Outreach Coordinator shall take place by an electronic ballot of the membership prior to, but within 3 months of, an Annual General Meeting of the Association.*

(b) *Each elected member of Council shall serve from the end of the Annual General Meeting immediately following their election until the end of the third Annual General Meeting after that.*

Statute D4: The Annual General Meeting shall have the following functions:

(a) **to report the election of the Officers and other members of the Council;**

Statute F5: Voting for elections to the BCA Council will normally be conducted by electronic ballot of the BCA membership.

Statute E2 (d) Three further Ordinary Members who shall be elected by vote of the membership of the Association.

By-law D3 The agenda for an Annual General Meeting shall include at least the following items:

(a) Appointment of a chair, if neither the President nor the Vice-President is present.

(i) **Report results of elections of Officers.**

(j) **Report results of elections of further Council members.**

By-laws section E with addition of E3

1. The Council shall take account of the terms of office of its existing members and, if appropriate, may then make nominations for each vacancy, subject to **Statute E.2**, and with a view to ensuring a **balanced representation of fields of interest, geographical areas and the diversity of the BCA membership**. The nominations of Council shall be circulated to members at least **two weeks before the nomination deadline**.

2. Any two Members may make nominations for any vacancy. Such nominations shall be accompanied by the written consent of the candidate to serve if elected, and must be received by the Secretary by **the nomination deadline**.

3. **The nomination deadline will be 30th September in the calendar year before the AGM, unless an alternative deadline is proposed and approved at an AGM.**

Sandy Blake asked what would happen in the event of a tied election. The current situation is that the President does not have a vote unless tied and no change to this is proposed. It was clarified the terms in office would be unchanged with elected members of council taking office at the AGM following the vote following a question from Dave Keen. Anthony Philips queried whether the relative numbers of members who took part in the questionnaire suggest a similar turnout for elections. It was commented that it works well for other organisations and has done for some time, for example the ACA and SCANZ and was impossible to answer. Andrew Goodwin suggested that it should be reviewed. It is also open to groups of 5 members to bring forward proposals not just Council.

A vote was taken by a show of hands with 75 in favour and no one against. The proposal was approved.

Proposal 2: Establishment of a Nominating Committee

The BCA Council proposed establishing a BCA Nominating Committee with the purpose of ensuring BCA members are presented with a choice of candidates for all elections to BCA Council. If approved these changes would take place immediately following the current AGM.

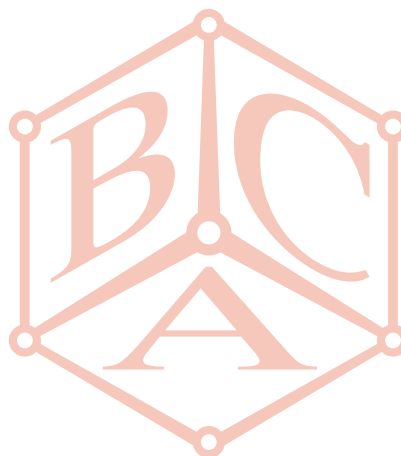
It was proposed that By-law E1, be completely replaced with a new By-law which defines the remit and composition of the Nominating Committee. These changes also correct the reference to statute E.2, which is written as E.3 in the current By-laws, and clarify what is meant by balanced representation.

1. *The Council shall appoint a Nominating Committee whose role shall be to secure the nomination of two candidates for each Council vacancy, subject to Statute E.2, and with a view to ensuring a balanced representation of fields of interest, geographical areas and the diversity of the BCA membership. The nominations should be accompanied by the written consent of the candidates and shall be sent to the Secretary by the nomination deadline. The Nominating Committee shall consist of 5 members, normally the Past-President of the BCA and one member from each of the BSG, CCG, IG and PCG groups. Terms of membership will be staggered over a 3-year cycle such that in one year the Past-President will be replaced and in the other years two of the other four members will be replaced. The Past-President will be limited to one 3-year term. Members of the nominating committee are not eligible for nomination to any position on BCA Council until after the AGM following the completion of their term on the committee. Current members of the BCA Council are not eligible to serve on the Nominating Committee.*

Details of the composition and terms of the proposed Nominating Committee were given. A discussion took place. It was noted that the existing route for nominations from two members remains open and that all nominations would come to the BCA Secretary as is currently the case. Charlie McMonagle asked whether the origin of the nomination would be clear on the ballot and it was noted that it had been decided that this would not be on the ballot but would be reported at the AGM.

A vote was taken by a show of hands with 57 in favour, none against and 1 abstention. The proposal was approved.

There was no other business and the meeting closed at 19:15.



BCA Council Elections 2018

AT the AGM in April 2017, changes to the BCA Statutes and Bylaws were approved in order to establish a new procedure for elections to the BCA Council. A Nominating Committee was established and elections will take place by electronic ballot of the membership. Nominations for the following positions on Council were invited from the Nominating Committee and from members of the BCA by the nomination deadline of September 30th:

President (Lee Brammer completes his 3-year term at the AGM 2018).

Education and Outreach Coordinator (Simon Coles completes a 3-year term and is eligible to stand for a second term).

Ordinary Member (Mark Senn completes a 3-year term and is eligible to stand for a second term).

Elections will take place at the start of 2018 with voting by electronic ballot. Details of the voting procedure will be sent to all BCA members by email. The results of the election will be announced and elected members of Council will start their terms at the 2018 AGM.

We encourage all BCA members to participate as the wider participation, beyond those present at the AGM, was one of the motivations for changing the election process as well as providing for a better handover to new members of Council.

The following nominations were received and in subsequent pages statements from each of the candidates are published to enable members to make informed decisions when voting.

Candidates for:

President: Mike Hough, Simon Philips, Pierre Rizkallah.

Education and Outreach Coordinator: Simon Coles.

Ordinary Member: Cheryl Doherty, Christoph Salzmänn, Mark Senn.



Mike Hough

Current Position:

Senior Lecturer in Structural Biology, School of Biological Sciences, University of Essex.

Education and Career:

BSc(Hons) Physics, University of Leicester; PhD in Structural Biology, De Montfort University (based at STFC Daresbury Laboratory); Band 5 then Band 4 Research Scientist, STFC Daresbury Laboratory; Post-doctoral fellow, University of Liverpool; Lecturer, University of Essex; Senior Lecturer, University of Essex; Fellow of the Royal Society of Biology; Member of the Institute of Physics; Member of the Royal Society of Chemistry, Member of the Biochemical Society.

Professional Activities:

Active member of CCP4 Working Group 2; Co-Organiser of the 2017 CCP4 Study Weekend 'From Crystals to Structure'; Programme committee member, 2018 BCA Spring Meeting; UK representative to the European Synchrotron User Organisation (ESUO); Session chair for IUCr Congress 2017, Hyderabad and CCP4 study weekend 2014.

Research Interests:

My main research interest is in combining synchrotron and XFEL X-ray crystallography with complementary methods such as single crystal spectroscopy to understand the structure, dynamics and function of metalloproteins. Related to this, I have an interest in experimental validation of crystal structures, specifically of the identity, redox and ligand states of metal centres. Most recently I have been involved in advancing high-throughput high-hit rate XFEL (SFX) structure determination. I have a strong interest in method developments in structural biology. I have been involved in developing methods to drive redox reactions in crystals using X-ray generated photoelectrons (the 'many structures from one crystal' approach) to produce dose-dependent structural movies of catalysis in redox enzymes. My work has focused on a wide variety of metalloproteins, including those from the nitrogen cycle (nitrite reductases, cupredoxins, cytochromes), antioxidant enzymes (copper, zinc superoxide dismutase) and haem enzymes and proteins involved in binding to small gas ligands such as nitric oxide and carbon monoxide.

Statement:

This is an exciting time for crystallography, with new synchrotron, X-ray free electron laser (XFEL) and neutron facilities coming online around the world together with highly capable home lab sources and detectors. Increasingly powerful computation, databases and bioinformatics tools allow us to exploit structural data in novel ways while methods such as electron crystallography are undergoing a resurgence. The BCA has a leading role to play in the coming years in all of these areas and as president, I would promote our activities and the central relevance of crystallography across the sciences. The BCA has a proud record in crystallographic education and this is increasingly important in ensuring that the underlying principles of crystallography remain understood by newcomers to the field in an age of increasing software automation. As president, I would support and push to increase the summer schools and workshop programmes organised by the different groups of the BCA as well as further developing the online resources related to education on the BCA webpages.

I would continue the excellent work of the BCA in strongly promoting gender balance in conference speakers and organising committees, on journal editorial boards and other representative roles. For BCA-organised meetings, I would seek to make public the gender statistics for all conferences/meetings as well as working closely with the programme committees throughout the process of inviting contributors.

It is critical for the future of the BCA that we continue to promote engagement with younger scientists, particularly as crystallography becomes one of a platform of tools used by a

particular researcher to address a particular physical, chemical or biological problem. I would work closely with the YCG to promote crystallography as a discipline and a fascinating field of research to postgraduate students and postdoctoral scientists in particular. I am enthusiastic about promoting outreach of our fascinating field to the general public and more broadly of communicating the central role of science in our community and society. The International Year of Crystallography and activities arising from it were very successful in this regard and it is important to maintain the momentum that was created by this. I would work closely with the YCG in particular to promote outreach to young people in schools and other venues.



Simon E.V. Phillips

Current positions:

Visiting Professor in Molecular Biophysics, University of Oxford (2008-); Visiting Professor of Biophysics, University of Leeds (2008-); Adjunct Fellow, Linacre College, Oxford (2015-).

Previous positions:

Director, Research Complex at Harwell (2008-2016); Associate Member, Christchurch College, Oxford (2008-2011); Dean for Research, Faculty of Biological Sciences University of Leeds (2001-2004); Director, North of England Structural Biology Centre (1995-2005); Director (and Founder), Astbury Centre for Structural Molecular Biology, University of Leeds (1999-2001); Astbury Professor of Biophysics, Department of Biochemistry and Molecular Biology, University of Leeds (1996-2008); Director, Leeds Centre for Molecular Recognition in Biological Systems (1993-1999); International Research Scholar of the Howard Hughes Medical Institute (USA) (1993-1997); Professor of Molecular Biophysics, Department of Biochemistry and Molecular Biology, University of Leeds (1992-1996); SERC Senior Fellow (1989-1994); Reader in Biophysics, Department of Biochemistry and Molecular Biology, University of Leeds (1989-1992); EMBO Fellow (Short-term), Institut Pasteur, Paris (1985); Lecturer in Biophysics, Astbury Department of Biophysics, University of Leeds (1985-1989); Chargé de Recherche, Immunologie Structurale, Institut Pasteur, Paris, France (1982-1985); Visiting scientist, Brookhaven National Laboratory, Long Island, NY, USA (1980); Scientist, MRC Laboratory of Molecular Biology, Cambridge, England (1976-1982); Teaching Post-doctoral Fellow, Department of Chemistry, University of British Columbia, Vancouver, BC, Canada (1974-1976).

Education:

BSc (Hons) Chemistry (1971) and PhD Chemistry (1974), Thomas Witherden Batt Scholarship (1971-1972), University College London.

Professional activities:

Awards – 2001 Royal Society of Chemistry Award for Peptides and Proteins (sponsored by AstraZeneca); 1990 Rapkine Lecturer, Institut Pasteur, Paris; **Societies** – Fellow of the Royal Society of Chemistry; Member of European Molecular Biology Organisation (EMBO); British Biophysical Society; British Crystallographic Association; The Biochemical Society; International Structural Genomics Organization; Biophysical Society; **Editorial Boards** – Associate Editor of Macromolecular Structures (1991-2000); Editorial Board,

Structure (1990-); **Examining** – External Examiner (taught courses) University of Manchester (2009-2011) and Imperial College London (2010-2014); **Committees (Current)** – I23 User Working Group, Diamond Light Source; Scientific Advisory Board, Membrane Protein Laboratory, Diamond Light Source; Scientific Advisory Board, Centre for Structural Systems Biology (CSSB), Hamburg, Germany; Scientific Advisory Board, P I E R: Partnership for Innovation, Education and Research DESY and Universität Hamburg, Germany; **Committees (Past)** – MRC Oxford Protein Production Facility Review Committee (2015); Co-chair, Wellcome Trust Biomedical Resources and Multi-User Equipment Committee (2012-2014); Protein Crystallography Beamlines Working Group, Diamond Light Source (2011-2012); Chair, Bragg Lecture Fund committee (2006-2009); Council, ESRF, Grenoble, France (2005-2007); BM14 Steering Group, ESRF, Grenoble, France (2000-2008); Scientific Advisory Committee, e-HTPX, E-Science Resource for High-Throughput Protein Crystallography (2003-2006); CCP4 Executive (2007-2010); Chair, Life Science Peer Review Panel, Diamond Light Source (2006-2009); Scientific Advisory Committee, Diamond Light Source (2006-2009); University of Leeds Senate (2007-2008); BBSRC Tools and Resources Strategy Panel (2004-2006); Chair, BBSRC Biomolecular Sciences Committee (2001-2006); BBSRC BioScience2006 Advisory Panel (2005-2006); Member, BBSRC Strategy Board (2001-2004); BBSRC Review of Structural Biology (2002); BBSRC Review of Neutrons in Biology (1996); BBSRC Biology Programme Joint Steering Committee (Synchrotron Radiation) (1994-2000); Scientific Advisory Committee, ESRF, Grenoble, France (1995-96); MRC Molecular and Cell Advisory Board (1997-2001); CCP4 Working group 1 (1996-2016); MRC Molecular and Cell Grant Committee (1996-97); BBSRC Equipment and Facilities Committee (1994-97); Chair, Life Sciences Beamtime Allocation Committee, ESRF, Grenoble, France (1994-96); College 8 (Biochemistry) Neutron Beamtime Allocation Committee, Institut Laue Langevin, Grenoble, France (1991-95); BCA Biological Structure Group (1988-91); CCP4 Working group 2 (1985-1996); Meetings Secretary, British Biophysical Society (1988-92).

Research Interests:

I started out as a small molecular crystallographer working on specific recognition of alkali metal ions by small organic ligands, and then topochemical control of photochemically induced reactions of small organic molecules in the crystal. I had a long-term interest in biology and computer programming, so I moved into protein crystallography, initially in structure determination and refinement of oxymyoglobin using both X-ray and neutron crystallography at low temperature. Working with haemoglobin sparked my interest in molecular recognition, the binding of small ligands to proteins and drug design. My metalloprotein work has continued ever since, through copper oxidases, magnesium containing nucleases, superoxide dismutase and NiFe hydrogenase. Crystal structures are essentially static, or more correctly time and population averages, but function, such as catalysis, often implies dynamics. In order to address this my structural enzymology work included methods for observation of catalytic intermediates to try to follow structural changes through reaction cycles, focusing in particular on metalloenzymes. In molecular recognition my work has centred on antibody-antigen complexes, as well as how nucleic acid binding proteins recognize specific DNA and RNA sequences in repression, activation, restriction and recombination. This led to an interest in virus structure and assembly, with high resolution structure determinations of viruses by crystallography and

cryo-EM. I have 214 publications (H=50). **Current interests:** crystallography, cryo-EM, structural enzymology and use of XFELs to investigate catalytic intermediates, virus structure and assembly, ligand binding and drug design.

Statement:

I have been committed to crystallography since a eureka moment as a chemistry undergraduate at UCL in 1970. We had reached the end of a seven-day practical, starting with mounting our crystals and ending with preparing a photographic print of an electron density map, using an optical Fourier summation device (von Eller photosommateur) with our own eye-estimated reflexion intensities. I was able to place a ruler on this print and measure the C-N bond length in hexamethylenetetramine. I found this magical, and I still do. Since structure underpins the properties of matter, crystallography is important to all the molecular sciences. The BCA is key to its advancement and, especially, promotion both nationally and internationally. I have been a BCA member continuously since its establishment, and served on the BSG committee in the 1980s. I have direct experience of both small molecule and macromolecular crystallography, with X-rays and neutrons, as well as, more recently, cryo-EM, so I understand the requirements and challenges in all these fields. I also believe passionately in multi-disciplinary science, since a chemist should see no fundamental distinction in the importance of structure for, say an enzyme or an A380 jet engine turbine blade.

My main interests are now in structural biology, but when I founded the Astbury Centre for Structural Molecular Biology in Leeds in 1999, we recruited members from Chemistry, Physics and Engineering as well as Biological Science departments. At the Research Complex at Harwell I was lucky to lead an even wider community focused on structural science, including strong industrial links. Interactions across that community generated unexpected new collaborations and projects, and the BCA should provide similar forums for ideas, especially at the Spring Meetings, and help to drive them forward. Catalysis, for instance, is a good example of an area that interests chemists, industrialists and biologists, and depends critically on structure.

The BCA should also have an eye for new technologies. Synchrotron radiation has revolutionised x-ray crystallography, but also brought new opportunities such as adding a fourth dimension, time, to allow dynamic studies of chemical and physical change. In addition, it stimulated new areas, such as diffractive imaging and microtomography, that bear a relationship to crystallography (or perhaps 'crystallographic imaging'). We can add to this the possible uses of X-ray free electron lasers (XFELs), particularly for studying fast processes, improved neutron sources such as the European Spallation Source and cryo-EM (where the Nobel Prize for Chemistry was recently awarded for developments in physics applied to biology). The BCA should ensure its horizons encompass these new developments and help stimulate their integration into wider structural science. The IUCr has, for instance, now launched a cryo-EM section in IUCrJ.

As a society, the BCA should seek to grow its membership still further, building on the success over the last few years, and exploiting the new opportunities in structural sciences. This would also help to improve the financial position, where serious challenges await as the result of currency fluctuations and research funding issues flowing from recent political decisions. The BCA should use its influence in the political arena, and co-operate with other learned societies to ensure its views are heard by policy makers. This is an area where

outreach is important, including to the public and, especially, the younger generation, who are the scientists of the future, and will soon be voters. The BCA is currently doing well in this area but we should retain a strong focus on it. It should also pay special attention to its own younger members, since they are its future. Once again the BCA does quite well in this, but we should continue to treat it as a priority.

I believe I have the knowledge and skills to help the BCA move forward in these uncertain times. I have experience of leadership in large organisations, and of science funding and the politics behind it. While the science is my first love, I realise we also have to look beyond the lab to ensure a healthy future for our science. I would be honoured to serve as BCA President and make a positive contribution to its future.



Pierre Rizkallah

Current position:

Senior Lecturer – Structural Biology, Cardiff University School of Medicine, since 2008. RCUK Senior Research Fellow, 2008-2011.

Education:

BSc Chemistry, 1st Class, Lebanese University, Beirut, Lebanon, 1979. PhD Chemistry, Nottingham University, UK, 1984. PDRA, Biophysics, Leeds University, 1984-1987. Senior Fellowship, Liverpool University and SRS Daresbury Laboratory, 1987-1989.

Career path:

Higher/Senior Scientific Officer, SRS Daresbury Laboratory, 1990-2008. Higher Scientific Officer, AFRC Shinfield, Reading UK, 1990. Production line manager, International Cosmetics Manufacturers, Beirut, Lebanon, 1979-1980.

Professional Roles:

Secretary, Beamtime Allocation Panel E, Protein Crystallography, SRS Daresbury, 1990-1997; Coordinator, SRS User Forum 1997-2002; Associate editor, Synchrotron Radiation News, 2004-2008; Member, Science Advisory Committee, SESAME Synchrotron, Jordan, 2000-2004; Co-Author of Life Sciences Program at SESAME, 2000; Coordinator, Commercial access to Protein Crystallography SRS facilities, 1990-2008. Coordinator, Beamtime Allocation Group for Diamond access, Cardiff University, since 2008; Public engagements with schools, newspapers, television and radio, throughout my career; Conference organiser for the South West Structural Biology Consortium, 2017.

Research Interests:

Macromolecular Crystallography, Immune System Proteins (MHCs, TCRs and complexes), Non-canonical amino acid incorporation into GFP, Drug design (anti-inflammatories), Bicolouration, Carbohydrate Recognition (lectins), Vaccine development (virus based), Ecological insecticides (bacteria), Cancer related research, modelling, Technology development (crystallisation screen design), Diamond and XFEL developments for Structural Biology, Cryo-EM.

Statement:

My association with BCA goes back to its roots. Stephen Wallwork, my PhD supervisor, persuaded me to go to the very first meeting of the BCA, held in Feb 1981 in the Royal

Society buildings in Piccadilly, London. He became the first treasurer, and life member as a founder, while I thought this thing was way above my head. A view I later corrected, as my first PDRA post was a direct result of being at the BCA Spring meeting in 1984, held at Nottingham University. There I met Tony North, and I launched myself into the world of macromolecules, and never looked back. I went to most of the BCA meetings since then, and particularly, the one-day Winter meetings organised by the Biological Structures group. Unfortunately, I don't have the full set of the annual meeting booklets, as I missed a few. I did help organise the program of the Biological Structures Group in the Spring meeting at Loughborough, 2009. Eventually, I decided to help run the committee of the BSG, first as an ordinary member, then as treasurer over three terms, which finished at the end of 2016. I am now an ordinary member of the BCA again.

I was always in awe of the galaxy of great scientific minds and luminaries, in crystallography and allied sciences, that were invariably drawn to this buzzing society over the years, particularly the eminent speakers who went on to become Nobel prize winners. I heard them first at the BCA meetings! The air of expectancy is always present, and I hope to savour it for some time to come. I hope the membership will also realise the timeliness and relevance of presentations made at BCA meetings, which can only be sustained by continuous effort, over an extended period, by a large number of people who make this atmosphere materialise.

At the other end of the scale, I observed many students and young scientists make poster and oral presentations, on their path to become established scientists later. I always felt the BCA was a forum that nurtured well the rising talents. The youth element has been the lifeline of the BCA, and it continues to be, and the BCA recognised that through the establishment of the Young Crystallographers Group, yet another activity that appears a natural extension to BCA work. I feel this area is deserving of great support.

The outreach activities, started in recent years, have also added an extra string to the bow of the BCA, bringing the immediacy and relevance of our chosen science to the masses. We must communicate the beauty of symmetry and the elegance of solutions used by Nature to conduct life. We must also tell the story of enterprising activities employed by scientists and engineers to create solutions for today's world, with myriad applications in communications, transport, construction, manufacturing and just about everything. Crystallography's contribution must be highlighted. This way, we can bring on board the public to support our activities and encourage more budding minds to continue where we leave off. Crystallography is still the preserve of Higher Education Institutes, when we should try to extend it to pre-university levels.

I am truly honoured to have been nominated for the post of President of BCA. If elected, I would use all my power and I will exert all the effort I can muster, to advance the work of the BCA. Challenges appear at every turn, not least the XFEL and cryo-EM developments. I hope to be able to steer the BCA on a comfortable path to the future, with the help of all the other members of Council, the special interest group officers and all the members of our association. The BCA has grown a long way from its humble roots in 1981, and has become an international organisation, with links to various crystallography associations across the world. I shall strive to keep the international aspect of the BCA alive and well, so it can continue to influence the science agenda and the perception of UK scientists by other practitioners of crystallography. The above list of aspirations may seem daunting, but our collective

effort could well see us through many of these challenges. I rely on your involvement.



Simon Coles, FRSC, SFHEA

Current position:

Professor of Structural Chemistry and Director of the National Crystallography Service, Chemistry, Faculty of Natural and Environmental Sciences, University of Southampton.

Professional Activities:

Since 2015 I have been a member of the RSC Local Section committee, since 2013 Director of an MSc in Instrumental Analytical Chemistry and since 2010 Director of Southampton Diffraction Centre. I am a visiting academic at the Universities of Cagliari (Italy), Gebze (Turkey) and Sydney (Australia). I am an Editorial board member for 4 journals (Crystallography Reviews, Supramolecular Chemistry, Chemistry Central & International Journal of Digital Curation) and my peer review panel membership has included EPSRC, ARC, JISC, ISIS, Diamond and ALS. I also serve as a member on 8 large project and facility management steering groups (external and internal to my university).

BCA positions held:

2015-Current National Education and Outreach Coordinator; 2013-2015 Chair, Chemical Crystallography Group; 2011-2013 Vice Chair, Chemical Crystallography Group; 2009-2010 Chair, Spring Meeting Programme Committee; 2006-2008 Chair, Young Crystallographers Group; 2000-2003 Ordinary Member, Chemical Crystallography Group Committee; 1995 Member Local Organising Committee BCA Spring Meeting.

Research Interests:

I am author on around 800 publications in journals, conference proceedings, periodicals and books, with an H-Index of 48 and >10000 citations. A significant proportion of these arise from being at the leading edge of service crystallography since the early 1990's. However my research interests beyond service crystallography are numerous. Structural chemistry research interests include the study of solid-state reactions and transformations, structural systematics, the determination of charge density distributions and their application to solid state reactivity and behaviour, discovering and investigating structure-property relationships and crystal growth. In the last 15 years I have diversified my research from conventional crystallography into interdisciplinary work with Libraries & Information Science, Archaeology, Statistics, Computer Science, Physics and Engineering. This has resulted in working in CT Imaging, SHG Laser Spectroscopy, Dynamic Light Scattering, Computational Modelling, Additive Manufacturing, Formulation, eLearning, Data Management, Data Science and Chemical Informatics areas.

Statement:

I am committed to enhancing education and understanding of chemistry and crystallography at all levels and to the broadest possible audience. Relevant to this BCA Council position, I have strong interests in Technology Enhanced Learning and routes to developing and enriching practical- and problem- led learning. I have won grants, mentored UG and PhD students and written papers while developing this

area. In 2013 I founded a fully equipped laboratory, including powder and single crystal benchtop diffractometers, dedicated to education and outreach around 'chemistry of the solid state'. This laboratory has seen many school children, undergraduates, masters students, members of the public and PhD students introduced to crystallography for the first time through hands-on learning. These activities contributed significantly to me attaining Senior Fellow of the Higher Education Academy status in 2016: the first non-education based member of staff in my university to do so. I am also committed to the BCA, having served in numerous committee positions and attended every Spring Meeting since 1992! I will bring all this background and experience to the position.

As the current incumbent of this position, I have spent time making sure education and outreach is firmly knitted into the agenda, infrastructure and working of the BCA. I have also strived to develop routes by which more members can get involved with education and outreach, including inaugurating a bursary scheme for developing activities. This work is now beginning to come to pass (we are on the verge of launching an online way to share teaching resources) and I would like to take the opportunity in the next phase to build on this momentum. The key now is to concentrate on making sure as large an audience as possible engages with this work and thereby enable this important aspect of BCA work to become fully mainstream. In recent years I have been involved in education and outreach in developing countries, particularly in Africa. I will strive to develop the BCA education remit further afield, particularly in the developing regions of the world.

These are important and exciting times for promoting our subject areas and I relish the opportunity to be fundamentally involved in developing this aspect of the BCA.



Cheryl Doherty

Current position:

Principal scientist at Pfizer Global R&D Sandwich in Pharmaceutical Sciences Small Molecule.

Education:

MChem in Chemistry at the University of Bath (2001); PhD in Chemistry, University of Bath (2005); Materials Scientist at Pfizer (2006- present day).

Professional Activities:

British Crystallographic Association industrial group committee member 2009-present day, chair (2013-2016), vice-chair (2016-present day). Meeting and session organiser of numerous Industrial group meetings during this time. Diamond Industrial Science Committee DISCo (2013-present day). Royal Society of Chemistry Chartered Chemist (2011-present day).

Research/Professional Interests:

Materials Scientist at Pfizer with 12 years' experience in the Pharmaceutical Industry. Primary focus on developing dosage forms for drug candidates. This includes using molecular modelling, crystallographic data and statistical analyses of structural information to design a program of action and guide dosage form development for these projects as well as guiding the experimental screening, characterisation and analysis of these candidates. This can be on candidates from early research (before first in human studies) through to those in Phase III clinical trials. Focus areas include using laboratory

and synchrotron source small molecule crystallography of pharmaceutical organic materials, quantitative phase analysis and identification of pharmaceutical powders and drug products and the use of structural data in statistically based computational models to rationalise and predict complex behaviour in pharmaceutical products.

Personal Statement:

I first joined the BCA as a student member and what struck me most at those early meetings was the very real sense of community that is, I think, still a strength of the group. Since those early years as one of the Young Crystallographers I moved from the Chemical group to the Industrial as I started my career in the pharmaceutical industry. I am grateful for the invitation from the nominating committee to stand for a position on council and would welcome being trusted with this opportunity to continue to work with and support my fellow members.

I work primarily with formulators, medicinal chemists and process chemists with little background in the structural sciences. The impact crystallographic information can have on all these other areas is profound and I have supported outreach efforts in this area, such as by contributing to the RSC Medicinal Chemistry Residential School last year. Membership of the BCA has provided a vital contact with structural scientists in academia and industry for me, and has been the source of several fruitful collaborations.

I have been an active member on the Industrial group for several years, first as an ordinary member, then as chair and finally as vice chair of the group. I was the webmaster for some of that time and I have also been able to organise a number of our meetings, primarily but not entirely pharma focussed. By our nature the Industrial group are a diverse bunch and I have found we have much in common, no matter how different the industry specifics first seem.

I would be honoured to serve the BCA as a member of this committee.



Christoph G. Salzmann

Current position:

Associate Professor in Physical and Materials Chemistry & Royal Society University Research Fellow, Department of Chemistry, University College London

Education:

MSc and PhD in Chemistry at the University of Innsbruck (Austria), Postdoctoral Researcher & Junior Research Fellow at the University of Oxford (working with John Finney, Paolo Radaelli and Malcolm Green).

Professional Activities:

Chairman of the Molecular Spectroscopy user group at ISIS (since 2013), Member of the Physical Crystallography Group committee of the BCA (2011-2016), Member of the ISIS Disordered Materials Facility Access Panel (2014-2016), Organisation and Chairman of Sessions at BCA Spring Meetings (2016, 2015 & 2012), Co-organiser of the CECAM meeting "From atoms to clouds: bridging the gap between atomistic simulation, surface science, atmospheric observation and climate modelling" in Zurich (2014), BCA Prize for Physical Crystallography (2010), BCA and RSC member (since 2006).

Research Interests:

The research activities of my group at UCL Chemistry focus on the structural characterisation of a wide range of materials including disordered crystals, amorphous and nanomaterials as well as liquids. Our keen ambition is to establish links between the atomic structure of materials, and their chemical and physical properties and performances. Naturally, X-ray and neutron diffraction are at the very heart of our research activities. But the group makes also extensive use of vibrational spectroscopy, calorimetry and transmission electron microscopy to name a few complementary techniques. Our love for the disordered makes us power users of total-scattering software packages such as RMCProfile, EPSR and DIFFaX. Sample preparations include high-pressure as well as low- and high-temperature procedures, inert-gas chemical syntheses and vapour deposition techniques. I am quite proud in thinking that there is not much which we cannot achieve in our lab in terms of sample preparations.

Research highlights from the group include the recent discovery of a new allotrope of phosphorus inside carbon nanotubes which we named 'pink phosphorus', the classification of high-density amorphous ice as a 'derailed state' along the ice I to ice IV crystalline to crystalline pathway, the discovery of 'super-dipole' aggregates in liquid chloroform as well as the first structural insights into azeotropes by using diffraction techniques. Stacking disorder is a particular pet topic in the group – we could recently show that Lonsdaleite is not actually hexagonal diamond but should be classified as stacking-disordered diamond. In fact, no one seems to have achieved a 'hexagonality' greater than 60% for diamond so far. For ice, the story is similar but with reversed roles – making hexagonal ice is easily achieved by simply putting water in a freezer. However, we could show that what was previously thought to be cubic ice is in fact stacking disordered ice. Making the perfect cubic ice is there still one of the holy grails in ice research which we are chasing relentlessly. The fact that snowflakes are sometimes found with only three-fold rotational symmetry was interpreted by us that stacking disordered ice may exist in the upper atmosphere of our planet. Clarifying this question would obviously be important with respect to the surface chemistry of atmospheric ice as well as its light scattering properties. However, the definitive proof is still missing – carrying out X-ray diffraction measurements at high altitudes is not going to be easy. But we are not going to give up! Ice has actually always been a very fascinating material to me and my early work included the discovery of three new polymorphs which we named ices XIII, XIV and XV. Last year, I was awarded an ERC Consolidator grant which will now enable my group at UCL to investigate the structure and dynamics of water and ice at the carbon interface in great detail. One aspect, for example, will be to try and make new types of clathrate hydrates with large cages – and then of course to solve their crystal structures.

Statement:

I am delighted to have been nominated for a position on the BCA council. Following the award of the BCA Prize for Physical Crystallography in 2010, I thoroughly enjoyed being a committee member of the Physical Crystallography Group for the last six years. My highlights were the organisation and chairing of sessions at the BCA Spring meetings which focussed on "hydrogen bonding", "liquids and amorphous materials" as well as "phase transitions". I would now be looking forward to taking my enthusiasm for crystallography to the BCA council. Apart from continuing to be engaged in the organisation of the spring meeting, there are three topics that would be of particular importance to me: The first one is

with respect to constantly continuing to improve and modernise the teaching of crystallography at the undergraduate level. Secondly, considering the firmly established importance of pdf methods, I think there is now an urgent need to develop a CIF-file analogue for pdf data. In the same way as we can currently download crystal structure information, I believe that data and key parameters from pdf studies need to be made publically available as well in a well-defined, 'clever' file format. Also, we now need to somehow develop an analogue to the R-factors in traditional crystallography for pdf data indicating how reliable the reported data is. Finally, given my experience with complementary techniques such as electron microscopy, atomic force microscopy and vibrational spectroscopy, I will remain dedicated to further exploring the interface between crystallography and other techniques, and to reach out to other research communities. My overarching aim is to promote the importance of crystallography and diffraction techniques as widely as possible also with the thought in mind to continue growing our membership.



Mark S. Senn

Current position:

Royal Society University Research Fellow,
Department of Chemistry, University of
Warwick (2017 – present).

Education:

MChem degree, Chemistry, Durham
University (2008); PhD in Chemistry, University of Edinburgh
(2012).

Professional activities:

Member of the Royal Society of Chemistry and the British Crystallographic Association, Ordinary Member of BCA Council (March 2015 – March 2018), teacher at the biennial BCA intensive school on crystal structural analysis (March 2015 – present), ordinary member of the Physical Crystallography group of the BCA (March 2014 – March 2020), organiser of the 2018 intensive school in physical crystallography.

Research Interests:

Solid state chemistry and condensed matter physics; crystallography; symmetry and Irreducible representation analysis; phase transitions; ferroelectric, magnetic and multiferroic order; charge orbital and molecular-like ordering; perovskites; soft mode lattice dynamics and negative thermal expansion; superconductivity and the thermoelectric effect.

Statement:

I am pleased to stand for re-election as an Ordinary Member on the BCA Council. I will aim to bring my experiences in research, teaching and organisation within the crystallography community to this position, as well as my strong ties with the PCG community.



Call for Nominations for BCA Named Lectures

THE BCA awards and hosts a number of named lectures at its annual Spring Meeting. These lectures are now scheduled on a regular cycle. The Dorothy Hodgkin Prize, The Bragg Lecture, and The BCA Prize Lecture are awarded once in a 3-year cycle. The Lonsdale Lecture, presented during the main meeting, and The Parkin Lecture, presented during the YCG Satellite Meeting, are awarded annually. Details of each award and previous winners are available on the BCA website crystallography.org.uk/prizes/.

The Parkin Lecture, 2018

Nominations are sought for the annual Parkin Lecture, due to be presented at the 2018 BCA Spring Meeting. The Parkin Lecture is awarded by the Young Crystallographers Group of the BCA. This lecture is named in memory of the late Dr Andrew Parkin and recognises his outstanding achievements as scientist and teacher, and his role in public outreach. Nominations of early career scientists who have had significant involvement in teaching and outreach activities should be submitted by email to the YCG chair (sam.horrell@desy.de) with a short (< 250 words) case for support. **The deadline for nominations is February 2nd 2018.**

The BCA Prize Lecture, 2019

Nominations are sought for the triennial BCA Prize Lecture, due to be presented at the 2019 BCA Spring Meeting. This is the first occasion in which nominations have been sought from the membership. The awardee will be someone who has made a notable contribution to scientific research in which crystallography has played a central role. Nominations are welcomed from any part of the crystallographic community and should be sent by email to the BCA President (president@crystallography.org.uk) together with a short (< 500 words) case supporting the nomination. **The deadline for nominations is February 23rd 2018.**

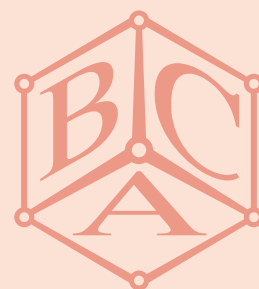
The Lonsdale Lecture, 2019

Nominations are sought for the annual Lonsdale Lecture, due to be presented at the 2019 BCA Spring Meeting. The Lonsdale Lecture is awarded by the BCA on the recommendation of the Young Crystallographers Group. The range of topics that may be presented by the awardee encompasses all areas of crystallography and diffraction and the lecture is expected to have an element of teaching. Nominations for The Lonsdale Lecture should be sent to by email to the BCA President (president@crystallography.org.uk) and include a short (< 500 words) case supporting the nomination. Awards are made in consultation with and upon the recommendation of the Young Crystallographers Group. **The deadline for nominations is February 23rd 2018.**

Puzzle Corner

THE 2018 European Crystallographic Meeting will take place in a very pleasant corner of Spain. From the following chemical or crystallographic clues derive symbols that give them a holiday message.

- ___ ___ Main ingredient of steel
- ___ ___ Its ions power highly energy-dense batteries
- ___ ___ Number of formula units in the unit cell
- ___ ___ Related to the element in the second clue; too much could give you high blood pressure
- ___ ___ Transition metal next to titanium
- ___ ___ Represents a body-centred cell
- ___ ___ Big brother of element 1
- ___ ___ Abbreviation for the base that pairs with thymine
- ___ ___ You need to breathe this
- ___ ___ That transition metal again
- ___ ___ Halogen you need to prevent goitre
- ___ ___ It's equal to mc^2
- ___ ___ Schoenflies symbol for a vertical (diagonal) mirror plane between 2-fold axes
- ___ ___ Schoenflies symbol for an octahedral group



Latest Developments in Education and Outreach

A CURRENT aim for Education and Outreach is to be able to support and empower as many people as possible to get out there and spread the word – to as large and diverse an audience as possible. Most of us will have small scale science fairs and outreach events or opportunities happening close by at some time or other and the BCA wishes to help maximise the promotion of crystallography at these. A significant barrier that most encounter when presented with this opportunity is not having an activity to run – and so the opportunity goes begging. We have set out to address this problem by establishing a mechanism whereby outreach activities can be made available online as ‘activity packs’ for anyone to use.

If aims, instructions, supporting resources (physical or electronic) and model risk assessments are readily available, then all the hard work is done already and all that remains is for you to get out there and talk about crystallography! It is early days, but an online repository at <http://learn.crystallography.org.uk/LearningResources> has been established and has a few examples of what these resources, or activity packs, can be.

We are now looking for contributions to help build up this resource. They can be big or small activities, aimed at diverse audiences from school children and the general public to politicians or other scientists. This resource can also be used for spreading of best practice in our university teaching – do you have an activity or a demo that you give in your lectures that could be shared? Please get in touch with **Simon Coles** (s.j.coles@soton.ac.uk) if you have material that can be shared in this way and we will look at what would be required to turn it into an activity pack.

Alternatively, if you have an idea that needs working on in order to develop it into an activity pack, then why not apply for a BCA Outreach Bursary to do so...

BCA Outreach Grants and Bursaries

APPLICATIONS to the BCA Outreach fund are sought to develop Education and Outreach resources for reuse within and beyond the community. Details of the schemes can be found at <http://www.crystallography.org.uk/bursary-scheme/>, however in summary:

Funding would support development of activity packs to support Outreach activities. These can range from physical materials made available via the inventory or electronic resources such as downloadable activity packs, guidance materials for conducting an exercise or software applications. These can be applicable to any age group or audience i.e. school teachers or scout leaders are as relevant as academics! It is a condition of the funding that the resources are openly available so that they can be reused by anyone, however, trialing and evaluating them at specific outreach events as part of a funded project is perfectly acceptable.

Funding is available at two levels. **Bursary** support may be sought for 8 week internships to fund undergraduate students to develop resources – these would normally be up to a level of £2500 for a stipend and materials. Alternatively, an individual may request **Grant** funds of the order of £300 to purchase materials required to develop an activity. These costings are indicative only and a funding breakdown summary will be required as part of the application.

Applications from Early Career Researchers are particularly favoured, either to perform the work or to supervise an intern. However, a supporting statement is required from a supervisor to indicate that the appropriate environment to conduct the work will be provided.

Applications or enquiries should be emailed to **Simon Coles** (s.j.coles@soton.ac.uk) and the closing date for the 2018 round will be **17:00 on Friday 2nd March 2017**. Applications will be reviewed by the Education committee (comprising the Education and Outreach Coordinator and the education representatives from the BCA groups) and potentially in some cases also by BCA Council.

Answers to September Puzzle Corner

THE venues (and waterways) for the European Crystallographic Meeting of 2016 and the American Crystallographic Association meetings of 2017, 2018 and 2019 are:

Basel (Rhine, river)
New Orleans (Mississippi, river)
Toronto (Ontario, lake)
Covington (Ohio, river)

The names require the following 27 letters: A x 1, E x 1, H x 2, I x 7, M x 1, N x 2, O x 4, P x 2, R x 2, S x 4, T x 1.

The element symbols are: Ne, Ar, Mn, Rh, Th, P x 2, O x 4, S x 4, I x 7, giving the same individual letters as above.

IUCr 2017 Hyderabad

Blog Day 1, Monday 21 August: International crystallography, collaboration and community



THE opening of the 24th congress and general assembly of the International Union of Crystallography was marked by a splendid programme that stressed, time and again, the international nature of our crystallographic community. When Professor

Gautam Desiraju, the organising committee chair and immediate past president of the IUCr, quoted one of the discipline's founding fathers, **W. L. Bragg**, in his welcome address: "At a scientific conference nationality disappears" he could have been summing up the whole event.

Certainly, this is the most diverse IUCr congress yet, as Desiraju explained. There are representatives of 73 countries here in Hyderabad, more than the 58 national members of the International Union. India is represented by over 500 delegates and the other BRICS countries – Brazil, Russia, China and South Africa – have all sent substantial delegations. The challenges and opportunities for scientists in these very different but in many ways surprisingly similar emerging countries will be discussed later in the week. Several countries including the Cameroon and Myanmar have sent a single delegate, but the most significant example of the 'borderless' nature of crystallography might be the 17 delegates from Bangladesh. Three of these are students who have joined the band of enthusiastic conference volunteers on equal terms with their domestic counterparts.

The IUCr President, **Marvin Hackert** of the University of Texas, Austin, gave a talk running through the history of the Union and its congresses. Like independent India, the IUCr was 'born' in 1947, and its international congress has taken place every third year since 1948. It has grown out of recognition since those early days but its basic roles are essentially unchanged: maintaining standards, publishing books and journals (including the International Tables) and promoting international collaboration. And a number of new initiatives have been started in or after the highly successful International Year of Crystallography in 2014. These include the LAAMP project – or the Lightsources for Africa, the (Southern) Americas and Middle East Project – to provide greater access to advanced synchrotron sources for scientists working in these disadvantaged regions. India already has two such sources, with others planned.

Paul Peter Ewald, a pioneering crystallographer known to students of structural science throughout the world for his 'Ewald sphere', was one of those principally involved in setting up the IUCr. Since 1986, his memory has been honoured by the award of the Ewald Prize at each congress to a distinguished crystallographer. The 2017 prize was therefore the eleventh in the series; it was awarded to Sir **Tom Blundell** from the University of Cambridge, UK, a pioneering structural biologist and a co-founder of Astex Pharmaceuticals.

Blundell's prize lecture was a tour de force, a whirlwind summary of half a century at the forefront of structural biology. Time and again, he came back to the importance of collaboration, both between nationalities and between academic and industrial scientists. And time and again he came back to his mentor, Nobel laureate **Dorothy Hodgkin**. He joined Hodgkin's lab as a student in 1964, the year in which she won the Chemistry Nobel, and became a member of the group that solved the 3D structure of insulin. He described giving his first plenary lecture at an international conference as a 27-year-old in 1969, showing delegates at the eighth IUCr congress the newly-solved structure of that vitally important biological molecule.

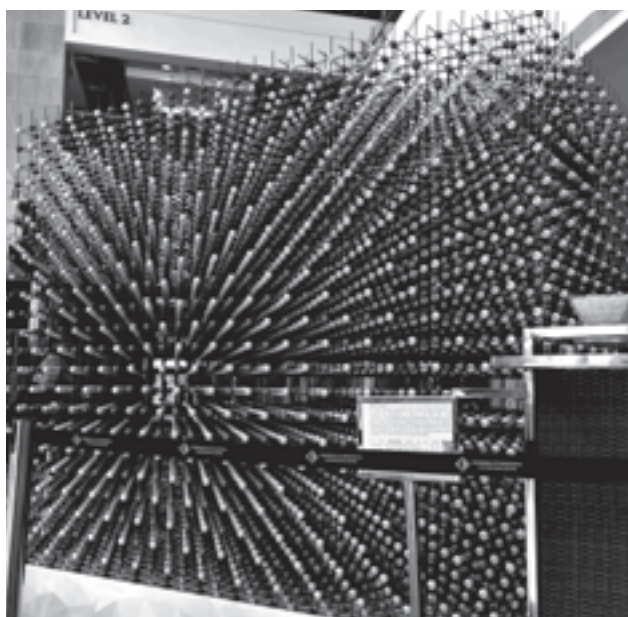
During his talk, he drew out four 'lessons' from Dorothy Hodgkin's example and the insulin story, illustrating them with anecdotes from throughout his career. Firstly, he explained that good science requires a long-term vision by citing the thirty years between the first insulin crystals and the first publishable 3D structure. There are lessons here for today's grant agencies and journal editors. His second point stressed the value of international and interdisciplinary teams and his third the importance of writing up experimental methods: Protein Crystallography, the book he co-authored with **Louise Johnson** in 1976, was the first authoritative textbook on this subject.

Blundell devoted most time to the fourth 'lesson', on the value and quality of industrial science. He has collaborated with the pharma industry since the Seventies – then perhaps rather improbably as a left-wing firebrand of an Oxford City councillor. His was one of the groups that simultaneously solved the structure of HIV's protease, paving the way for some of the most successful drugs for AIDS. In 1999 he and two ex-colleagues, **Harren Jhoti** and **Chris Abell**, founded Astex to pioneer the technique of fragment-based drug discovery. This company is now wholly owned by Otsuka Pharmaceuticals in Japan, and eighteen years after the program was launched, its first drug, ribociclib, has just received FDA approval for breast cancer. Dorothy Hodgkin herself would recognise this time-scale. Blundell is now taking the technologies pioneered at Astex back into academia for complex targets and neglected diseases, the latter with generous funding from the Gates Foundation. Despite passing the 'official' retirement age he still has plenty of plans for his international, interdisciplinary team, and for what his mentor might have called 'useful' crystallography; I will be reporting on more of both throughout the meeting.

Dr Clare Sansom, Department of Biological Sciences, Birkbeck College, London, UK

(The rest of Clare's blogs can be accessed at <http://blogs.iucr.org/crystallites/>.)

THE beep of horns and balmy temperature confirmed my arrival in Hyderabad, India for the 24th Congress and General Assembly of the International Union of Crystallography. Despite being monsoon season, we had sunny clear blue skies to accompany us on our journey into the city. The triennial IUCr conference, hosted at Hyderabad's International Convention Centre within the tech district, commenced on the Monday night with a drinks reception and welcome ceremony. Here the world's largest crystal structure was unveiled, a sodium chloride structure boasting 11.8km of sticks and 42,875 balls! Sir Thomas Blundell, who determined the crystal structure of insulin along with Dorothy Hodgkin, was the recipient of the 11th Ewald prize and gave an engrossing first talk. The welcome ceremony then drew to a close with a traditional Indian musical performance.



The conference continued over the next week with three plenaries, 40 keynotes, countless microsymbiosia and satellite meetings, all of which provided a fantastic platform for exploration of the latest cutting edge research in the field of crystallography, covering life sciences, physics and chemistry. From membrane protein structure determination to computational materials design the breadth of information available was astounding. With participants from over 60 countries including students, professors, exhibitors, and industry representatives, the opportunity for networking and collaboration was superb. Poster sessions were held each day during lunch and coffee breaks within the exhibition hall, creating a lively hub of scientific discussion. For busy delegates, novel E-poster screens were dotted around the conference centre, allowing delegates to easily select and access posters from throughout the week. In keeping with current technology, there was also a mobile app available which contained information on talks as well as facilitating contact between speakers and delegates, with a daily quiz for the competitive among us.

As a reminder to our location, somewhat forgotten within the air-conned halls, were frequent art and culture talks delving into the rich history of India. Daily trips were also available for delegates to experience India's culture first hand. A steady climb up the 365 steps to the top of the Golkonda Fort was rewarded with an impressive and breathtaking view over the whole city.

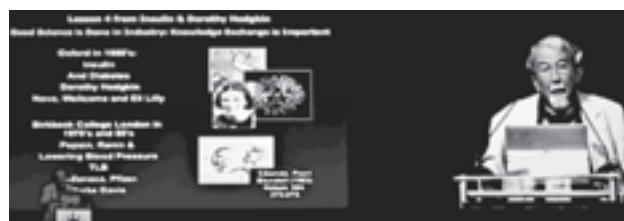
An elaborate banquet hosting dishes from regions across India was held on the penultimate night, where parrot fortunes were read, jewellery was forged, and Mehendi, Hyderabad's form of henna, decorated hands. The end of the conference was marked by the closing ceremony, where a multitude of poster prizes were awarded and the 2023 IUCr host country was announced as Melbourne, Australia.

The quality and diversity of topics presented at this conference provided a well-rounded and in-depth understanding of the processes undergone from protein expression and purification all the way through to the diffraction data analysis, beneficial to both early stage researchers and experts in the field.

Amy Danson
University of Reading

USUALLY going to the International Union of Crystallography's Congress, the largest meeting for crystallography in the world and held only once every 3 years, is a momentous occasion in itself. My lone previous experience attending the meeting in Montreal in 2014 was incredible, and the sheer quantity of and quality of excellent science being presented was overwhelming. Now take this, and add the fact that this year's conference was being held for the first time in India (a country that I had never visited before) and you have quite the combination.

Held in Hyderabad in August of this year, the conference started with an inspiring Ewald lecture by Sir **Thomas Blundell**, highlighting a career over many decades in which crystallography gave a unique insight into the structure and function of proteins. What was particularly inspiring was Sir Thomas's clear acknowledgement of the valuable mentorship of Dorothy Hodgkin and her influence over many different strands of his research, reminding the audience of her transformational effect on the field. We were also treated to a wonderful performance of Indian music, a mixture of centuries old poetry and improvisation in what was a completely new style to me.



My invited talk was the very next day, and I was fortunate to be part of a really insightful microsymposium covering computational materials design, from first-principles calculations to strategies for crystal structure prediction. I had some great conversations with some attendees after the session, and have some new ideas to work on once I get back to the lab!

Over the next seven days there were far too many excellent talks to list them all, but some highlights for me included **David Bryce's** ingenious way of combining solid-state NMR information to obtain better structural refinements, **Branton Campbell's** clear and insightful presentation of a new method to consider coupled rigid unit modes for structural distortions in tungsten bronzes, and **Andrew Goodwin's** always enjoyable exploration of the world of disorder in crystallography, accompanied by some beautiful tilings.



Away from the science, the week was filled with a lot of new and amazing food experiences, first and foremost being the local Hyderabad specialty, biryani. The conference dinner was part Bollywood spectacle, part street food market, and above all an excellent way to relax and socialise with some new friends from all around the world. This IUCr was special in its efforts to invite participants from around the world, with around 500 participants from India alone (a record), as well as many crystallographers from Africa and South and Central America. It certainly felt like a truly global community brought together by their love of science.

Now that I'm back in Cambridge, I have a notebook full of new ideas to explore, a number of email threads with new possible collaborators, and a mind full of fond memories. What more could one want?

Matthew Dunstan
University of Cambridge

THE vibrant, southern Indian city of Hyderabad was host to the 24th Congress and General Assembly of the International Union of Crystallography. Much like Hyderabad itself, the international convention centre was a hubbub of excitement and activity over the 8 days the conference took place. With over 1700 participants from 73 countries, the conference was successful at bringing together scientists from diverse backgrounds, unifying them with one common scientific theme, crystallography. The 3 plenaries, 40 keynotes, 119 microsymposia and hundreds of posters ranged in topics from 'Crystallography of materials for energy' to 'Crystallographic patterns in art and cultural heritage', reflecting the broad scope of applications for crystallography.

The conference kicked off with a short speech by **Gautam Desiraju**, who gave us a brief history on the origins of IUCr and its growth over the past 70 years. This was followed by an awe-inspiring Ewald Prize lecture given by Sir **Tom Blundell**. In addition to the several humorous and remarkable anecdotes about his 40 year career in crystallography (as well as a jazz musician/political activist), Tom emphasized a number of important issues in the field. The first issue highlighted was the importance of diversity in science; in particular, the participation and, notably, the recognition of women in science, especially in a 'field that was pioneered by women'. Other issues included the importance of knowledge exchange between academia and industry, the importance of international and interdisciplinary collaborations, the requirement for long term vision, and the importance of documenting crystallographic methods. Overall, the opening ceremony had set the standard for what was to be an excellent congress.

The high calibre of presentations continued throughout the week. As well as the session on the 'Analysis and validation of protein ligand structures', which was most relevant to my current research interests, I was especially impressed by the session on 'Techniques and insights into macromolecular crystallization', chaired by **Abel Moreno** and **Anna Schenk**. It was both exciting and intriguing to hear about the innovative strategies and novel technologies being developed for crystallization experiments. These included the use of gels, Molecularly Imprinted Polymer nucleants, luminescent lanthanide complexes, a novel Cross-Diffusion Microbatch plate and Designed Ankyrin Repeat Protein crystallization aids to obtain high quality crystal structures, all demonstrating the significant advances in macromolecular crystallization.

The city of Hyderabad offered ample opportunities for sightseeing in the evenings and downtime. The rich culture and history of the city meant that there was something for everyone to enjoy; from tombs to temples, to the markets and bazaars, and even the largest film studio complex in the world. We were even lucky enough to experience some of the celebrations for the Ganesh Chaturthi religious festival that took place while we were there.

As a first year PhD student, and newcomer to the world of crystallography, IUCr2017 was extremely educational, interesting and enjoyable. It was incredibly encouraging to see such an extensive, but friendly community of crystallographers who actively welcome the participation of young investigators. Presenting my research as a poster was a valuable experience, not only in allowing me to exchange thoughts and ideas with others interested in the same field, but also in allowing me to develop my confidence as a crystallographer. Without the Arnold Beevers Bursary Fund, this trip to Hyderabad would not have been possible, and for that I would like to sincerely thank BCA for their support.

Dannielle Kydd-Sinclair
University of Reading

THIS year's IUCr Congress was held in the amazing city of Hyderabad, India and gathered together 1827 delegates from 73 countries. The conference featured 666 speakers talking in a diverse and interesting programme.

Right from the opening ceremony, it was clear this conference would be one to remember. We were treated to the Ewald Prize Lecture by Sir **Tom Blundell** from Cambridge University on "Crystallography, structural biology and drug design". This looked at developments in structure guided and fragment based approaches to identifying and targeting molecules for drug design, focusing on the collaboration between academia and industry to achieve the best results. This is particularly relevant to my PhD and was without a doubt a highlight of the conference. This was followed by a welcome to the conference including the opportunity to view a small sample of the amazing Indian dance and music, as well as for our first taste of real Indian food.

The conference continued with a huge variety of exceptional speakers talking across 9 parallel streams. This ensured there was always something fascinating and relevant to listen to. I particularly enjoyed the session on structural immunology and receptor signalling, in particular a talk on T-Cell receptors by Dr **Stephanie Gras** from Monash University, Australia. This work investigating the modes of recognition of antigens by

T Cells featured diverse and impressive structural work to establish the molecular basis of this interaction.

The session on “Cryo-EM: Method of the Decade” was also a highlight, along with the preceding lecture by now Nobel Prize winner Dr. **Richard Henderson**, looking at the work done in advances in Cryo-EM, along with a number of the incredible discoveries found using this amazing technique.

In addition to traditional research talks there was also a special activities programme which included talks on less traditional topics. I found the session of new approaches to crystallographic teaching particularly informative, and it was very interesting to see the range of software and tools being used to teach crystallography across all ages. A Dragon’s Den style competition also occurred in this parallel programme which allowed early career researchers the opportunity to pitch for funding for a scientific research proposal. Ideas covered a huge range of topics and it was fascinating to hear snippets of ideas from so many areas.

The congress featured a large number of networking breaks in addition to a large industry fair. This allowed for discussion about new developments in technology as well as the opportunity to pick up some freebies!

The conference concluded with a spectacular banquet, with different stands with food from all over India available to try. There was also entertainment in the form of Indian dancers and singers, with the chance to try our hand at some Bollywood dancing! The range of topics and standard of speakers at the conference was both spectacular and stimulating, providing a great opportunity to experience more of the field and help aid with decisions of what to do following my PhD.

Rebecca Eno
Durham University

55th EHPRG Meeting, Poznań, 2017

THE 55th European High Pressure Research Group (EHPRG) Meeting was held in the historic Polish city of Poznań by the Adam Mickiewicz University in Poznań. The venue was the Department of Chemistry situated on a modern well equipped campus a short tram ride north of the beautiful old market square and ancient cathedral island.

The conference started on Monday September 4th and was opened by Dr **Ho Kwang Mao** on hydrogen generation in the deep lower mantle and then straight into 4 parallel sessions for the rest of the morning and afternoon. Dr **Kamil Dziubek** gave an interesting presentation on the importance of recording all the possible metadata alongside raw data and raising the controversial point of open access to raw data. Kamil also reported on the efforts of the International Union of Crystallography Commission on High Pressure to encompass all the vital aspects of high pressure data and metadata within the Crystallographic Information Framework, CIF. This was followed by the first of two lively poster sessions accompanied by a good Polish beer or two.



In a Tuesday morning session I presented my recent work on developing a new moderate pressure capillary cell for I19 at Diamond Light Source. This session was devoted to new high pressure instrumentation from a wide range of different fields and pressure regimes, and I received great feedback and lots of interest in what we are working on. The afternoon followed

quickly with an update on recent developments at high pressure central facilities around the world. Then it was off back into town for an open lecture from Professor **Leonid Dubrovinsky** entitled ‘Journey to the centre of the Earth 150 years after Jules Verne: Science - not fiction’ in the beautiful opera hall of Poznań University.

On the Wednesday there were talks in the morning followed by a fun, if slightly soggy, trip to Rogalin Palace, a large stately

home south of the city that has recently been restored to its former glory. Thursday’s afternoon plenary was given by Professor **Elena Boldyreva** who gave a very interesting retrospective on organic and coordination compounds at high pressure, a very similar field to my own group, and her perspectives on future challenges and goals in this area. More posters followed and then it was time for the Gala dinner. The last evening was opened with a fantastic concert from an award winning classical pianist followed by food and a great jazz band to get the night started. Friday was the last day of the conference and time for me to head home to Edinburgh.

This was the first EHPRG meeting I have attended and also my first visit to Poland. However, I am sure it will not be my last visit to either. I am extremely grateful to the BCA for awarding me an ABBF Bursary that made it possible for me to attend. I must also thank the organisers for accepting my talk and for putting on a really great, well organised, and friendly meeting. As a result of this trip I met and was able to present my work to many interesting and eminent scientists in the field of high pressure research; in particular, instrument development, a field that I aim to pursue in my own career.

Charlie McMonagle
University of Edinburgh

(Photos by Michal Kalet – website: <http://michal.kalet.pl/>)



CCP4 Protein Structure Workshop

THE annual CCP4 Protein Structure Workshop, in its long-time home of Carlisle, was held for the 24th time on September 6-8th. Organised by **Arnaud Baslé** (Newcastle), **Steve Prince** (Manchester) and **Khushwant Sidhu** (Leicester), this year's meeting was an intimate gathering of around 40 delegates from a spread of universities, from Glasgow in the North to Birmingham in the South, Manchester in the West to York in the East, although 'Northern-ness' is not a requirement for attendance with several delegates from Cambridge and Oxford.

Primarily a platform for PhD students (who can attend for free thanks to generous CCP4 sponsorship) and research associates, the workshop is an opportunity for early career researchers to present their work in a supportive, collaborative environment to an audience of peers – as well as a number of senior researchers. It was especially exciting this year to be treated to talks from many first-year PhD students just embarking on their research careers.

The theme of this year's meeting was "Complementary techniques" and the talks certainly delivered in diversity, with cryo-electron microscopy featuring heavily alongside X-ray and neutron crystallography (**Chris Millard**, **Peter Moody** (Leicester)), drug discovery (**David Hargreaves** (AstraZeneca)), SAXS (**Steve Prince** (Manchester)) and computational chemistry (**Andrew Leach** (Liverpool JMU), **Natalie Tatum** (Newcastle)).

The program for the 2017 meeting featured 13 students eligible for the prize for best presentation, and after much deliberation, the chairs chose first year PhD student **Charles Tomlinson** (Durham) as the well-deserved recipient for his talk on the use of fluorescent probes for studying retinoic acid binding proteins. Honourable mentions were also given to third year PhD student **Daniel Wood** (Newcastle) for his outstanding contributions to discussions over the three day workshop, and to first year **Freya King** (Manchester) for excellent communication of the context to her PhD research on the engineering of new vaccines. As ever, the standard of talks from our doctoral student delegates was truly exceptional.

The first of two plenary talks was delivered by Prof. **Neil Ranson** (Leeds) on the subject "What cryo-EM can do for you"; with recent advances in hardware and software transforming the field, Neil predicted that the next great leap will be in sample preparation. Neil demonstrated, using his group's work on BK polyomaviruses, the quality of biological information we can gain from cryo-EM, and his talk served as a great primer for any in the audience not yet privy to the 'cryo-revolution'.

The second plenary (pictured) was given by Dr. **Allen Orville** (Diamond Light Source) who dazzled us all with the power and progress of X-ray free electron lasers and the work of the XFEL Hub at Diamond. By implementing acoustic dispensing techniques among a host of other developments, Allen showed us how the careful synchronicity of crystal, XFEL beam and light can give us not only time-resolved diffraction data, but simultaneous single-crystal spectroscopic data.



Dr. Allen Orville

Other honourable mentions are made for Dr. **Andrew Leach** (Liverpool John Moores University), who showed us how quantum mechanics can be used alongside our current refinement methods to improve the quality of the ligands in our protein-ligand structures; Dr. **David Hargreaves** (AstraZeneca) who took us through the highs and lows of drug discovery using both DNA-Encoded libraries and antibody-assisted crystallography; and Dr. **John Berrisford** (PDBe) who demonstrated all new things bright and beautiful at PDBe.

With a CCP4i2 workshop and a poster session in addition to the program of talks, the success of the 24th meeting was made possible by the generous sponsorship of CCP4, Astex, AstraZeneca, the BCA Biological Structures Group and our commercial exhibitors, and we look forward to the next meeting – the 25th anniversary – to be held in 2018.

Natalie Tatum
Newcastle University

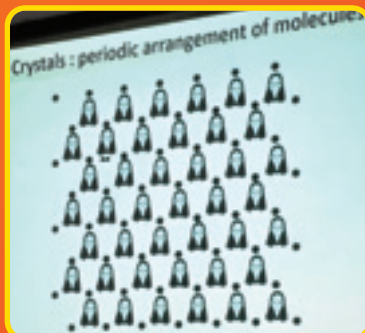
Memories of **INDIA**



Our photographer Helena Taberman, an innovative e-poster, more scenes of Hyderabad including the Chowmahalla Palace and the Qutb Shahi Tombs.



Bangalore, the venue for the Crystallographic Computing School, including one very keen would-be participant.



Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com. Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

10-15 December 2017

High-Accuracy CLEM: Applications at Room Temperature and in cryo, Heidelberg, Germany.

https://www.embl.de/training/events/2017/LEM17-01/index.html?_ga=2.263148357.87988381.1493825942-1740041149.1491823482

18 December 2017

BCA Biological Structures Group Winter Meeting, Cambridge.

<http://bsg.crystallography.org.uk/>

9-10 January 2018

Real-time cryo-EM image processing with SIMPLE, Oxford.

<http://simplecryoem.com/Oxford/workshop2018.html>

10-12 January 2018

CCP4 Study Weekend: Multi and Serial Crystal Data Collection and Processing, Nottingham.

<https://eventbooking.stfc.ac.uk/news-events/ccp4-study-weekend-2018-384>

27 January – 2 February 2018

2nd NEUBIAS. The Bioimage Analysis Community Conference, Szeged, Hungary.

<http://eubias.org/NEUBIAS/neubias2020-conference/szeged-hungary-2018/>

4-8 February 2018

Cryo-EM from Cells to Molecules: Multi-Scale Visualization of Biological Systems (F1). A Keystone Symposium on Cryo-EM, Tahoe City, CA, USA.

<http://www.keystonesymposia.org/index.cfm?e=web.Meeting.Program&meetingid=1576>

17-21 February 2018

Biophysical Society Annual Meeting. Fuelling Discovery through Biophysics, San Francisco, CA, USA.

<http://www.biophysics.org/2018meeting/Home/tabid/7117/Default.aspx>

18-23 February 2018

Photoionization & Photodetachment (GRC), Galveston, TX, USA.

<http://www.grc.org/programs.aspx?id=12840>

26 February – 9 March 2018

49th IFF Spring School 2018: Physics of Life, Juelich, Germany.

http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/_node.html

27 February – 2 March 2018

ICON Europe 2018. 2nd International Conference on Nanoscopy: Beyond the Diffraction Limit, Bielefeld, Germany.

<http://www.icon-europe.org/>

5-8 March 2018

26th Annual Meeting of the German Crystallographic Society, Essen, Germany.

<http://www.dgk-conference.de/>

20-23 March 2018

International Conference on Nanofilms 2018, Cranfield.

<http://www.ecnf2018.org/>

21-24 March 2018

3rd International Symposium on Cryo-3D Image Analysis, Lake Tahoe, CA, USA.

http://cryoem.bcm.edu/cryoem/events/view_workshop/1

26-29 March 2018

BCA Spring Meeting, Warwick.

<http://www.bcaspringmeetings.org.uk/>

8-13 April 2018

Powder Diffraction & Rietveld Refinement School, Durham.

http://community.dur.ac.uk/john.evans/webpages/riet_register.htm

16-17 April 2018

The Astbury Conversation 2018, Leeds.

<http://www.astburyconversation.leeds.ac.uk/index.php>

24-27 April 2018

XOPT'18. International Conference on X-ray Optics and Applications 2018, Yokohama, Japan.

<https://opicon.jp/info/20170601-876/>

20-25 May 2018

12th New Diamond and Nano Carbons Conference (NDNC 2018), Flagstaff, AZ, USA.

<http://www.mrs.org/ndnc-2018>

27 May – 1 June 2018

Fatigue 2018, Poitiers, France.

<https://www.sf2m.fr/Fatigue2018/Organization.htm>

1-10 June 2018

Electron Crystallography. 51st Erice Course, Erice, Italy.

<http://crystalalice.org/2018/>

1-10 June 2018

First Erice International School on Quantum Crystallography. 52nd Erice Course, Erice, Italy.

<http://crystalalice.org/2018/>

4-5 June 2018

Applied Crystallography, London.

<http://crystallography.euroscicon.com/>

11-16 June 2018

13th International Conference on Synchrotron Radiation Instrumentation (SRI 2018), Taipei, Taiwan.

<http://sri2018.nsrc.org.tw/site/page.aspx?pid=901&sid=1157&lang=en>

18-21 June 2018

PCG Intensive School in Physical Crystallography: From Phonons to Phase Transitions

Cosener's House, Abingdon, Oxfordshire.

<http://pcgschool2018.wordpress.com/>

18-22 June 2018

2018 E-MRS Spring Meeting and Exhibit, Strasbourg, France.

<https://www.european-mrs.com/meetings/2018-spring-meeting>

18-26 June 2018

The 14th European Summer School on Scattering Methods Applied to Soft Condensed Matter, Carcans-Maubuisson, Gironde, France.

<https://indico.ill.fr/indico/event/86/page/2>

24-28 June 2018

American Conference on Neutron Scattering (ACNS 2018), College Park, MD, USA.

<http://www.mrs.org/acns-2018>

25-28 June 2018

DSL2018. 14th International Conference on Diffusion in Solids and Liquids, Amsterdam, Netherlands.

<http://www.dsl-conference.com/>

26-29 June 2018

UKSR50. 50 years of Synchrotron Radiation in the UK and its global impact, Liverpool.

<http://www.uksr50.org/>

1-4 July 2018

EPDIC16 – The 16th European Powder Diffraction Conference, Edinburgh.

<http://epdic16.efconference.co.uk/>

9-13 July 2018

SIAM Conference on Mathematical Aspects of Materials Science, Portland, OR, USA.

<http://siam.org/meetings/ms18/>

11-13 July 2018

Methods and applications of crystal structure prediction: Faraday Discussion, Cambridge.

<http://www.rsc.org/events/detail/24508/methods-and-applications-of-crystal-structure-prediction-faraday-discussion>

20-24 July 2018

ACA 2018, Toronto, Canada.

<http://www.amerocrystalassn.org/2018-meeting-homepage>

29 July – 3 August 2018

Diffraction Methods in Structural Biology (GRC), Lewiston, ME, USA.

<https://www.grc.org/diffraction-methods-in-structural-biology-conference/2018/>

19-24 August 2018

XRM2018: 14th International Conference on X-ray Microscopy, Saskatoon, Saskatchewan, Canada.

<http://xrm2018.com/>

22-27 August 2018

31st European Crystallographic Meeting (ECM31), Oviedo, Spain.

<http://ecm31.ecanews.org/en/index.php>

26-30 August 2018

7th EuCheMS Chemistry Congress, Liverpool.

<https://www.euchems2018.org/>

2-6 September 2018

SMARTER6, Ljubljana, Slovenia.

<https://smarter6.ki.si/index.php/smarter6/>

7-12 October 2018

SAS2018. XVII International Conference on Small-Angle Scattering

<http://sas2018.anl.gov/>

2-5 December 2018

AsCA 2018/Crystal32: 15th Conference of the Asian Crystallographic Association and 32nd Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ), Auckland, New Zealand.

<http://asca2018.org/>





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