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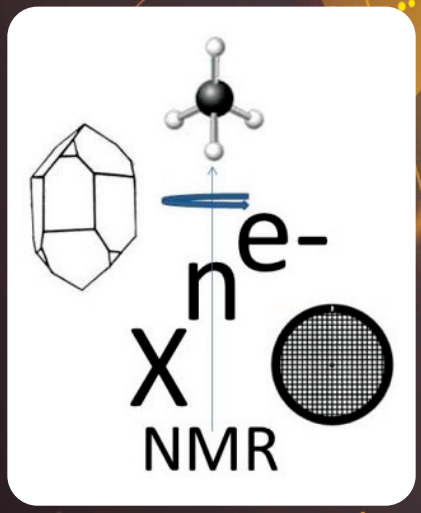
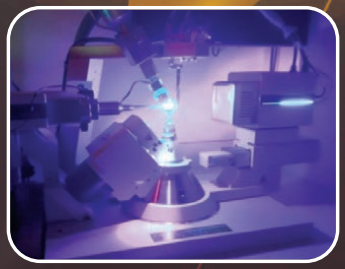


WORLDWIDE PDB PROTEIN DATA BANK 20 Years



Twenty years of the Worldwide Protein Data Bank

Twenty years of the wwPDB p6
Crystallography in Cardiff p7
BCA Spring Meeting 2024 p8
2023 Spring Meeting reports p11
Bursary winner reports p16
ACA 2023 Baltimore p17
Inaugural by Brendan Howlin p19
Down memory lane p20
Meetings of interest p22

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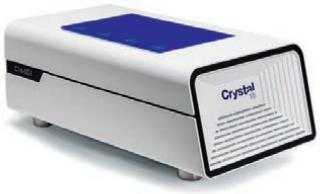

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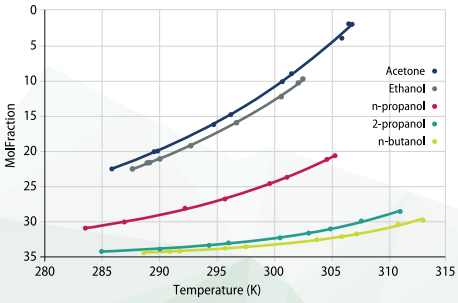

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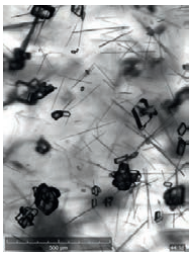
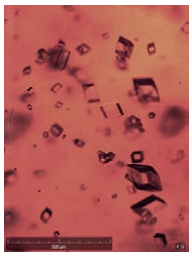


Polymorphic transformation



Coloured compounds

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British Crystallographic Association

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Further information on the eligibility criteria and the application portal is available here:
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https://industrial.crystallography.org.uk/bursaries-and-awards/

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the December 2023 issue are sent to the Editor to arrive before 25 October 2023.

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Contents

From the President 2
BCA Council 2023 3
From the Editor 4
Answer to last issue's problem 5
Twenty years of the Worldwide Protein Data Bank 6
Macromolecular Crystallography in Cardiff 7
BCA Spring Meeting 2024 8
Reports on the BCA Spring Meeting, Sheffield 2023 11
Bursary winner reports 16
ACA 2023 Baltimore 17
Inaugural Lecture by Prof Brendan Howlin, Surrey 19
Down memory lane: Snapshots of a sage 20
A challenging plane group and a history quiz question 21
Meetings of interest 22

This month's cover:

A selection of photos and logos from articles in this issue including John Helliwell's entry for the ACA logo competition two years ago (top centre).

From the President

BY the time you read this, the IUCr Congress in Melbourne will be over. I hope you enjoyed it and would invite attendees to share short reports on aspects of the meeting with *Crystallography News*. I would like to thank Suzanna Ward for leading the UK delegation to the IUCr General Assembly meetings. We are grateful, as always, to the Royal Society for matching funding for our IUCr subscription, which enables us to send a total of five voting delegates to these meetings. The Assembly receives reports from the IUCr journals, commissions and committees and makes decisions regarding, *inter alia*, approval of applications of states to join the IUCr, locations of future congresses, approval of new journal editors and international programmes of education.

Looking ahead to next year, I'm keen to encourage eligible BCA members to upgrade their membership to Fellowship status. This option recognises an established career in crystallography and offers a simple way to support the BCA through membership subscriptions. An online application form will be made available as we approach the membership renewal date.

I'm also looking forward to next year's BCA Spring Meeting in **Leeds** from **25th-28th March 2024**. There is such a rich crystallographic history at Leeds that chancing upon significant anniversaries is more likely than not: Next year is 100 years since the publication by Astbury and Yardley (later Lonsdale) – both of whom soon after relocated their research to the University of Leeds – of "Tabulated data for the examination of the 230 space-groups by homogeneous X-rays"[1] which introduced a simple and intuitive notation to display the symmetry elements of the 230 space groups, and which became the basis for the International Tables of Crystallography.

Thank you to our scientific programme chairs **Peter Moody** and **Hanna Kwon** along with **Suzanna Ward** and the rest of the Programme Committee, who have devised a great draft programme for the meeting which is outlined in this issue. I am pleased to note that **Arwen Pearson** will deliver the 2024 Bragg Lecture – a triennial lecture hosted by the BCA and awarded by the external Bragg Committee – and that keynote lectures are confirmed in the main BCA and ESCG programme from **Simon Coles**, **Syma Khalid**, **Aurora Cruz-Cabeza**, **Silvia Ramos**, **Helena Shepherd**, **Helen Ginn**, and **Lukáš Palatinus**. Your support by attending the meeting, inviting colleagues and submitting abstracts is always valued.

I was sad to learn of the passing of Professor Bruce Forsyth, age 91, a few days before this issue went to production. A short announcement, in French, is accessible in the ILL website.[2] Many BCA members and researchers in the neutron diffraction community will have known Bruce, who was one of the very first Honorary Members of the BCA. An article commemorating his life and work will be published in a future issue. If you are able to contribute, then please get in touch.

As I based a recent column on the influence of large language models (ChatGPT) on scientific publications, I was pleased to see an editorial in the current *IUCrJ* by Read, Baker, Bond, Garman, and Raaij[3] which set out a sensible and balanced view on the recent successes and subsequent hype of another opaque computational model – AlphaFold. The authors note that *"… recent anecdotal reports suggest that some scientists reviewing grants and papers believe that AlphaFold is so powerful that it has made experimental structural biology redundant."* This, perhaps unintended, side effect of the excitement surrounding a poorly understood new technology is sadly real, at least in the short term. Furthermore, according to the often-cited model from US IT consultants Gartner, the initial hype will be followed by a precipitous drop from the "Peak of Inflated Expectations" to the "Trough of Disillusionment". However, as the IUCrJ article is keen to point out, there are real opportunities for structural biology to exploit information from AlphaFold, including assisting with structure solution of experimental X-ray and cryo-EM structures, allowing researchers to make faster progress with analysis and to use the insights to address deeper biological questions. Gartner calls this recovery "The Slope of Enlightenment" which rises gently to "The Plateau of Productivity" at which point the true value of a technology emerges and gives rise to improved efficiency and results. It seems like a good idea to keep one eye on when and where new methods will eventually make a real impact, to avoid being blinded by either the hype or the disillusionment extrema.

A reminder that as of the BCA AGM 2024, Council will have vacancies for one Ordinary Member, one Outreach and Education Coordinator, and one President. There is no direct succession from Vice-president to President – anyone may be nominated for any vacancy. Nominations may be made by any two members and should be accompanied by an email or letter from the nominee giving their consent to serve if elected. Nominations must be sent to the BCA Secretary (secretary@crystallography.org.uk) by September 30th. The nominating committee will also work to secure nominations for these vacancies. Candidates will provide short statements to appear in the December issue of *Crystallography News* in advance of voting in the new year.

In response to changes made following the takeover of twitter last year (now known as 'X'), a significant number of users have left or reduced their engagement, and advertisers have distanced themselves from the platform as banned accounts were reinstated and standards of content moderation dropped. As an organisation that has historically used the platform for alerting members to news and for promoting crystallography to a wider audience, as well as for occasional 'live tweeting' of meetings, this has left us hunting for new platforms to reach members who have chosen to move on. For the time being you can follow meeting announcements and discussions by joining the British Crystallographic Association group on LinkedIn[4] or following @britcryst on Instagram[5] or Threads. These links, and any others that may be needed in future, are available at crystallography.org.uk, which is not due to be taken over by any billionaires in the near future.

Richard Cooper
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4. https://www.linkedin.com/groups/126033/.
5. https://instagram.com/britcryst.

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Full committee details on the BCA website **www.crystallography.org.uk**

From the Editor

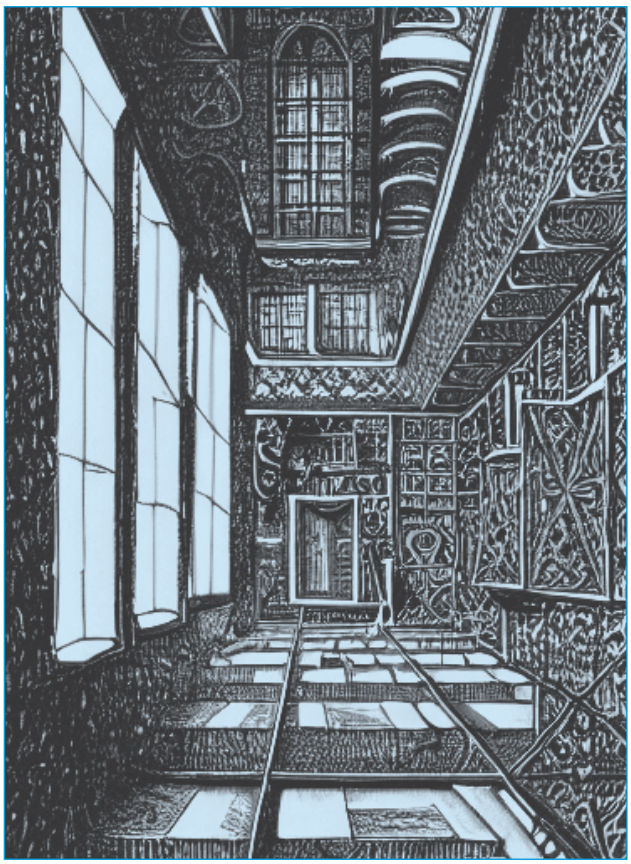
I am delighted to bring you my second issue of *Crystallography News* which begins with an article by Deborah Harrus (PDBe) commemorating 20 years of the wwPDB – an achievement for the structural community which is surely worth celebrating in earnest. We then have an article describing just some of the very exciting crystallographic work ongoing at the University of Cardiff. The draft programme for the 2024 BCA Spring Meeting has been very kindly provided by Peter Moody (Leicester) and Suzanna Ward (CCDC) and is a reflection of their hard work and commitment to the cause. We continue to provide group and bursary winner reports on this year's excellent Spring Meeting in Sheffield and we have a fascinating account by John Helliwell (Manchester) of the 2023 ACA meeting in Baltimore. We then wrap up this issue with a summary of an inaugural lecture given by Brendan Howlin (Surrey) and a look at one or two historical observations of the life and achievements of Prof John Desmond Bernal FRS, a key early figure in the structural field. If you only read this far, rest assured, that is enough.

Having offered to instantiate a new column on *Crystallographic Forteana*, my efforts to deliver a novel contribution in this field are, despite appearances, firmly on course – it will happen. Already I have generated a piece of artwork which I am proposing should accompany the series. It was created by typing the phrase "Crystallographic Forteana" into one of the websites which allegedly use artificial intelligence to generate relevant imagery (https://www.deepai.org). After several attempts it came up with this somewhat haunting dream-like picture. However, it's clear to me that for all its great intelligence and ability to predict protein structures, AI cannot quite draw windows properly! Never mind. Secondary modern technical drawing lessons spring to mind at this point, but draughtsmanship wasn't quite my *forte* either. Maybe these minor but quintessential failings of such a powerful technology add to the overall sense of mystique!

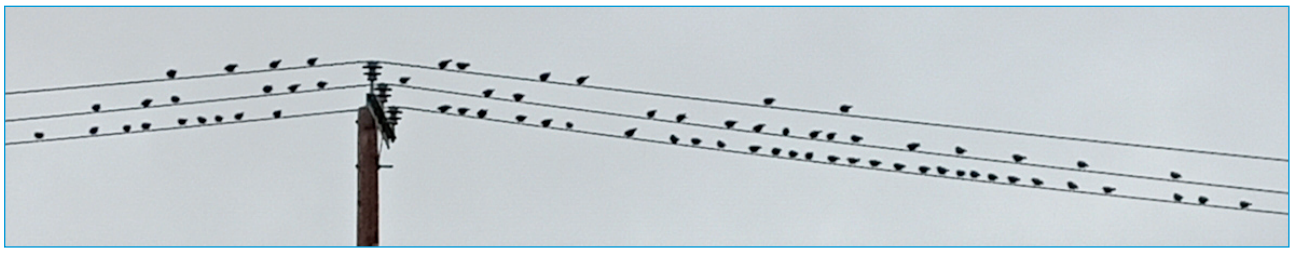
I just about started the Fortean ball rolling in the last issue with a picture of a partially ordered array of starlings. A look at Wikipedia (the free encyclopedia) shows that the swarming behaviour of these birds is well-known and has been studied by the best brains in science, even using computational simulation. They certainly seem to stick together and, truly, the phrase "swarm intelligence" has already been coined. Biologically it is claimed that swarming constitutes a defence mechanism to hypnotise and therefore confuse predators. I struggle to believe this one as surely the best way to escape the enemy's attention is to never congregate at all? Anyway, for these birds to land on a regularly spaced array of telephone wires coupled with the need to maintain a minimum distance to avoid wing-contact are probably the main factors in the partial ordering observed in my photograph in the previous editorial. A more recent one shows similar behaviour but this time they are being even more tantalising. Spotting order in this array is surely a frustrating process, but I believe it is there! It is also worth mentioning their ability to exchange places dynamically, sometimes leaving vacancies in the lattice. Maybe there are parallels with physical or chemical systems – just let me know, but regardless, it really is an intriguing sight to be seen.

Read on now for some proper crystallography.

Jon Cooper
UCL



An AI-generated image derived from the phrase "Crystallographic Forteana" (above) and another murmur of starlings demonstrating, I think, at least partial order (below).



Answer to last issue's problem

The following formula is given on page 54 of *Crystals and X-rays* by the late Dame Kathleen Lonsdale FRS (Bell, 1948). The challenge was to describe its symmetry and propose a rule for memorising it.

$$\frac{1}{d^2}=\frac{\begin{vmatrix} \frac{h}{a} & \cos\gamma & \cos\beta \\ \frac{k}{b} & 1 & \cos\alpha \\ \frac{l}{c} & \cos\alpha & 1 \end{vmatrix} + \frac{k}{b}\begin{vmatrix} 1 & \frac{h}{a} & \cos\beta \\ \cos\gamma & \frac{k}{b} & \cos\alpha \\ \cos\beta & \frac{l}{c} & 1 \end{vmatrix} + \frac{l}{c}\begin{vmatrix} 1 & \cos\gamma & \frac{h}{a} \\ \cos\gamma & 1 & \frac{k}{b} \\ \cos\beta & \cos\alpha & \frac{l}{c} \end{vmatrix}}{\begin{vmatrix} 1 & \cos\gamma & \cos\beta \\ \cos\gamma & 1 & \cos\alpha \\ \cos\beta & \cos\alpha & 1 \end{vmatrix}}$$

The highest symmetry determinant is the denominator which has a diagonal mirror. One rule-of-thumb for remembering the formula (which I only noticed when typing it into an equation editor) is to start with the denominator, and imagine that the top 3 determinants are empty. We can simply drop all of the denominator terms into each empty determinant and replace one column with *h*/*a*, *k*/*b* and *l*/*c* depending on whether it is the first, second or third term of the numerator, as shown by the columns in light blue. **What do members think?**

BCA Corporate Membership

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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Photonic Science: **https://photonicscience.com/**

The Cambridge Crystallographic Data Centre (CCDC): **https://www.ccdc.cam.ac.uk**

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- A broad range of meetings organised by the BCA and its subject groups
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- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Twenty years of the Worldwide Protein Data Bank

IN July 2003, the Worldwide Protein Data Bank was launched as a partnership between RCSB Protein Data Bank (RCSB PDB, USA), Protein Data Bank in Europe (PDBe), Protein Data Bank Japan (PDBj) in the management of the essential Protein Data Bank Core Archive of atomic-level, three-dimensional (3D) structures of biological macromolecule experimentally determined by macromolecular crystallography (MX), nuclear magnetic resonance (NMR) spectroscopy, or three-dimensional cryo-electron microscopy (3DEM).[1,2]

Since then, the wwPDB collaboration has expanded to include additional Core Archives as partners: BioMagResBank (BMRB, USA) Core Archive of spectral and quantitative data derived from NMR spectroscopic investigations of biological macromolecules and metabolites; and Electron Microscopy Data Bank (EMDB, UK) Core Archives of 3D volumes and associated information of macromolecular complexes and subcellular structures from 3DEM and electron cryo-tomography. wwPDB partners adhere to the FAIR principles of Findability, Accessibility, Interoperability, and Reusability,[2] and ensure that all archival data can be accessed at no charge and with no limitations on usage under the most permissive Creative Commons CC0 1.0 Universal License.

As the wwPDB celebrates its twentieth year of operations, wwPDB is pleased to welcome Protein Data Bank China (PDBc) to the organization as an Associate Member. PDBc is based in the National Facility for Protein Science in Shanghai which is associated with Shanghai Advanced Research Institute of Chinese Academy of Sciences, and the SIAIS and iHuman Institutes of ShanghaiTech University. An announcement describing the process of PDBc joining the wwPDB has been submitted to *Acta Cryst D* (pdf).[3] PDBc has received training and support from the wwPDB partners, and it is expected that PDBc will process most, possibly all, depositions made by structural biologists working in the People's Republic of China to all three wwPDB Core Archives.

Since its inception, the PDB has been an international archive and the establishment of the wwPDB ensured that valuable data contained in these Core Archives will continue to be stored, managed and kept freely available for the benefit of scientists worldwide.

Deborah Harrus
PDBe, Cambridge

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Macromolecular Crystallography in Cardiff

CRYSTALLOGRAPHY at Cardiff University has been growing in recent years, with researchers in both chemical and biological disciplines studying reaction dynamics in crystals using diffraction techniques. Meetings of the Cardiff University Dynamic Structural Sciences and Biophysics Network (CUDSSBN – run by Senior Researchers Ben Bax, Georgina Menzies and Pierre Rizkallah), bring together researchers from across the University to learn from each other (e.g. in June 2023 a talk was given on 'Using serial femtosecond crystallography to solve the structures of pesticidal proteins from natural crystals' by Lainey Williamson and Hannah Best; from Prof Colin Berry's group) or external speakers (e.g. in February 2023 we had an 'Overview of MX data collections and facilities at Diamond Light Source' by Anna Warren, Diamond).

Complementing crystallography in Cardiff University, Georgina Menzies pursues research interests in molecular modelling and molecular simulations and Marcella Bassetto, an organic chemist, uses structures in designing antiviral compounds. Mark Young has recently determined the structure of a slipper limpet haemocyanin with cryo-EM, complementing his expertise in P2X receptors.

Researchers at Cardiff University continue to use facilities at Diamond Light Source for Macromolecular Crystallography and other applications. A large number of research programs have benefited from this (e.g. immune system studies, virology, green fluorescent protein, bacterial insecticidal proteins, calpain inhibitors, biotechnological applications, etc). Over 100 researchers in the schools of Medicine, Biosciences, Chemistry, Pharmacy and the Medicines Discovery Institute, have used the facility to collect data from crystals, leading to over 60 publications and 200 PDB depositions in the last 15 years.

One of the earliest projects, led by Prof Andrew Sewell, involved elucidating how a T-cell receptor (TCR) isolated from a patient with type I diabetes recognised a small peptide from pre-pro-insulin presented by a disease-risk human leukocyte antigen. Subsequent structure determinations showed how pathogen-derived peptides could be strongly recognised by this same TCR and provided a potential mechanism for disease initiation via molecular mimicry. Prof Andrew Godkin's group has had a long-standing interest in modifying antigens to enhance CD4+ T cell responses, and structural studies looking at HLA-II presented peptides has enabled the design of unique vaccines for both cancers and infections such as influenza A virus. This work has been extended by Bruce MacLachlan who has used HLA-II-peptide structures to identify completely novel mechanisms of escape by SARS-CoV-2.

The virology studies of human adenoviruses, led by Prof Alan Parker, identified receptor targets on human cells. Judicious mutations rendered the virus unable to leave infected cells, while modulation of the binding epitope redirected the virus to cancer cell lines, producing a viral onco-therapeutic agent. The chimpanzee adenoviral vector 'Chadox1', widely used for COVID19 vaccination, produced some rare but serious side effects. We contributed to the structure determination of this virus, to understand the basis of the problem. Vectored vaccines derived from human adenovirus serotypes are under development in collaboration with Carly Bliss. We are now pursuing the structure determination of whole human adenovirus 10, using cryo-EM techniques, with the help of EBIC (Electron Bio-Imaging Centre, Diamond Light Source).

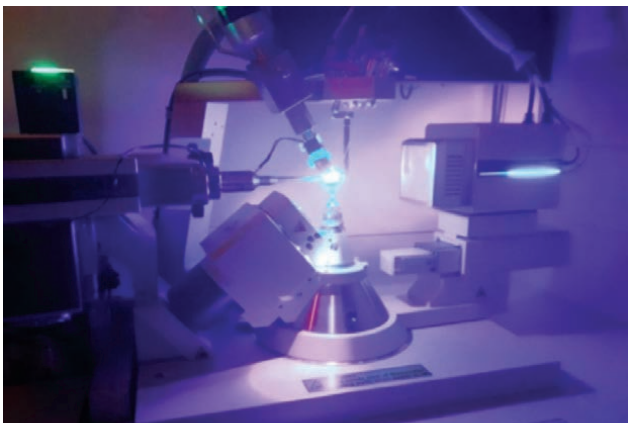
The highest resolution structure determination of enhanced green fluorescent protein (GFP, project led by Prof Dafydd Jones), at 1.35Å, demonstrated its mechanism of action, and led to a programme of manipulation involving mutations and deletions to modify fluorescence energy. Click Chemistry was used to modulate the GFP oligomeric state and further enhance spectral properties. Prof Colin Berry used access to Diamond and the European X-ray Free-Electron Laser Facility (European XFEL) to enable the determination of *Bacillus thuringiensis* insecticidal protein structures to understand their mechanism of action and develop applications in environment friendly pesticides. Applications in the field of onco-therapy are also being pursued.

The aim of structural biology group in the Medicines Discovery Institute (MDI), Cardiff University (run by Profs John Atack and Simon Ward) is to enhance the quality of lead molecules (both by understanding their binding mode and by using structure guided drug design). For example, the phase I compound MDI-478, followed from understanding of the binding mode of AMPA receptor positive allosteric modulators (PAMs). The MDI used a fragment based screen (XChem) to identify fragments binding in the PAM/NAM pocket of NMDA receptors. XChem screens have also been used to discover a druggable pocket in serine racemase. The crystal structure of ebselen covalently bound to Cys 141 of inositol monophosphatase (IMPase) suggested that ebselen, a compound that has been through a phase 2 clinical trial, may function as an allosteric inhibitor. More recently a Creoptix WAVE was used to measure affinities of the C-terminal (non-kinase) domains of SPAK and OSR1 kinases for WNK derived peptides, complementing structural studies for these kinases which are potential targets for both breast cancer and stroke. Current MDI targets being worked on include targets involved in lysosomal disorders and DNA gyrase.

In the School of Chemistry, a time-resolved instrument for X-ray structures (TRIXS) has been recently installed, as part of a project led by Lauren Hatcher, with input from the Schools of Chemistry, Biosciences and the Medicines Discovery Institute. In collaboration with Rigaku Europe, a rotating anode diffractometer has been specially modified to collect time-resolved single-crystal X-ray diffraction data in the home laboratory. In this new instrument, an LED light "pump" is synchronized with a gated response from a HyPix-6000HE detector to facilitate "pump-multiprobe" experiments, with single-crystal datasets obtained down to millisecond time-resolution. Thanks to further funding from the Royal Society, a Raman probe will soon be integrated into this time-resolved

laboratory set-up, allowing the simultaneous collection of complementary diffraction and spectroscopic data from the same sample position. The School of Chemistry is also involved in several other dynamic X-ray diffraction projects that utilize both laboratory and synchrotron X-ray sources. In the Hatcher research group, PhD student Sam Lewis is developing fixed-target serial synchrotron photocrystallography measurements, in collaboration with Mark Warren on Beamline I19 at Diamond Light Source. These experiments utilise so-called "diffract-and-destroy" approaches to collect pump-probe diffraction data at very fast time resolution, merging the response from hundreds of photoexcited microcrystals.

Pierre Rizkallah, **Ben Bax** and **Lauren Hatcher**
Cardiff



The Rigaku time-resolved instrument for X-ray structures (TRIXS) at the University of Cardiff.

BCA Spring Meeting 2024

PLANNING is underway for the 2024 BCA Spring Meeting to be held in Leeds, so please put the dates in your diary. Details and titles for sessions are given below to inspire you to start thinking about contributing oral or poster abstracts. Remember that the abstract deadline early in the New Year always seems to arrive sooner than expected.

Early Stage Crystallographers Group (ESCG)

Monday 25 March 2024

13:00 – 21:00

The ESCG satellite meeting is an opportunity for all early-stage crystallography researchers, from across the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

13:00 – 13:30

ESCG Opening Plenary:

Session Chair: **Rebecca Clulow** (Uppsala University)
Speaker: **Dr Lukáš Palatinus** (FZU – Institute of Physics of the Czech Academy of Sciences)

Title TBC

13:30 – 17:15

ESCG Research Sessions

Contributed talks from the ESCG community.

Session 1 Chair: **Joshua Morris** (Cardiff University)
Session 2 Chair: **Olivia Breen** (University College Dublin)
Session 3 Chair: **Sam Lewis** (Cardiff University)

17:15 – 17:45

ESCG Annual General Meeting

18:30 – 21:00

Flash Poster Presentations

Session Chairs: **Phillipa Partridge** (University of Edinburgh) and **Julia Gascol Cardona** (University of Strathclyde)

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide.

19:00
Poster Session with Dinner and Wine

21:00
Evening Concludes

Tuesday 26 March 2024

09:00 – 09:30
Parkin Lecture
Session Chair: **Thomas Hitchings** (University of Kent)
Speaker: *TBC*

09:30 – 10:30
Session 4
Session Chair: **Anna Herlihy** (ISIS Neutron & Muon Source/Diamond Light Source)

10:30 – 11:00
Closing Plenary
Session Chair: **Jake Hill** (University of Bradford)
Speaker: **Dr Helen Ginn** (Hamburg Advanced Research Center for Bioorganic Chemistry)
Teasing out the secrets of subtle protein dynamics

BCA 2024 Main Meeting

11:30 – 12:15
Lonsdale Lecture
Session Chair: **Dr Anthony Carter** (Pharmaron)
Speaker: **Dr Helena Shepherd** (University of Kent)
Thermally Responsive Molecules and Materials

13:00 – 13:45
CCG Plenary
Session Chair: **Mike Probert** (Newcastle University)
Speaker: **Aurora Cruz-Cabeza** (University of Durham)
Title TBC

14:00 – 15:30
Parallel Sessions

BSG: Getting the most from your protein crystals at the synchrotron
Session Chair: **Adam Crawshaw** (Diamond Light Source)

CCG: Dynamics and Reactivity in Solids
Session Chair: **Erli Lu** (Newcastle University)

PCG/ESCG: Recent Developments in Software
Session Chairs: **Dan Porter** (Diamond Light Source) and **Ben Tragheim** (University of Warwick)

16:15 – 17:45
Parallel Sessions

BSG/ESCG: Joint Session – Breaking the field boundary: careers between chemical and biological crystallography
Session Chair: **Jake Hill** (University of Bradford)

CCG: Mechanochemistry
Session Chair: **Guilio Lampronti** (University of Cambridge)

PCG: Phase Transitions
Session Chair: **Nilanthy Balakrishnan** (Keele University)

18:00 – 18:45
BSG Plenary
Session Chair: **Rachael Wilkinson** (University of Oxford
Speaker: **Prof. Syma Khalid** (University of Oxford)
When structural data gets messy: insights from molecular simulations

19:00 – 21:00
Poster Session with Dinner and Wine

Wednesday 27 March 2024

09:00 – 09:45
IG Plenary
Session Chair: **Tony Bell** (Sheffield Hallam University)
Keynote: **Simon Coles** (Southampton University)
TBC (Micro ED NCS topic)

10:15 – 11:45
Parallel Sessions

CCG: Framework Materials
Session Chair: **Georgia Orton** (University of Birmingham)

IG/BSG: Exploring synergies at the small molecule-biomolecule boundary
Session Chair: **James Gordon** (Rigaku)
Keynote: **Duncan Johnstone** (GSK)

PCG: Electron Crystallography
Session Chair: **Matt Cliffe** (University of Nottingham)

11:45 – 12:15
CCG Annual General Meeting
BSG Annual General Meeting
PCG Annual General Meeting

13:00 – 14:30
Early Career Prize Lectures

Biological Structures Group Early Career Prize
The BSG will award a prize to someone who has had an impact in the field of Structural Biology (with an emphasis on crystallography) and recently obtained a personal fellowship, a lectureship or equivalent position.

Chemical Crystallography Group Prize for Younger Scientists
The CCG will award a prize to a younger scientist who has performed original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry.

Physical Crystallography Group Early Career Prize
The Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field.

14:30 – 14:45
Exhibitor Forum
Session Chair: **TBC**

15:15 – 16:45
Parallel Sessions

BSG: Artificial intelligence in Structural Biology
Session Chair: **Georgina Menzies** (Cardiff University)

IG/CCG: Crystallography and Systems under Mechanical Stress
Session Chairs: **Tony Bell** (Sheffield Hallam University) and **Adam Michalchuk** (University of Birmingham)

PCG: Analysis of Local Structure
Session Chair: **Anna Herlihy** (STFC)

17:15 – 18:00
Bragg Prize Lecture
Session Chair: Richard Cooper (University of Oxford)
Speaker: Professor Arwen Pearson (University of Hamburg)
Title TBC

18:00 – 19:00
BCA Annual General Meeting

19:30 – 01:00
Conference Dinner & Cèilidh

Thursday 28 March 2024

09:00 – 09:45
PCG Plenary
Session Chair: **TBC**
Speaker: **Silvia Ramos** (University of Kent)
Structural Signatures of Metal-Insulator Transitions as seen by Polarisation Dependent X-ray Absorption Spectroscopy

10:15 – 11:45
Parallel Sessions

BSG: Breaking Barriers with Emerging Technology in Structural Biology
Session Chair: **Hanna Kwon** (University of Leicester)

CCG: Molecular Interactions and Supramolecular Chemistry
Session Chair: **Krešo Bucar** (University College London)

PCG/IG: Energy & Sustainability
Session Chair: **Glen Hebberd** (Durham University)

12:15 – 13:45
Parallel Sessions

BSG: Open Session
Session Chair: **TJ Ragan** (University of Leicester)

CCG: Open Session
Session Chair: **Sam Chong** (University of Liverpool)

PCG: Open Session
Session Chair: **Lewis Owen** (University of Sheffield)

CLOSE OF CONFERENCE

Reports on the BCA Spring Meeting, Sheffield 2023

BCA Prize Lecture

The BCA Prize Lecture was awarded to **Aurora Cruz-Cabeza** (Durham), and she delivered a whirlwind tour of topics related to "Beyond the bulk: when shall we care about surfaces in molecular crystals?", drawing on examples from her past and present research. Aurora began by introducing the thermodynamics of crystal growth, relating bulk and surface effects, and showed how these equations can be exploited to predict new polymorphic forms stabilised by surface effects and experimentally accessed using techniques such as mechanochemistry. Next the relationship between surfaces and nucleation was explored. She showed an experimental link between computational measures of crystal growth surface 'roughness' and difficulty of crystal nucleation for individual polymorphs. Finally the connection between surfaces and crystal growth was investigated using several example systems, including a study of selective inhibition of paracetamol polymorph growth using a metacetamol impurity to inhibit growth of form I and favour form II. This was a fascinating lecture and wonderful career summary, which made a strong link between the sometimes seemingly quite separate fields of crystal structure and crystal growth.

*The BCA Prize Lecture awarded to **Aurora Cruz-Cabeza** (Durham) by the BCA President **Richard Cooper** (Oxford).*

Richard Cooper
Oxford

Industrial Group XRF Session

The Industrial Group (IG) organised two sessions and one plenary lecture at this year's BCA. The plenary lecture was given by **Ahmad Sheikh**, a senior research fellow and the global head of molecular profiling and drug delivery at AbbVie. Dr Sheikh presented virtually (at 3 am his time!) a talk entitled "From computational solid state chemistry to molecular design – leveraging opportunities in contemporary small molecules drug discovery and development." After an introduction to crystal structure prediction (CSP) and the development of the technique, Dr. Sheikh detailed the application of CSP workflows used at AbbVie. Some of the examples covered included the improved sampling of hydrated crystal structures in order to predict stable hydrate structures. Additionally, a method of 'Quick-CSP' was presented, where the study of structurally related models can be aided by using transferable tailor-made forcefields. This method resulted in significant CPU savings whilst providing a similar accuracy to standard methods.

The "Industrial Crystallography for Pharmaceuticals" session was opened by **Andrew Maloney** (CCDC), who spoke about "From crystal structures to particle properties: applying informatics approaches to pharmaceutical development and manufacturing challenges." Understanding particle properties is very important to aid development of new or improved drugs. This talk demonstrated how tools using information from the Cambridge Structural Database can help gain insights into the stability and properties of a crystal structure. The new CSD-Particle suite of tools was also highlighted. This allows users to gain further understanding by visualising and analysing surface properties and calculation of crystal morphologies as

well as the identification and analysis of potential slip planes. Next **Colin Seaton** (Bradford) presented "Hunting elusive co-crystals: The impact of crystallisation kinetics on solid form screening." The formation of co-crystals of caffeine-benzoic acid has been described as 'elusive' within scientific literature. Through the construction of ternary phase diagrams of caffeine-benzoic acid, however, it was shown that it was possible to identify suitable conditions for co-crystal growth of this combination of materials. This was followed by **Julia Gasol Cardona** (Strathclyde) who gave a talk titled "From crystal to tablet – linking structure to function through compression studies." It is very important to understand the behaviour of pharmaceutical agents under pressure like that applied during the tabletting process. This presentation detailed the study of pharmaceutical compounds, ofloxacin and levofloxacin, under both moderate and high pressure to understand the compressibility of these crystals. Finally, **Fraser White** (Rigaku) presented "XtaLAB Synergy-ED: To cryo, or not to cryo, that is the ED question" which described two applications of performing electron diffraction experiments at low temperatures using the Rigaku XtaLAB Synergy-ED electron diffractometer. The talk demonstrated that freezing samples prior to performing the experiment allows the study of hydrated crystals with electron diffraction, despite the requirement for the sample to be studied under high vacuum.

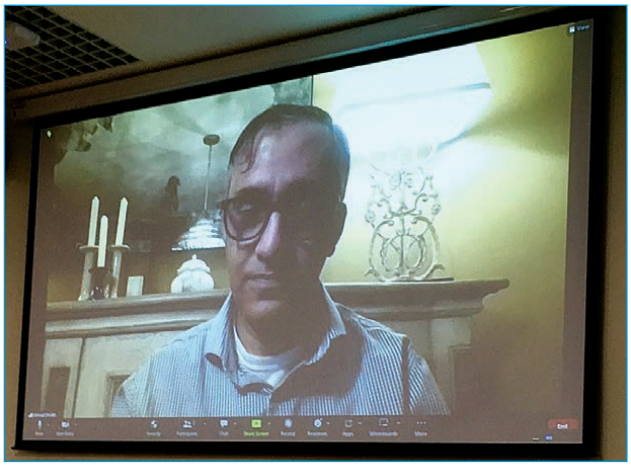
The IG usually organises a stand-alone X-ray fluorescence (XRF) meeting every year. This year, in an attempt to bring the XRF community closer to the rest of the BCA industrial community it was decided to dedicate one of the IG sessions to XRF and there were three speakers in this session. The keynote speaker was **Paul Bingham** (Sheffield Hallam) who spoke on "XRF analysis of feldspars and silicate glass: effects of melting time on fused bead consistency and volatilization." Fused beads are a common way of sample preparation for XRF as it produces homogenous samples by mixing with a flux material and then heating in a furnace. This mixture melts and cools to produce a sample. However, it should be noted that the heating time can affect the XRF results for fused beads. If the heating time is too short the sample may not form a homogenous mixture and crack on cooling. The longer the heating time the greater the chance of volatile components of the sample leaving the sample. Variation of fused bead melting times showed changes in XRF analyses of a number of certified reference materials. Next, **John Austin** (SciMed) gave a talk entitled: "A comparison of energy-dispersive (ED) and wavelength-dispersive (WD) X-ray fluorescence spectrometers" which provided an overview of these two types of spectrometers. Energy dispersive XRF spectrometers rely on detectors to separate and resolve differing X-ray energies to understand the composition of a sample. Wavelength dispersive XRF spectrometers utilise X-ray diffraction to separate X-rays according to their wavelength prior to detection, using specialised crystals. This presents different approaches of non-destructively quantifying sample composition based on the XRF signals detected. The optical pathways of the two techniques were compared along with X-ray tubes, sample presentation, resolution, and detection. The application of the techniques, along with advantages and disadvantages of their usage were shown. Finally, **Archibald Harris** (Bruker) presented a talk on "Using XRF for rapid elemental analysis QC in Food and Feed" demonstrating the many applications of XRF spectroscopy in the food industry, such as its use in quality control, identifying traces of toxic elements and the identification of raw materials. Many different examples were given into how and why to use XRF to the best advantage.

This year's IG poster prize was given to **Carissa Ponan** (UCL) for a fantastic poster titled "The future of pharmaceutical solid-state chemistry: hyphenated *in situ* diffraction techniques."

Tony Bell, Sheffield Hallam
and **Natalie Johnson** CCDC

*Speakers in the IG XRF session from left to right: **Archibald Harris** (Bruker), **Paul Bingham** (Sheffield Hallam), **John Austin** (SciMed) and session chair: **Tony Bell** (Sheffield Hallam).*

*Speakers in the Industrial Crystallography for Pharmaceuticals session, session chair: **Natalie Johnson** (CCDC), **Colin Seaton** (Bradford), **Andrew Maloney** (CCDC), **Fraser White** (Rigaku) and **Julia Gasol Cardona** (Strathclyde).*



*Plenary lecturer **Ahmad Sheikh** (AbbVie) speaking via video conference.*

Physical Crystallography Group Sessions

The BCA Spring Meeting 2023 was a fantastic event. After the YCG meeting, the main BCA spring meeting on Tuesday was kicked off with the PCG plenary. This year we had the pleasure to invite as speaker **Bo Brummerstedt Iversen** (Aarhus). Professor Iversen gave a fantastic talk entitled "Toward XFEL crystallography for small-unit-cell systems." His incredibly engaging talk reflected back over his career, exploring developments that had occurred over that time and the current exciting opportunities available with XFELs. He highlighted some of the challenges associated with data reduction, and potential possibilities including pair distribution function (PDF) analysis.

The full PCG programme was varied, with three sessions in collaboration with another of the BCA subject groups. The PCG and CCG held joint sessions on "Software for Data Processing and Analysis" and "Teaching Crystallography". The YCG also lead a joint session with both the CCG and PCG on Central Facilities. This took the opportunity to explore a different format – being led as a panel discussion. Further sessions were also held on "Phase Transitions", "Sustainability", and an "Open Session" where talks were encouraged on a topic related to physical crystallography. Overall, there were excellent talks across the board and we hope we gave to everyone the opportunity to find something interesting with a broad programme.

The joint PCG/CCG session on "Software for Data Processing and Analysis" saw an exciting mix of talks on the history, recent developments, and the future direction of the field. To kick things off, **Jeremy Frey** (Southampton) asked the rather pertinent question "Will an AI win a Nobel prize?" He introduced and reviewed some current aspects of machine learning and spoke about the need for well-curated metadata in order to leverage the huge amounts of scientific data being collected in labs every day. He concluded that although we may be entering the fifth paradigm of scientific discovery, it would be very unlikely that an AI wins a Nobel prize – and ChatGPT agrees with this conclusion (although apparently it can convincingly write slides for a BCA spring meeting presentation!)

The first contributed presentation was by **Richard Waite** (ISIS) whose talk was entitled "Summing up: How many ways can there be to integrate peaks?" He described new peak finding and integration algorithms implemented in MANTiD which can identify weaker, and therefore significantly more single crystal reflections, and integrate and validate those reflections more accurately. Next was a presentation by **Niklas Ruth** (Durham) who introduced a new software framework: "QuantumBox: Unlocking (Quantum) crystallography". This project is in its infancy but aims to facilitate fully-parameterised data processing across multiple software applications with full provenance. He showed a proof-of-principle demonstration of well-known applications running in containers, with data seamlessly being passed from one application to the next. Finally, **Tobias Bird** (DLS) speaking on "Symmetry adapted pair distribution function analysis" presented a new technique for modelling pair distribution function fits by leveraging irreducible representations. This technique, and the python package he has authored, allow users to extract directly from PDF data the distortion mode amplitudes and therefore describe dynamic distortions and order parameters which occur on the local scale.

*Speakers in the PCG session "Software for data processing and analysis" from left to right: **Niklas Ruth** (Durham), **Tobias Bird** (DLS), **Richard Waite** (ISIS) and **Jeremy Frey** (Southampton).*

The PCG session on Phase Transitions, chaired by **Nikolaj Roth** (Oxford) presented a wide variety of talks, showing that there is still much to be understood about phase transitions, both in terms of their nature and how we can measure them. **Siân Dutton** (Cambridge) presented her work on exploring the phase transition in layered $NaNiO_2$ in a presentation entitled: "Jahn-Teller distortions in $NaNiO_2$." At ambient pressure, this material undergoes a phase transition from a monoclinic to rhombohedral structure, which is associated with the loss of long-range orbital ordering. In the talk, Siân discussed the nature of the phase transition using variable temperature and pressure neutron measurements, which showed that the Jahn-Teller transition changes with pressure. Additionally, ambient pressure experiments, including neutron-PDF, EXAFS, and solid-state Na NMR, were used to discuss whether the phase transition was of displacive or order-disorder type. Convincing evidence was presented for a displacive phase transition. Next, **Emma McCabe** (Durham) presented work on the "Phase transitions in corundum-derived $Fe_{2.5}Sn_{0.5}InO_6$." With the addition of Sn to $Fe_{2.5}InO_6$, the compound becomes polar and shows second harmonic generation. The presentation focused on the phase transitions, as the compound orders magnetically below 432 K and shows evidence of magnetoelectric coupling. The structural characterization using X-ray and neutron diffraction data was presented to explain its second harmonic generation activity. **Cameron Wilson** (Edinburgh) presented a new method for identifying crystallographic signatures of subtle high-pressure phase transitions in molecular materials. In the talk entitled "Characterisation of subtle phase transitions at high pressure" it was shown that some phase transitions that are observable using spectroscopy can be hard to identify in diffraction data. By partitioning the unit cell volume into void space and occupied space using van der Waals radii, small changes in the void space volume were able to identify some phase transitions that would otherwise be hard to find. The talk discussed the sensitivity of the method and its limitations. **William Brant** (Uppsala) presented a talk on the impact of cation ordering on the performance of transition metal (TM) oxide electrodes in batteries, with a particular focus on $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO). In the talk entitled "Cationic disorder drives non-equilibrium phase transformations during electrochemical cycling of $LiNi_{0.5}Mn_{1.5}O_4$" it was shown that higher cation disorder results in a narrower miscibility gap and more stable lithium storage capacity for a greater number of cycles, but TMs tend to gradually order during the electrochemical cycling process, which reverses the benefits. William presented two phenomena related to TM cation

ordering in LNMO: the mechanism responsible for TM ordering and the narrowing of the miscibility gap between compositional end members based on TM ordering and applied current density.

Nikolaj Roth (Oxford) chaired while Cameron Wilson (Edinburgh), Siân Dutton (Cambridge), Emma McCabe (Durham) and William Brant (Uppsala) spoke in the PCG session on "Phase Transitions."

With the previous year's success of a newly introduced Q&A panel session (focusing on careers), this year saw the return of the same format for the YCG/PCG/CCG "Central Facilities Panel Discussion". The theme of the session revolved around central facilities and their instrumentation, facility developments and the exciting science that comes from performing experiments using them. The 5 panellists: **Chris Milne** (European XFEL), **Gema Martinez-Criado** (ESRF), **Simon Coles** (Southampton, NCS), **Lucy Saunders** (DLS) and **Pascal Manuel** (ISIS) each gave a 10 minute introduction to their respective facility discussing current techniques, recent developments and stimulating science arising from their establishment. As examples, Chris discussed the benefits of using XFEL techniques for *in-situ* and operando-based studies; Gema highlighted the ESRF's new Extremely Brilliant Source (EBS) upgrade and its elevation to a 4th generation synchrotron; Simon praised electron diffraction (ED) techniques leading the way in revolutionising crystallographic study, with new ED diffractometers being installed at both Southampton and Warwick universities; Lucy provided a 'whistle-stop' tour of Diamond's suite of crystallography instruments and Pascal detailed the new polarisation and thin-film upgrades to the WISH diffractometer, WISH-II.

During the Q&A portion of the session, many stimulating topics were discussed, both about specific instrumentation/facilities and also more general questions about central facilities themselves. For example, discussions with Simon around ED techniques ranged from the sample preparation methods to perform a successful experiment, to the capability of resolving and studying diffuse scattering features. Chris addressed how access to the European XFEL facility proceeds from a UK user perspective, encouraging these users to apply for experimental time. Conversations with Lucy around various sample environments used in the Diamond crystallography group were had, including those involving total scattering measurements on I15-1 under applied electric fields, similar to those highlighted for single crystal and powder diffraction measurements on I19 and I11, respectively.

More general questions posed to the panel included those of the current limitations that prevent each facility extracting the most science out of their experiments, and how this could be improved. A common answer from the entire panel focused on the data obtained from an experiment in terms of both storage and processing, while Gema and Pascal highlighted additional limitations of engineering challenges associated with the maintenance and upgrades of central facilities in general. Overall, the session provided a great opportunity for those working directly in central facilities to highlight the exciting new developments and scientific curiosities occurring within these establishments. The Q&A portion of the session gave an inclusive platform to allow both experienced and early-stage researchers to engage in the conversation about central facilities.

Panellists of the Central Facilities Discussion: Chris Milne (European XFEL), Simon Coles (Southampton), Lucy Saunders (DLS) and Pascal Manuel (ISIS) with chairs: Ben Tragheim (Warwick) and Natalie Pridmore (Bristol).

The first talk in the session entitled "Sustainability" and chaired **Gabriel Perez Garcia** (ISIS) was given by **Xiao Hua** (Lancaster) who spoke on the "Application of a big data approach to study lithium-ion battery materials." Xiao talked us very eloquently through the exciting methodology that he developed for investigating structurally complex battery materials. This is built on the PDF technique and is particularly concerned with addressing the challenges of characterising phase-heterogeneous and disordered materials. Xiao presented his big-data approach demonstrating how non-negative matrix factorisation can be used to model the PDF of phases that can potentially exist in various metal fluoride cathodes and metal oxide anodes. Particularly fascinating was Xiao's demonstration of using his methodology to find the possible formation of an intermediate bcc-FeO phase, previously not considered, in $LiFe_2O_3$ during cycling. This demonstration was accompanied by elegant animations that served as an excellent visual aid for the audience. We anticipate Xiao's novel methodology to be instrumental to guiding the design of better materials both for and beyond energy storage. Next, **Nicolas Bristowe** (Durham) spoke on "Revisiting magnetoelectricity in perovskites from first principles." Nick discussed his work on extending group-theoretical studies into octahedral distortions in perovskites to include magnetism. This topic is highly relevant as ABX_3 perovskites have been intensively investigated with the aim of finding new magnetoelectric multiferroics, which could potentially lead to more sustainable microelectronics. However, no single component material at room temperature whose M can be reversed with an electric field has been found, likely due to the complex microscopic origin of the perovskite's magnetoelectric mechanisms. By expanding the energy landscape around the parent perovskite phase, in terms of displacive, occupational and magnetic modes, Nick's group identified several magnetoelectric coupling schemes. Nick also discussed which ones could allow for the reversal of M with an electric field. Moreover, he illustrated the concept of using first principle calculations on a candidate perovskite. Nick's approach to the identification of different schemes is an excellent example of how *ab initio* DFT calculations can be used to simulate combined structural and magnetic phenomena in complex structures. **Theodosios Famprikis**

(Delft) then spoke remotely on the subject of "Structure and dynamics of rotationally disordered ionic-molecular ion conductors." The speaker compared the differences in the local and average structure of three different plastic crystals, α-Li_2SO_4, α-Na_3PO_4, and γ-Na_3PS_4. These peculiar types of materials are polyanionic crystalline solids containing mobile cations, such as Li^+ and Na^+, that exhibit phase transitions at high-temperature with distinct rotational polyanion disorder. What is enticing about this, is that such disorder induces a commensurate increase in mobile cation conductivity, making this type of ion conductor a potentially good candidate for energy generation and storage applications. Theo showed how using a simple average structure analysis approach, such as Rietveld refinement, is unsuitable to accurately characterise these complex materials. Instead, a multi-technique approach including total scattering analysis, spectroscopy, and computational simulation is needed to fully understand the dynamics of such disordered structures. It was clear that Theo's research has been highly thorough as he has gone as far as calculating ion diffusion coefficients in these materials and suggesting how polyanionic rotational diffusion may be correlated with the cationic translational diffusion in these materials. Last but not least, **Martin Adam** (Bruker AXS) spoke pertinently on "How to reduce the electrical power requirements for high-intensity X-ray sources", taking a very different approach towards how crystallographers can contribute to an improved sustainable future. Martin presented Bruker's range of energy-saving X-ray diffractometers. The audience found the content of Martin's talk highly relevant not only to the sustainability goals that the scientific community is working on, but also to the energy consumption needs of these times. I was particularly impressed by the IμS DIAMOND II diffractometer, which consumes less than 3% of the energy of the standard 1.2 kW microfocus rotating anode. One of the key features behind this machine's impressive high efficiency is its multilayer mirrors and microfocus sources, which are almost a perfect match for a monochromatic beam with a tailored beam-cross section and divergence. The other feature is its Diamond Hybrid Anode, whose thin target layer allows it to dissipate heat much more efficiently. This talk provided the perfect closure to a very interesting session that, although faced some technical issues at the beginning causing it to have a delayed start, kept the audience engaged until the very end.

*Speakers in the PCG session on "Sustainability." **Theodosios Famprikis** (Delft) who presented remotely with **Nicolas Bristowe** (Durham), **Martin Adam** (Bruker AXS), **Xiao Hua** (Lancaster) and the session chair **Gabriel Perez Garcia** (ISIS).*

The final PCG session of this year's Spring meeting was an "Open session" chaired by **Alex Browne** (St Andrews). The aim of this session was to provide a home for any contributions that fell outwith the more well-defined topics of the other sessions, and we were treated to four excellent talks. So as not to bias the definition of 'open' no keynote speaker was selected. The first talk was by **Paul Henry** (ISIS/Uppsala) and was entitled "When is size mismatch good? The anomalous behaviour of scandium in titanate-based proton conductors." Paul presented neutron diffraction and local-structure studies of scandium-doped barium titanate perovskites with promising solid-state ionic conductivity properties. Resolving the vacancy distributions in three phases with different levels of doping offers routes to the rational design of materials with improved functionality. Secondly, **Nikolaj Roth** (Oxford) explored the fundamental effects of correlated disorder in crystals with a talk entitled "Tuning electronic and phononic states with hidden order in disordered crystals." By demonstrating how different patterns of correlated disorder affect the electronic and phonon structures of model structures, exciting possibilities for the 'disorder engineering' of the physical properties of real materials were raised. The third talk was a dive into symmetry-mode -driven design of new magnetoelectrics, with a particular focus on tetragonal tungsten bronze phases. The talk, entitled "Symmetry design of novel magnetoelectric tetragonal tungsten bronze oxides: a first-principles approach", was given by **Urmimala Dey** (Durham). A combination of group theory and DFT calculations were used to predict new target materials, and the results of ongoing collaboration to experimentally verify these predictions are eagerly awaited. Finally, **Vitaliy Kurlin** (Liverpool) took us back to our roots by examining the question of how to define a crystal uniquely with a talk entitled "The crystal isometry space continuously extends Mendeleev's table to all periodic materials." Data from the CSD were used to demonstrate the mapping of the unique positions of all real materials in a common crystal isometry space, and examples in both materials discovery and the verification of reported 'new' materials hint at the implications of this computationally-inexpensive approach.

*Presenters in the PCG open session: **Alex Browne** (St Andrews, chair), **Urmimala Dey** (Durham), **Paul Henry** (ISIS/Uppsala), **Vitaliy Kurlin** (Liverpool) and **Nikolaj Roth** (Oxford).*

Alex Browne, St Andrews, **Lewis Owen**, Sheffield and **Arianna Minelli**, Oxford.

Bursary winner reports

I arrived in a sunny Sheffield and hopped off my delayed train to head straight the venue. A talk by **Mark Senn** (Warwick) opened the YCG (now ESCG) meeting. The full day dedicated to those at an early stage in their crystallography career makes the BCA Spring meeting an excellent opportunity to present work and contribute from the audience. It's surely one of the most welcoming and friendly conferences in the calendar.

In the main meeting one session in particular stood out as a personal highlight. The PCG: Phase Transitions session opened with a lecture by **Siân Dutton** (Cambridge) on her group's work looking at Jahn-Teller distortions in $NaNiO_2$. With two topics close to my heart: Jahn-Teller distortions and Na-ion batteries making up the backbone of this talk I was delighted to hear Siân's insight into these materials from a fundamental crystallographic perspective. The use of big-box fitting in TOPAS to capture both the global and short-range ordering was particularly impressive. Brilliant talks by **Emma McCabe** (Durham) and **Cameron Wilson** (Edinburgh) followed before concluding with a presentation from **William Brant** (Uppsala). Will's work on $LiNi_{0.5}Mn_{0.5}O_4$ used synchrotron XRD to study this cathode material cycling at high rates. The evolution of metastable phases occurs when the movement of Li^+ ions exceed the movement of the coherent interphase. This is an excellent example of the importance of in operando characterization where one can capture the dynamic system rather that the system at rest as is the case for ex-situ characterization. Although I have picked out one session to highlight, I would like to state just how high the standard of talks was at the meeting, and on such a wide range of topics.

The conference dinner was an excellent evening with speeches and poster prizes followed by the much-anticipated return of the cèilidh. Overall, Sheffield provided an excellent venue for the BCA Spring meeting and I'm already looking forward to next year.

John Cattermull
Oxford

The YCG Satellite Meeting brought many early career crystallographers together for a fascinating, fun and inspiring couple of days. Many researchers were given the opportunity to present their work, resulting in a series of engaging short talks, including those from **Thomas Roseveare** (Sheffield), who gave insight into the design of porous materials, and **Eliza Dempsey** (Edinburgh) who shared her work looking at functional materials in extreme conditions. I very much enjoyed presenting and discussing my own work in a friendly and supportive environment, and through this have been given fresh ideas for my research. The evening poster session was a great opportunity to meet fellow researchers, discuss ideas and read about a range of areas within crystallography, all over food and wine. It was overall a very enjoyable event, and I would like to thank the organisers who would have worked so hard to make it happen. I'm looking forward to next year!

Suzannah Hughes
Birmingham

Straight off the back of the Durham school, two weary eyed members of the Hatcher group arrived in Sheffield by train on a gorgeous spring Sunday afternoon, tired but excited to continue the whistlestop crystallography tour of the North of England. The first thing on the agenda was to put the bags in our rooms at the Jonas Hotel before meeting up with another group member to survey our new surroundings for the following couple of days before grabbing some dinner and eyeing up the tremendous scientific programme.

The conference then started off on Monday afternoon in the Edge building with the (now newly renamed!) YCG satellite meeting opened by the fantastic **Mark Senn** (Warwick) delivering a talk on symmetry assisted insights into ferroic materials which set the tone for what would be a great conference. Between the sessions it was great to catch up with friends made at the Durham school and my MChem supervisor **Mark Elsegood** (Loughborough), who I can thank for setting me on the path of crystallography during my undergraduate studies!

Following the sessions, and an admittedly last minute entry to the flash presentation from myself, the evening poster session proceeded in the Edge dining room. It was a great opportunity to see the broad range of research being done by others, accompanied by a glass of wine or two. As a first opportunity to present my work, it was a superb experience to get some insight from the community, which has definitely helped to direct my research going forward.

The next 3 days covered a wide variety of different topics, and I particularly enjoyed the central facilities discussions and learning about the exciting developments in electron diffraction just on the horizon. Personal highlights of the conference were the inspirational talks of **Lucy Saunders** (DLS) and **Aurora Cruz-Cabeza** (Durham) delivering the CCDC and BCA prize lectures respectively.

The conference dinner was held towards the end of the conference at the wonderful INOX which was a lovely evening to celebrate with the community, awards be given out, and of course take part in the cèilidh, which admittedly I was far too uncoordinated for! The spring meeting was an incredibly enriching and motivational experience which by the end had me itching to get back to work and put all those new found ideas into practice, so my thanks go to the event organisers and the other delegates for making the event such a positive experience.

Sam Lewis
Cardiff / DLS

*Bursary winner **Sam Lewis** (Cardiff / DLS) at the 2023 Spring Meeting in Sheffield with **Ben Coulson** (Cardiff) and **Josh Morris** (Cardiff).*

I arrived in Sheffield late on the Sunday evening after a long drive up from Southampton for the annual BCA conference. I was nervous, as I was preparing for my presentation the next day, but I was also excited as the program had a particularly good line up of computational themed talks and I was looking forward to catching up with the people I had met the previous year in Leeds.

The conference kicked off with the YCG meeting, where we heard about all the fascinating research younger members of the community have been undertaking. I presented the work I have been undertaking for my PhD, which was a fantastic opportunity to share my research with the community. Although hugely nerve-racking, I was eased by the reassurance that everyone was feeling the same way. The day ended with an evening of drinks in the union bar and many games of pool.

The main meeting followed over the next three days with talks on a wide range of topics. Highlights of the meeting for me were the Parkin Lecture given by **Lewis Owen** (Sheffield) on science communication and the CCG plenary given by **Kim Jelfs** (Imperial), who spoke about exploring supramolecular materials with computation. Other highlights included the BCA Prize Lecture by **Aurora Cruz-Cabeza** (Durham) and also **Jeremy Frey** (Southampton) who gave a really insightful talk titled "Will AI win a Nobel Prize?", discussing the use of data-driven modelling and machine learning for scientific research.

During the meeting I also had the opportunity to present a poster to the community on my research. This was another a great chance to talk about my research with others, but it was also great to talk in-depth about all the amazing work that is going on within the community. There were lots of coffee breaks after each session to network and talk with some of the sponsors at their exhibition stands about their new equipment and technologies, in particular Rigaku and their exciting electron diffraction technologies. The conference dinner on the last night was a great evening and poster prizes were handed out. A highlight for me was the long-awaited return of the annual BCA cèilidh, which was great fun!

The final day of the conference closed with an excellent session on crystal structure prediction. We heard from **Lily Hunnisett** (Cambridge) about the results of the most recent CCDC Blind Test, highlighting its achievements and success but also its environmental impact, which was particularly eye-opening as a computational chemist myself. The breadth of topics covered and continuing to develop friendships within the community means I am greatly anticipating the next one in 2024.

Eleanor Soper
Southampton

ACA 2023 Baltimore

THE 73rd annual meeting of the American Crystallographic Association was held from Friday, July 7th to Wednesday, July 12th, 2023, at the waterfront in Baltimore, Maryland and was a fully in-person meeting. The scientific program spanned biological, chemical, and materials structural science. The Transactions Symposium was on cryo-EM and reflected the broadening of the ACA's coverage. The specific structural topics included quantum crystallography, structural genomics, artificial intelligence, and machine learning, MicroED, structure-based drug design, and the future of light sources.

The new ACA new logo is shown above and an entry I submitted for their logo competition in 2021 features on the front cover. Fair enough that four words proved more effective.

I tend to attend an ACA conference, which I find excellent, about once every three years, basically restricted by my available conference travel funds. I agreed to attend this conference and present a lecture within a session entitled *Validating Models from the Data, Other Data, and Theory* in the context of the new raw diffraction data, 'Big Data' opportunities that lie before all of us (see the IUCr Public Forum of the Committee on Data for postings on this https://forums.iucr.org/viewforum.php?f=39&sid=a8cd6420dc08410e9b5271bc1343ba58). This session was organised by ACA Past President **Joe Ferrara** (Rigaku, Texas) and **John Rose** (Georgia).

For ACA 2023 the organisers had expanded the parallel sessions from 5 to 6 and this naturally made my personal choices even more difficult than earlier conferences. The ACA prize lectures were plenaries, which all attendees could attend. Also, whilst I focussed on my own primary research activities for choosing sessions, I knew that the Transactions Symposium talks would be published, and I could catch up later.

The session on the "Economics of Structural Science: in memoriam of Carlos Murillo" I found especially interesting. Topics included: How does funding drive the need and availability of structural scientific results? Why support structural science? Funding a service lab and justifying the cost. How does a contract research lab make services economically feasible? Also, how do young investigators leverage the movement of government agencies funding centralized national centres or regional cores? Carlos Murillo had been highly thought of in his role as a government funding coordinator. Perhaps the one missing topic that I would have included would be the resilience of principal investigators to find ways to take forward those alpha rated proposals that we all make but in the end fall below the budget available cut off line of the funding agencies. Funding success rates basically are rarely above 25%. A current funding manager could have provided further insights on this aspect for sure!

Naturally I was very interested in the future of light sources. This topic featured in various sessions as well as in its own dedicated session. One emphasis was on the APS Upgrade which has

recently commenced. So, at the APS ChemMatCARS sector (chemical crystallography amongst other techniques) for example a thousand-fold increase in intensity at the sample is possible, reaching 10^{18} ph/sec/mm^2. In the questions I mentioned that, to set this in context, in 1981 the first SRS protein crystallography beamline had a source size to be worked with of 14 x 0.4 mm^2, instead of the 12 x 8 micron^2 at the new APS! In another talk a speaker from the IT and Data section at NSLS II envisaged use of an "Agent" to control the experiment and do the initial data processing. This "Agent" concept worried users in the audience who did not want to relinquish control of their experiments to such an Agent. The speaker responded that a human is being kept in the loop. In the artificial intelligence and machine learning (AI and ML) session itself (entitled *"Automation in Software, Hardware and Data Processing"*) several instrument scientists spoke including from NIST (National Institute of Standards and Technology) in Gaithersburg and Oak Ridge National Laboratory (ORNL) in Tennessee and again the facility view was planning extensive use of AI and ML. In my own session on *Validating Models from the Data, Other Data, and Theory* the discussion featured the recent White House announcement of its open publications and open data policy wherever government i.e. taxpayer funding was involved. The concept from mainland Europe's synchrotron, X-ray laser and neutron central facilities of Facility Data Catalogues, with full data release to the public after three years, that I briefly described, wasn't recognised as yet by the USA facility users present in the session.

The Patterson Award Lecture was given by **Tamir Gonen** (Los Angeles) and was chaired by the current ACA President **Cora Lind-Kovacs** (Toledo). The Patterson Award is given *"to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information."* Tamir described the structural biochemistry and membrane biophysics research he and his laboratory had conducted on the development and applications of electron crystallography from microscopic crystals now popularly known as MicroED. As the Patterson Awardee in 2014 I offered my hearty congratulations to him as the Patterson Awardee for 2023.

The Rognlie Award Lecture entitled was presented as a video recording by **Majed Chergui** (Lausanne). This award is

Outside the ACA Patterson Award plenary lecture room, ***Tamir Gonen*** *(Los Angeles) and* ***John Helliwell*** *(Manchester).*

"bestowed to a deserving individual, at any stage of their career, for an exceptional discovery or technical development of particularly high impact in any area of structural science." Majed described his pioneering time-resolved X-ray absorption spectroscopy (XANES and EXAFS) research at synchrotrons (SRs) opening the way to structural studies of chemical systems subject to an external perturbation (e.g. a pulse of light or a laser T-jump). Majed answered questions live by a telephone link to his home office.

The Elizabeth A. Wood Writing Award Lecture was presented by **Juan Ma Garcia Ruiz** (Granada). The award is named in honour of Elizabeth A. Wood, President of the ACA in 1957, and author of science books for lay readers. This award is for *"Persons who have written books or articles that bring science to the attention of a wider audience."* The detailed citation to Juan Ma's incredible work on such things as crystal growth and his education lectures, in Latin America, is described here https://acas.memberclicks.net/wood-ruiz-2023 and is well known all over the world.

The Exhibition was described at the ACA Annual Business Meeting as large and was indeed extensive. One exhibit stand was for the IUCr 2026 World Congress in Calgary, Canada. I was glad to lend my support at the stand.

The IUCr Calgary 2026 World Congress exhibit at ACA 2023 with ACA Past President ***Joe Ferrara*** *(Rigaku) and* ***John Helliwell*** *(Manchester).*

The conference hotel was the Baltimore Waterfront Marriott. This was where all the lectures, and the conference banquet, were held. The view from my room in the Baltimore Waterfront Hotel was a delight, stretching across to the quaysides and marina for yachts. A WaterTaxi made regular trips to and from the city as a short cut, avoiding a long walk around the waterfront. Of general interest I mention that Baltimore is the home of separate stadia for American football and baseball (the Baltimore Orioles). A plaque near the hotel described that in the American civil war Baltimore was split between Unionists and the Confederates. The point being that as 'border states' Maryland, Delaware, Missouri, and Kentucky were slave states whose people had divided loyalties to Northern and Southern businesses and family members (https://en.wikipedia.org/wiki/American_Civil_War). The Baltimore Washington International Airport was only 12 miles from the hotel making a relatively easy transfer by taxi. My flight coming in was unfortunately delayed by 5 ½ hours which meant I arrived at my hotel at 2 am. So, I missed the opening event, a lecture by Nobel Prize winner **Venki Ramakrishnan** and the reception. On my post-meeting feedback form to the ACA, I answered excellent to most all the questions except the dates of the conference which I think were too close to the IUCr Congress in Melbourne date; I recall the 1999 ACA in Buffalo which was held in May well away from the IUCr in Glasgow date.

My ACA 2023 talk slides can be downloaded here https://zenodo.org/record/8164848.

John R Helliwell, Manchester

Inaugural Lecture by Prof Brendan Howlin, Surrey

THE first in this year's series of Surrey Inaugurals was held on 7th June 2023 and was given by Brendan Howlin, an ex-colleague of mine from Birkbeck. The opportunity to visit leafy Guildford for Brendan's lecture entitled "Molecular modelling in drug design and energy" was not one to be turned down. The chair Ian Cunningham (Surrey) introduced the speaker by emphasising his track record of over 220 publications arising from research council and industrial funding. Brendan's work spans simulation of cross-linked polymers and superdielectrics with widely recognised contributions in the fields of sustainability and artificial intelligence.

The speaker began with a time-honoured quote by Democritus that "nothing exists except atoms and empty space, all else is conjecture." To give this statement some historical context, it has to be remembered that the ancient Greek philosophers argued as to whether matter e.g. sand, could be divided an infinite number of times into fragments of ever decreasing size or whether there was a limit as to how many divisions could be made until an indivisible fragment, the atom, was obtained. It took some 2000 years for the atomistic view of reality to be accepted.

The speaker described advances in computing since his first experiments in programming a Commodore PET in the late 70's through to his present day work with the UK's National High Performance Computing system in Edinburgh, Archer2 – an HPE Cray EX supercomputer with some ¾ of a million cores. He then moved onto the range of representations which computational chemists use to describe molecular structures from the simple 2D line formulae to ball-and-stick and space-filling models of their 3D structures.

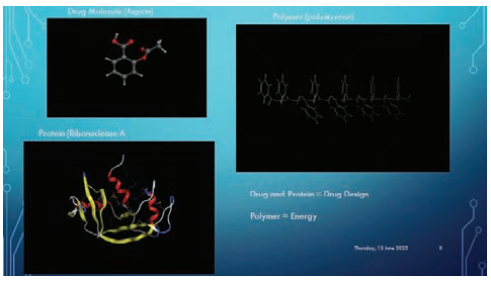
Brendan then outlined some of the underlying classical physics involved in molecular mechanics calculations such as the importance of Hooke's law in energy calculations and Newton's laws of motion in molecular dynamics. In the more sophisticated molecular orbital calculations, a quantum mechanical approach is taken and such studies are generally limited to relatively small molecules. Brendan's work spans studies of drug molecules, cross-linked polymers, proteins and enzymes as well as drug-receptor complexes. As a post-doctoral researcher working on ribonuclease with David Moss at Birkbeck, he was instrumental in development of the macromolecular refinement program RESTRAIN. This came very close to being CCP4's standard refinement shortly before the maximum likelihood-based refinement program REFMAC took the limelight. In recent work with Rex Palmer at Birkbeck, Brendan has been involved in further studies of ribonuclease, this time at atomic resolution.

Since the speaker's main interest is on design of anti-ageing drugs he outlined the basic principles of the lock-and-key hypothesis which emphasises the importance of the complementarity of the drug and its receptor molecule. Brendan then went on to outline his work on NADPH oxidase 2, or NOX2, which is an enzyme that catalyses the formation of harmful superoxide radicals and is therefore associated with oxidative damage. NOX2 is a transmembrane protein complex which is activated when the cytosolic multidomain protein p47 becomes phosphorylated upon activation of phagocytes. Phosphorylated p47 interacts with another cytosolic component, p22, and this leads to the binding of several other cytosolic components which associate with the membrane and trigger NOX2 activation. The superoxide produced plays a key role in killing of phagocytosed cells in the immune system. Drugs which interact with p47 and prevent this assembly process have therapeutic implications in treatment of inflammatory diseases and ageing.

Brendan then outlined studies using AI to analyse the results of compound screening in the search for substances which increase the lifespan of *C. elegans* worms. The average lifespan of this organism is 18 days but this can be increased to about 25 days in the presence of certain dietary supplements. AI analysis of compounds in the ChEMBL database has allowed the identification of chemical descriptors which are associated with an increased lifespan and such compounds are generally antioxidants, such as flavones or anthocyanins. Antibiotics were also found to increase the *C. elegans* lifespan, although since this effect was most likely to be due to their antibacterial effects, these compounds were removed during curation of the database.

The speaker also covered studies of cross-linking of thymine bases which occurs in DNA damage and how quantum mechanics is shedding light on the repair mechanism. Reactive molecular dynamics simulations of polyphenolic heat resistant coatings, such as those used in protective shields for space craft re-entry, have allowed the charring process to be modelled computationally over 2000 ps. Recent studies include the development of supercapacitors where the emphasis is on designing better electrolyte polymers using compounds originally developed for soft contact lenses. Future improvements in supercapacitor technology should allow these energy storage devices to compete with lithium-ion batteries as a source of electric power in transportation, with the benefit of much quicker recharging than conventional batteries. Brendan's lecture ended with an impressive video demonstrating the exciting potential of this new technology and a lively question and answer session ensued.

Jon Cooper, UCL



The first of the Surrey Inaugurals in 2023 was given by ***Brendan Howlin****.*

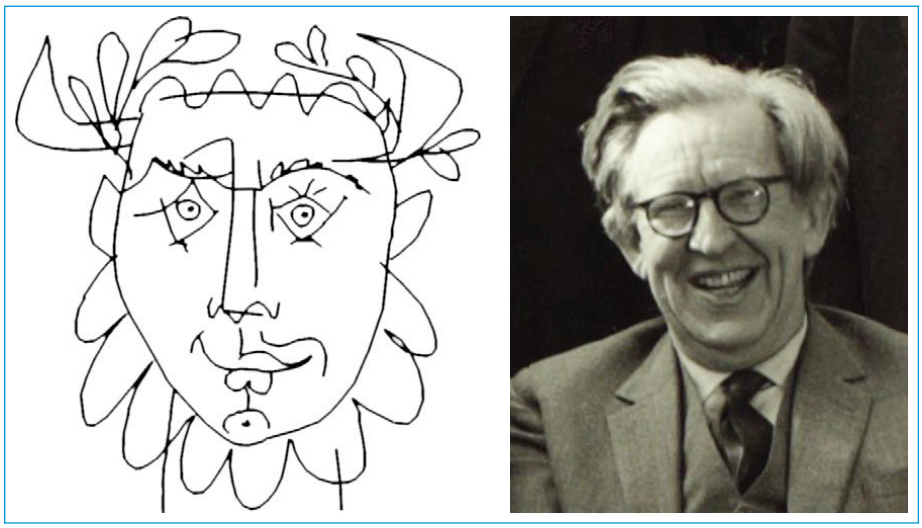
Down memory lane: Snapshots of a sage

THE late Uli Arndt (Cambridge) mentions Prof J. D. Bernal FRS (1901 – 1971) very briefly in the Introduction of his autobiography "Personal X-ray Reflections" (Athena, London, 2006) as follows: "I was sitting with a group of his Birkbeck College students after a conference session in which he made his usual brilliant contribution to the discussion. One of his people – to whom he was just 'Sage' – said to him, 'Sage, you are the most intelligent man I have ever met and you have made great contributions to science, but not quite as great as one might have expected from you; why is that?' After thinking for a moment he answered, 'I have always had a passionate interest in everything that goes on in science and I have found that in a given amount of time I can read very much more about what others have done than I can hope to do myself.'"

More light is shed on this question in the closing pages of C. H. Carlisle's unpublished work "Serving my Time in Crystallography at Birkbeck: some memories spanning 40 years, 1938 – 1978" (c/o Birkbeck College Library) in which the author states: "I believe that it was not only Bernal's past achievements that were the spur to us working together; … rather it was his capacity to give one the feeling of participating in a great venture. What was equally important was that he let you get on with the job, very rarely breathed down your neck, and trusted you implicitly with it. In other words he had what I would call 'influence'. He imparted ideas freely to anyone who asked for his opinion or advice. Lord [C. P.] Snow puts it succinctly in "J. D. Bernal, A Personal Portait" in "The Science of Science" (Ed. M. Goldsmith & A. Mackay, Souvenir Press, 1964) when he says "But he has suffered from a certain lack of obsessiveness which most scientists possess and which makes them want to carry out a piece of creative work to the end. If Bernal had possessed such obsessiveness he would have polished off a great deal of modern molecular biology and won Nobel Prizes several times over." C. P. Snow continues "He has also suffered from a grander reason. By temperament, by social passion, he was driven to give much of his energy to commitments outside science. This stopped him making the completest use of his scientific power… He has sacrificed perhaps half the pure science he might have done." Carlisle goes on to say that John Kendrew described how Bernal had explained to him in the jungles of Sri Lanka during the later stages of the war where the important advances in molecular biology might lie. Following Kendrew's receipt of the Nobel Prize in Chemistry along with Max Perutz in 1962, he wrote to Bernal expressing his appreciation for his help and advice adding that "… you have fathered five Nobel Prize winners." As Carlisle points out "The third was Francis Crick, the fourth was Maurice Wilkins and the fifth was James Watson. In fact there were six: Dorothy Hodgkin received the prize for Chemistry in the following year. What greater testimony could there be for one who gave freely of his ideas and never withheld them?" I would argue that there were seven if we include the 1982 Prize to Aaron Klug who worked with Bernal for 9 years from 1953.

Bernal's struggle with the professoriate at Birkbeck to form a Department of Crystallography that was distinct from Physics is described in Eric Hobsbawm's "Bernal at Birkbeck" chapter of the book "J. D. Bernal – A Life in Science and Politics" (Ed. B. Swann and F. Aprahamian, Verso, 1999). While speed-reading the book, one paragraph caught my eye simply because it describes a tragic event which occurred shortly before my date of birth. With some extemporisation, it reads: "I recall the Academic Board on 2 July 1963, which Bernal attended straight off an all-night flight returning from a lecture tour in New York, delayed for several hours of waiting in a heatwave, in an aircraft without air conditioning. He looked like death and I remember noticing his speech already seemed slurred. Indeed, halfway through the board, which he attended only because failure to fulfil his college duties might have been used against him, he asked a colleague to take over from him. That evening he had his first stroke."

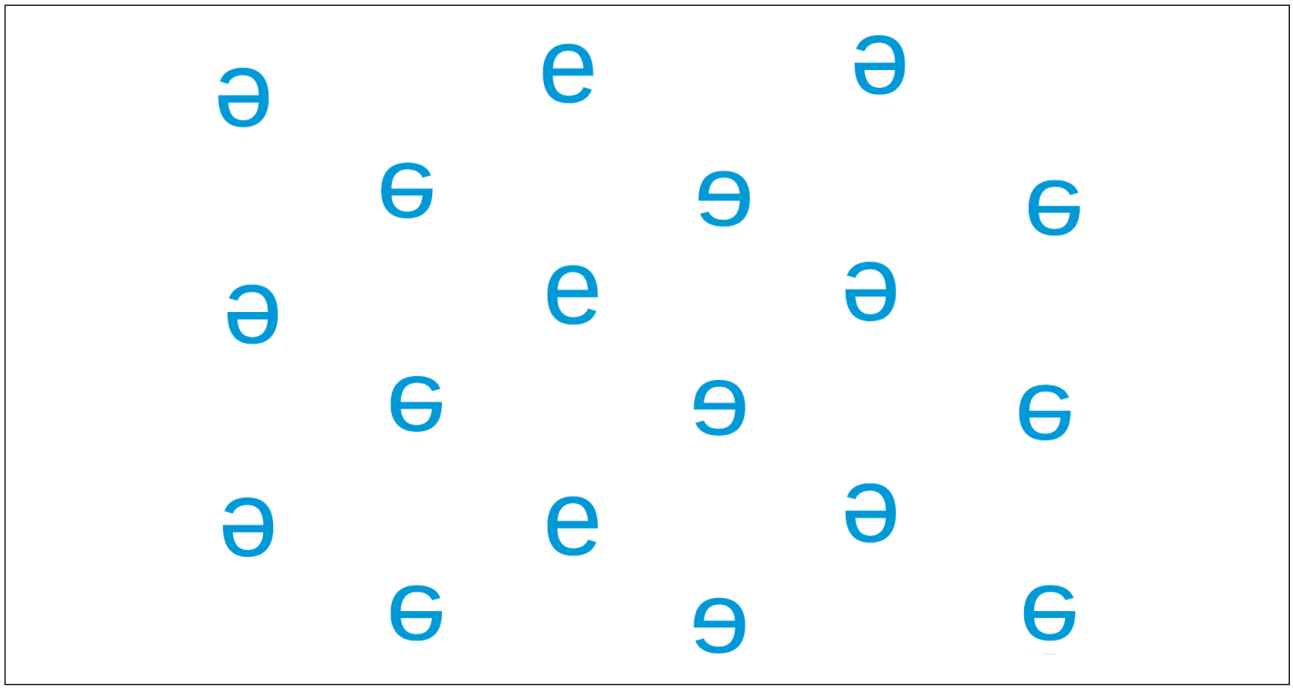
Jon Cooper
UCL



Part of a mural by ***Pablo Picasso*** *dated 12/11/50 showing Professor* ***J. D. Bernal*** *FRS (1901 – 1971) or 'Sage' humorously portrayed with devil's horns. The complete mural which includes an unknown woman, drawn as an angel, was removed from Sage's flat when the building housing the Department of Crystallography at Birkbeck (University of London) was demolished in the late 1960's. The section of wall with the mural on it was then transferred to the Institute of Contemporary Arts and later to the Wellcome Collection. A photograph of Bernal taken in 1962, a few years before the Department's move to new accommodation in Malet Street (c/o Birkbeck Image Collections).*

A challenging plane group and a history quiz question

A few issues back, Bob Gould (Edinburgh) left us with the cryptic problem of identifying the symmetry elements and finding the unit cell and plane group of a curtain pattern (see below).



The model answer which Bob very kindly provided is as follows "Though there are a lot of local symmetry elements, none of them are general. The unit cell is a rectangle that may be defined by 4 e's, and the plane group is p1." Now, to the editor anyway, this all seemed eminently sensible.

However, **Philip Bradfield** (Edinburgh) bravely sent in the following answer. "This puzzle is teasingly complicated by the presence of two independent – but seemingly alike – pairs of 'atomic species/motifs.' The (rectangular) 2D space group (plane group) is Pg, but the seductive relationship between the non-equivalent species is caused by the actual particular location of the one pair w.r.t. the second, and the similarity of the two distinct motifs. There are hints of un-fulfilled diad axes. I think a room so decorated would eventually distress any crystallographer!"

I decided to check this with Bob who very kindly replied: "I had a good long talk with Philip about this in May when we were both selling science books at the great Edinburgh Christian Aid book sale. He is quite correct. I accidentally simplified the actually even more annoying pattern, so what I drew is in fact pg (glide lines vertical). Happily, this is not a wallpaper, it is a net curtain material, so when it is hanging loosely, the pattern isn't so strident!"

Thank you to Bob and Philip for shedding light on this!

To round off this section, I am posing a less crystallographically rigorous question of my own and there are no prizes for guessing that it has more of a historical flair!

Which British scientist completed a PhD in what is now a rapidly advancing diffraction technique that was covered in the June issue, before going on to write a textbook on the subject and, in later life, becoming both the frontman and scapegoat for major infrastructure changes across the UK?

Jon Cooper
UCL

Meetings of interest

WITH much less concern about the virus, the conference scene seems to have been strongly revitalised, with a lot of new meetings being organised – so you might well find something new and interesting below. Most meetings are in-person ones, though some remain online or hybrid.

Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

If you have news of any meetings to add to future lists, please send them to the Editor, **jon.cooper@ucl.ac.uk**.

British X-ray Crystallographers

Peter Morris of the the Royal Society of Chemistry Historical Group has organised a free one-day meeting on the **18th October 2023** at Burlington House, London, which is likely to be of much interest to BCA members.

Registration closes soon (9th Oct 2023) and is available here: **https://www.rsc.org/events/detail/76719/british-x-ray-crystallographers**.

The programme is below.

- *John Desmond Bernal,* **John Finney** (UCL)
- *Kathleen Lonsdale,* **Jenny Wilson** (UCL)
- *Dorothy Crowfoot Hodgkin,* **Judith Howard** (Durham)
- *John Kendrew,* **Elspeth Garman** (Oxford)
- *Max Perutz,* **Georgina Ferry** (Oxford)
- *David Phillips,* **Tom Blundell** (Cambridge)
- *Rosalind Franklin,* **Stephen Neidle** (UCL)
- *Helen Megaw,* **Mike Glazer** (Oxford)
- *Judith Milledge,* **Ian Wood** (UCL)

CCG Autumn Meeting – Chemical Crystallography in the age of automation

This virtual meeting, **15th November 2023**, aims to highlight some of the cutting-edge work in experimental automation as well as computational automation and machine learning to better understand material structures and properties. We also hope to provide opportunities to stimulate some collaborations between crystallographers and computational scientists and the Materials Chemistry consortium.

The organisers are **Martin Ward** (Strathclyde) and **Anuradha Pallipurath** (Leeds).

The speaker programme is below.

- **Simon Parsons** (Edinburgh)
- **James Osbourne** (Liverpool)
- **Mark Warren** (DLS)
- **Jonathan Skelton** (Manchester)
- **Kasper Tolborg** (Imperial)
- **Taylor Sparks** (Utah)
- **Matthew Brown** (Sheffield)
- **Scott Woodley** (UCL) *tbc*

BCA-IG Autumn Meeting – Current X-Ray Crystallography Trends in Industry

The next BCA-IG meeting will be held on **28th November 2023** at Pharmaron UK in Hoddesdon. The in-person event will feature a series of talks focused on current industrial trends in X-ray crystallography with opportunities for networking with fellow industrial colleagues. There is no charge for this event and lunch will be provided.

Location: Pharmaron UK Ltd, West Hill Innovation Park, Hertford Road, Hertfordshire, EN11 9FH.

Date: 28th November 2023, 10:00 am.

Pharmaron is a leading, fully integrated pharmaceutical R&D services platform with global operations and has a well-established team of over 19,000 employees working in 20 different sites located in China, United States and the United Kingdom.

Registration details and agenda to follow, please check the following BCA link for future updates: **https://www.crystallography.org.uk/categories/#meetings**.

ECM34

The European Crystallographic Association (ECA) and the Italian Association of Crystallography (AIC) are hosting the 34th European Crystallographic Meeting in Padova (Italy) **26th-31st August 2024**.

The organisers of this event are **Gilberto Artioli** (Chair), **Giuseppe Zanotti** (Co-chair) and further details can be found here: **https://www.ecm34.org**

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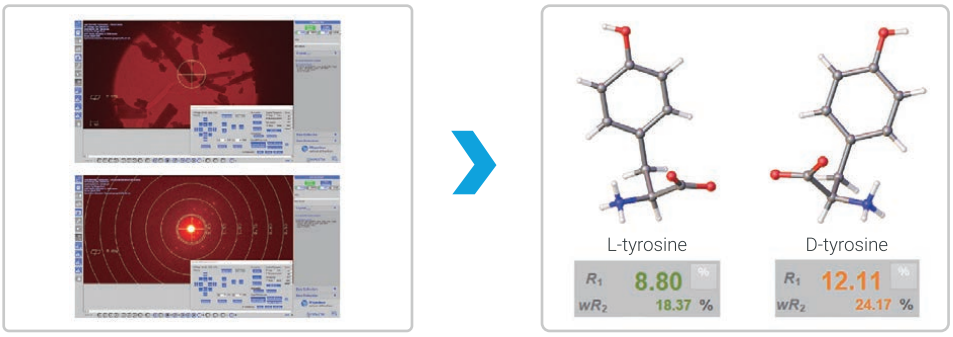

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