

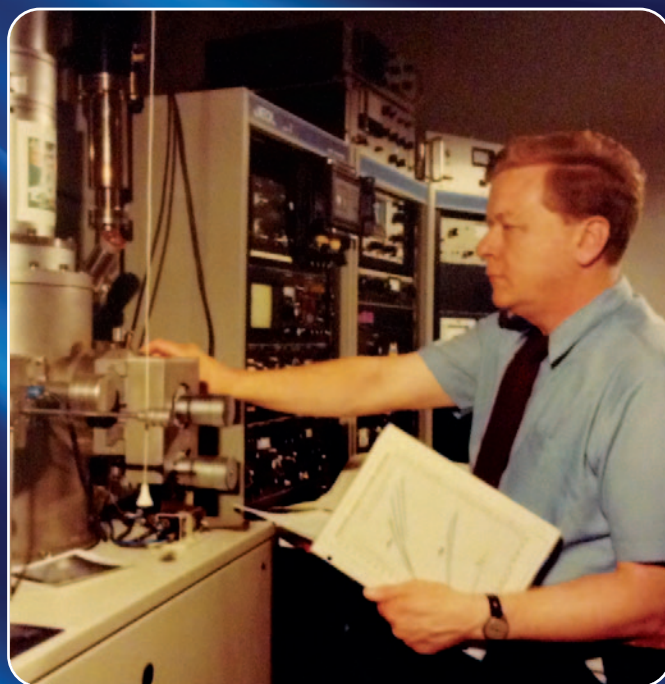
Crystallography News

British Crystallographic Association



Issue No. 160 March 2022

ISSN 1467-2790



Happy 40th Birthday BCA!

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2021 AGM

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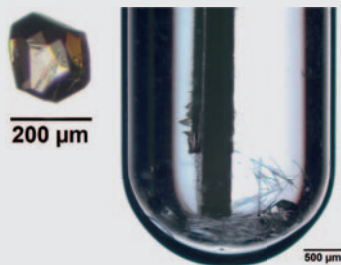
Meetings of interest

p22

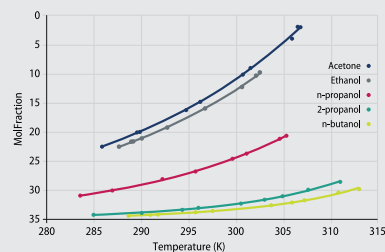
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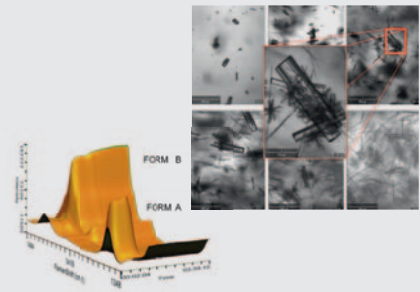
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- vapor diffusion
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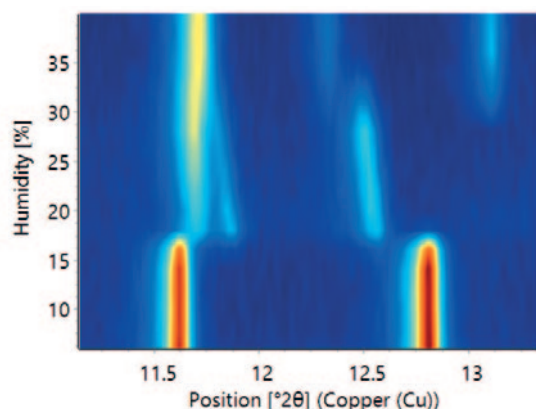
Come to see us at the BCA Spring Meeting – University Leeds

Learn more about

Water cluster structure in the MOF CAU 10-H: a powder diffraction perspective

and

In-situ XRD and PDF investigation of battery fluoride materials $\text{MF}_3 \cdot 3\text{H}_2\text{O}$ (M = Fe, Cr) in controlled atmosphere: accessing new phases with controlled chemistry



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British Crystallographic
Association

Conference Bursaries 2022

Bursaries are available for BCA members to attend national/international crystallographic meetings in 2022.

Local meetings and virtual meetings (with no travel) are supported. Eligible members may apply every year.

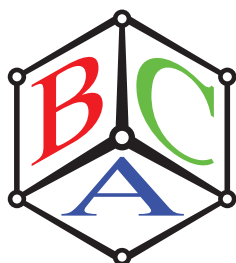
Apply early for in person attendance at international meetings. Successful local/virtual meeting bursary winners are still eligible.

Further information on the eligibility criteria and the application portal is available here:

<https://crystallography.org.uk/prizes/bursaries>

Additional carers grants are also available to BCA members at any career stage:

<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 June 2022 issue are sent to the Editor to arrive before 25 April 2022.

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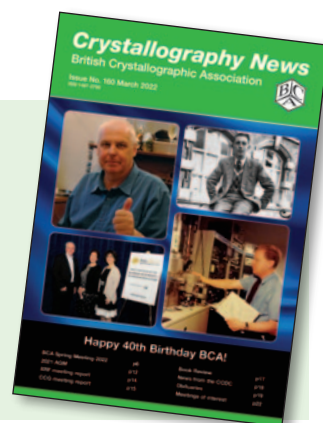
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These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

Printed by North Wolds Printers
83 Halifax Way, Pocklington Industrial Estate,
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Tel: 01759 303944
Web: www.northwolds.co.uk

This month's cover:

Four crystallographic stalwarts who have left their marks (see page 19). Clockwise from top left: Bernard O'Hara, Ron Patrick, Ian Ferguson, Graham Fisher.



From the President



IT would be daring (or even foolhardy) to attempt make a forecast (or even an observation) about the state of a pandemic in a column that is written over a month before it is published. Instead, I would ask you to read these words as a historical record, offering a glimpse of the different (or maybe similar) times we were living in way

back in January 2022.

I send sincere thanks to **Iain Oswald** for taking on the role of programme chair for the upcoming Spring Meeting in Leeds, and to all who have worked on the programme committee and behind the scenes organising the meeting. The frequent, albeit necessary, changes to rules relating to large gatherings of scientists have undoubtedly added pressure and uncertainty to securing speakers and attracting delegates, who would understandably rather wait before committing their time and funds to a meeting. I am looking forward to an excellent programme which spans an impressive range of subjects from the topical: room temperature biological systems and Covid drug discovery, to complementary and related techniques: nucleation, crystallisation, and extreme conditions.

This year is the 40th anniversary of the creation of the British Crystallographic Association. As previously promised, I have uploaded copies of the first three years of *Crystallography News* (June 1982 – March 1985) and some even earlier editions which pre-date the formation of the association, but are filled with exciting plans for its creation. These earlier issues were published jointly by crystallography groups of both the IOP and RSC. Issue 3/5 from October 1981 includes a thoughtful article ‘*Wither Crystallography Or Whither Crystallography?*’ by **Michael Woolfson**, which is still relevant today, as it envisages the crucial role of the soon-to-be-formed BCA in supporting both specialized meetings, and enabling sharing of ideas and methods on the common ground of crystallography, while recognizing that this task will require constant attention as crystallography and its application in related sciences are constantly evolving. He writes: “*It will be a major function of the British Crystallographic Association to hold together the various strands of crystallography, to provide a forum in which crystallographers can discuss common interests while, at the same time, through its groups [...] special sectional interests can be catered for.*”

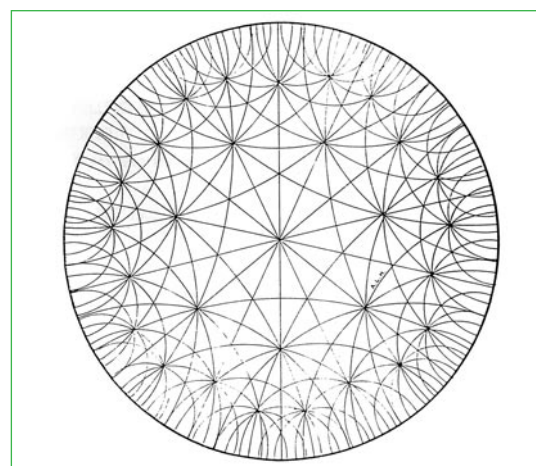
The other editions from that time capture concerns and artefacts of the time – there are advertisements from long disappeared or merged companies that have nevertheless left their marks on the industry – X-ray tubes from GEC Avionics, TV-camera based X-ray image detectors from Enraf-Nonius and powder diffractometers from Nicolet. The December 1982 edition contains an advert for the first BCA Spring meeting at Royal Holloway College. The meeting is advertised as running from 28-32 March 1983 – a typically understated April Fool’s joke presumably courtesy of **Moreton Moore** who was the *Crystallography News* editor and local organizer of the meeting. The total cost for registration, accommodation and dinner was £72.50 (which is £284 adjusted for inflation). Sadly, in the intervening years, university facilities have gradually increased

charges to cover the costs of administration setup to help recover those costs. The same edition also announces an afternoon meeting (£2 admission including tea) to discuss the new draft ionising radiation regulations from the perspective of X-ray crystallographers. The meeting includes contributions from university and industrial scientists, health physicists and the Health and Safety Executive.

Coincidentally, 2022 is also the 40th anniversary of the release of Jim Henson’s fantasy-based film ‘*The Dark Crystal*’, which at first glance may appear to have nothing more than the mention of a crystal in its title in common with the BCA. Yet the film tells the story of historically separate interest groups with different outlooks and objectives – the Skeksis and Mystics – which are eventually united to restore the balance of the universe. The BCA continues to provide opportunities to work together where it benefits all of us, and to pursue subjects at the forefront of our respective fields with colleagues from across the UK and beyond. This point is underscored by **David Philips** in the June 1982 edition of *Crystallography News*: “... we have tended increasingly to think of ourselves as physicists, chemists, mineralogists, metallurgists, biochemists, and so on, who happen to use crystallographic and diffraction methods in our researches... In part this is surely a natural and a healthy development, *but we neglect our base in crystallography at our peril.* Hence the need for the BCA.”

Past issues of *Crystallography News*, including those mentioned here, are available on the BCA website at <https://crystallography.org.uk/crystallography-news/>. The front cover of issue 1 is shown on page 10.

Richard Cooper



The March 1985 issue featured the first of many cover illustrations and images with the accompanying caption: “This picture was drawn by **Dr Alan Mackay** (Department of Crystallography, Birkbeck College) and it represents the packing of regular heptagons, each composed of seven equilateral triangles. It is shown in stereographic projection: (it is angle-true). Since in a plane the average coordination number is six, a coordination number of seven can only be achieved by curving the space, which is here hyperbolic. For equiangular triangles of unit area the radius of curvature is $\sqrt{(-7/\pi)}$. Sevenfold symmetry is quite possible in a lattice, but not in this world.”

BCA Council 2022

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

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

From the Editor



IN addition to the 'usual' items in the March issue (more information on the Spring Meeting, AGM minutes, group reports...) I'm pleased we have a book review – the first one since I took on the editor's job. *Crystallography News* welcomes not only book reviews like this one, but also (see the left hand column of page 1) technical articles, news about people (e.g.

awards, honours, retirements etc.), reports of meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor and hardware or software reviews. Copy deadlines are generally the 25th of January, April, July and September, though it helps me to plan if I know what is likely to come in before those dates. It's your 'News' so if there is something you want to tell the rest of the community, just drop me a line!

One kind of item that we – regrettably but inevitably – have regularly is obituaries. Looking back over the last four years, eight out of ten of these have been of academic research scientists. Of the remaining two, one worked in industry, the other in the public sector. This academic emphasis might give the impression that academia is the main area where excellent crystallography is done, whereas in reality crystallographic ideas and techniques are, as we all know, much used in both industry and the public sector. The four obituaries in this issue – and celebrated on the front cover – will perhaps help to recognise this as all the four crystallographers we are remembering this month were crystallographic stalwarts that have worked in either industry (one setting up his own instrument company) or the public sector. It's also perhaps worth noting that all four obtained their Ph.Ds through part-time study – three of them at Birkbeck (which incidentally celebrates its 200th anniversary next year – watch this space!).

What is more, I'm pleased that several of the authors have given us insights into our late colleagues' commitments to helping others advance educationally, in particular in crystallography – which is of course one of the BCA's charitable objectives. I'll choose but one example: **Graham Fisher** (declaration of interest – I was his Ph.D. examiner). In addition to his Trusteeship of the St Louis Academy of Science mentioned in Paul Barnes's article, Graham involved himself more widely in the local education scene, not only with respect to encouraging science (illustrated here judging a High School Honors Division Science Fair project at Webster University) but also concerning himself with those less favoured educationally – for example by funding buses to enable children from underserved schools to attend St Louis Science Academy events. Ashley Newport from the Academy put it squarely to me: "Graham was one of our favorites! Such a kind and gentle man". Many – both sides of the pond – will miss him.

Finally, reading the President's column reminded me of a copy of a letter I uncovered a year or so ago when sorting out boxes of old paperwork relating to the accounts of the Welsh upland sheep farm we* ran some 30 years ago. As there's no legal requirement to keep financial documents for more than seven years, I was just about to ditch the carbon copy (oldies will remember those – and the carbon paper and the typewriters that produced them...) when I saw it was typed on the reverse side of an A4 poster for the first BCA Spring Meeting that Richard mentions in his column. So I thought it might be fun to reproduce it alongside the front cover and contents of the first edition of *Crystallography News* that Richard has extracted from the BCA archives – see the centre spread! Applaud the expert calligraphy of **Moreton Moore**, who organised that first Spring Meeting! And perhaps – *cf.* the comment in the President's column – note that the dates on the poster are correct!

John Finney

**Actually my wife – I was the worker at weekends and during lambing...*



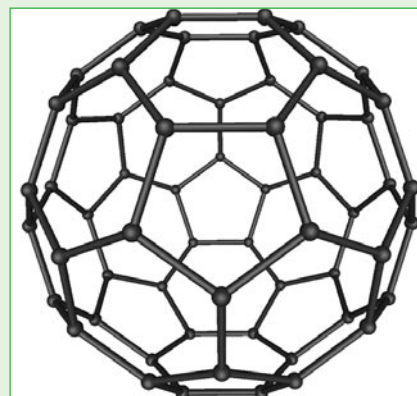
Picture courtesy of Academy of Sciences St Louis.

Puzzle Corner



THIS month, four questions about buckminsterfullerene ('buckyballs').

1. What is the point group of a buckminsterfullerene molecule?
2. If you could closest pack these molecules, what would be the highest symmetry space group you could obtain?
3. Many modern footballs share this symmetry. How long have these been official?
4. For a programme in the 1990s about buckminsterfullerene, the BBC chose various selections from a Mozart Mass (K.427) for background music. Why?



Picture courtesy of Michael Ströck.

Answer to December's puzzle:

In either case, one must have three of one kind, so one can start from there.

For four of a kind, there are two chances of getting the essential card out of the remaining 49 in the pack, i.e. one chance in 24.5.

For a full house, the first card can be anything except the one needed for four of a kind (48/49). There are then three cards left to give the pair so the overall probability is (48/49) x (3/48), or one chance in 16.3.

So the chances of a full house are indeed higher.

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.
- 10% discount on exhibition stands at the annual BCA Spring meeting.
- Two free registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

Corporate Membership is currently **£800** for one year.

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Benefits of Individual BCA Membership:

- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- 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/

BCA Spring Meeting 2022



CHECK out the Scientific Programme below to see the excellent range of talks and sessions that are sure to satisfy any conference hungry brain after a year online!

Full details and registration information is at <https://registrations.hg3conferences.co.uk/bca2022>.

YCG EARLY CAREER SATELLITE MEETING

Monday 11th April, 2022

Young Crystallographers Group (YCG)

13:00 – 21:00

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography, 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

YCG Opening Plenary

Session Chair: **Tom Roseveare** (*University of Sheffield*)

Speaker: **Dr Claire Hobday** (*University of Edinburgh*)

Pressure driven phase transitions – a look to the future of solid-state refrigeration

13:30 – 17:15

YCG Research Sessions

Contributed talks from the YCG community.

Session 1 Chair: **Tom Roseveare** (*University of Sheffield*)

Session 2 Chair: **Dr Natalie Pridmore** (*University of Bristol*)

Session 3 Chair: **Aly Abdeldaim** (*ISIS Neutron and Muon Source/University of Birmingham*)

17:15 – 17:45

YCG Annual General Meeting

18:30 – 21:00

Flash Poster Presentations

Session Chairs: **Dashnor Beqiri** (*University of Warwick*) &

Lee Birchall (*University of Kent*)

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide. A poster session (with buffet and wine) follows.

BCA 2022 MAIN MEETING PROGRAMME

Tuesday 12th April, 2022

09:00 – 09:30

Parkin Lecture

Session Chair: **Dr Rachel Wilkinson** (*Swansea University*)

Speaker: **Dr Alexander Tansell**

Peer review vs Public review: why we should care about both

09:30 – 10:30

YCG Research Sessions

Contributed talks from the YCG community.

Session 4 Chair: **Dr Charlie McMonagle** (*European Synchrotron Radiation Facility*)

10:30 – 11:00

YCG Closing Plenary

Session Chair: **Dr Charlie McMonagle** (*European Synchrotron Radiation Facility*)

Speaker: **Dr Sam Horrell** (*Diamond Light Source*)

10 things your beamline scientists wish you knew

MAIN MEETING

11:30 – 12:15

Lonsdale Lecture

Session Chair: **Tom Roseveare** (*University of Sheffield*)

Speaker: **Prof. Andrew Goodwin** (*University of Oxford*)

Disorder by design: from form to function

13:00 – 13:45

PCG Plenary

Session Chair: **Dr Alex Gibbs** (*University of St Andrews*)

Speaker: **Prof. Xiaodong Zou** (*Stockholm University*)

3D Electron crystallography: past, present and future

14:15 – 15:45 Parallel Sessions

PCG: Porous Materials

Session Chair: **Aly Abdeldaim** (*ISIS Neutron and Muon Source/University of Birmingham*)

Keynote: **Dr Sam Chong** (*University of Liverpool*)

The importance of cooperativity in understanding porous molecular crystals

The diverse functionality associated with the versatility of porous materials allows for the discovery and realization of properties that are crucial for advances in next generation applications. Specifically, their broad structural-property adaptability explains the enduring appeal of their research as porous materials find diverse applications ranging across, among others, energy storage, drug delivery, and nanotechnology. As such, this session will focus on exploring the ongoing trends in this field, delving into their synthetic complexity, structural-property relationships, and their relation to *ab initio* techniques.

BSG: RNA-Protein Interactions

Session Chair: TBC

Keynote: **Max Wilkinson** (*Massachusetts Institute of Technology*)

Snapshots of pre-mRNA splicing from cryo-EM studies of the spliceosome

CCG: Crystallography Under Extreme Conditions

Session Chair: **Dr Charlie McMonagle** (*European Synchrotron Radiation Facility*)

Keynote: **Dr Christine Beavers** (*Diamond Light Source*)

Extreme Conditions for All: Expanding the Exploration of Phase Space in a Multitude of Materials

Crystallography under extreme conditions comes with its own associated challenges. In this session we explore the advances in technique development and data analysis under non-ambient regimes that inform on interesting chemistry. Extreme conditions can provide critical insight into the structures, reactivity, and behaviour of molecules and materials. This session will cover scientific, technological, and methodological developments across a wide range of extreme experimental conditions including high magnetic fields, electric fields, high and low temperatures, high pressure.

16.30 – 18.00 Parallel Sessions

PCG: Structure-Property Relationships in Energy Storage

Session Chair: **Dr Karen Johnston** (*University of Durham*)

Keynote: **Prof. Laurence Croguennec** (*Institut de Chimie de la Matière Condensée de Bordeaux*)

Developing an in-depth understanding of new materials to optimise cathodes in metal-ion batteries

As we strive to achieve net zero emissions it is increasingly clear that energy storage will play a crucial role in addressing this global challenge, driving areas such as the electrification of transport and large-scale storage of renewable energy. Rechargeable Li- and Na-ion batteries will be key in delivering future energy storage demands. This session explores battery materials, their complex structure-property relationships and the methods used to characterise them. We are interested in new battery materials and technologies (beyond Li-ion). Examples where the combination of experimental and computational methods has resulted in significant structural understanding are also of interest.

BSG: Correlative Tomography

Session Chair: **Dr Maria Harkiolaki** (*Diamond Light Source*)

Keynote: **Peter Sadler** (*University of Warwick*)

Correlative synchrotron x-ray imaging of metal anticancer complexes in cancer cells

Correlative imaging is fast becoming an indispensable approach to understanding complex biological systems at the cellular and atomic levels. New synergies between microscopies are constantly documented highlighting the need for crossing contrast and resolution barriers to fully understand biological processes. This session focuses on applications and developments in 2D and 3D correlative imaging of cellular ultrastructure and chemical organisation within cells.

CCG: Nucleation & Phase Changes

Session Chair: **Dr Katharina Edkins** (*University of Manchester*)

Keynote: **Prof. Gérard Coquerel** (*Université de Rouen, Normandie*)

Polymorphic transitions in the organic solid state: two complex cases with simple molecules

The phase transitions between liquid and solid, or indeed between two solid phases, can have an immense impact on the manufacture and stability of organic materials. Most phase transitions include a nucleation step, while nucleation is best known as the first step in the generation of a crystalline material from solution or the melt. In this session, we will be looking at the impact and the underpinning fundamental science of phase transitions and their related nucleation in organic or organo-metallic materials for the application in pharmaceuticals, agrochemicals or fine chemicals, sensors and energy materials non-exclusively.

18:15 – 19:00

CCG Plenary

Session Chair: **Dr Michael Probert** (*University of Newcastle*)

Keynote: **Prof. Michael Hardie** (*University of Leeds*)

Supramolecular cages and networks with pyramidal ligands

19:00 – 21:00

Poster Session with Dinner and Wine

Wednesday 13th April, 2022

08:45 – 09:30

IG Plenary

Session Chair: **Dr Judith Shackleton**

Keynote: TBC

10:15 – 11:45 Parallel Sessions

PCG/CCG: Advances in Complementary Techniques and *In Situ* Crystallography

Chair: **Dr Hamish Yeung** (*University of Birmingham*)

Keynote: **Prof. Fiona Meldrum** (*University of Leeds*)

Using Coherent Diffraction and Super-Resolution Imaging Methods to Visualise the Internal Structures of Bio-Inspired Crystals

Advanced complementary techniques offer fantastic potential to improve our understanding of structure, mechanisms and processes far beyond what is possible using conventional crystallography. X-ray tomography, coherent diffraction imaging, NMR crystallography and electron diffraction are just four examples of emerging methods that give a wealth of information beyond long-range ordered structure and are all the more powerful when performed *in situ* or *in operando*. Such techniques push the boundaries of possibility with existing instruments and methodology, leading to advances across many diverse scientific disciplines including biological crystallisation, energy storage, catalysis and advanced materials.

BSG: Electron Diffraction

Session Chair: **Dr Peijun Zhang** (*Diamond Light Source*)

Keynote: **Dr Tim Gruene** (*University of Vienna*)

Instrumental requirements for electron crystallography are less demanding than you might think

The field of electron diffraction of micro/nanocrystals (microED) is emerging. A growing number of structures were determined by microED and several protocols and workflows for data collection and structure determination have been established. This session will be focused on advances in software/hardware for microED, results obtained and discussions of future development.

IG: Industrial Crystallography Metallurgical and Other Applications

Session Chair: **Dr Judith Shackleton**

Keynote: **Dr Will Bodel** (*University of Manchester*)

Graphitisation and neutron irradiation induced degraphitisation of near-isotropic graphites for next generation reactor design

This session will include industrial applications on a metallurgical/inorganic theme. It is intended to cover a wide range of topics and hopes to include laboratory X-ray, synchrotron, and neutron diffraction. There are already contributions covering reactor materials such as graphite, the application of the neutron diffractometer ENGIN-X as well as residual stress and preferential orientation, in shot-peened aluminium.

12:15 – 12:45

BSG Annual General Meeting PCG Annual General Meeting

12:45 – 13:15

CCG Annual General Meeting

13:15 – 14:45

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.

CCDC Chemical Crystallography Group Prize for Younger Scientists

The CCG and CCDC 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 Prize

The PCG 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.

15:30 – 17:00 Parallel Sessions

YCG+ Careers Session

Session Chairs: **Dr Natalie Pridmore** (*University of Bristol*) & **Tom Roseveare** (*University of Sheffield*)

Panellists: **Prof. Andrew Goodwin** (PCG, *University of Oxford*); **Dr Claire Hobday** (CCG, *University of Edinburgh*); **Dr Sam Horrell** (BSG, *Diamond Light Source*)

An opportunity to hear from, and pose questions to, the panellists about their jobs and career paths in various fields of crystallography.

BSG: Membrane Proteins

Session Chair: **Dr Julien Bergeron** (*King's College London*)

Keynote: **Dr Jamie Blaza** (*University of York*)

*Understanding the mechanism of the bifurcating hydrogenase from *Thermotoga maritima* through the application of cryo-EM and symmetry expansion*

IG: Industrial Crystallography: Changes and Challenges

Session Chair: **Dr Anthony Bell** (*Sheffield Hallam University*)

Keynote: **Dr Jeremy-Karl Cockcroft** (UCL)

The Changing Face of X-ray Crystallography: Are We Keeping Up-to-Date?

The session will include a wide range of topics covering many aspects of Industrial Crystallography.

Actually Industrial Crystallography includes pretty much anything from metals to minerals and pharmaceuticals. So there is plenty of scope. We are hoping to cover a range of measurements; those that went well and those very instructive ones which didn't.

The keynote talk will discuss the use of crystallography in the evaluation of patents and will also cover some of the errors which can occur in powder diffraction.

17:10 – 18:00

Hodgkin Lecture

Session Chair: **Prof. Richard Cooper** (University of Oxford)

Keynote: **Prof. Elspeth Garman** (University of Oxford)

Macromolecular Crystallography in 112 AD (After Dorothy)

18:00 – 19:00

BCA Annual General Meeting

19:30 – 01:00

Conference Dinner

Thursday 14th April, 2022

08:45 – 09:30

BSG Plenary

Session Chair: **Dr Katherine Brown** (University of Cambridge)

Speaker: **Prof. Randy Read** (MRC, Cambridge)

Structural biology in a post-AlphaFold world

10:15 – 11:45 Parallel Sessions

PCG: Extracting information from disordered and poorly crystalline solids

Session Chair: **Dr Arianna Minelli** (University of Oxford)

Keynote: **Dr Kirsten Jensen** (University of Copenhagen)

Materials on the nanoscale: Total scattering analysis for nanoparticle chemistry

Increasingly, materials with structural disorder are studied with diffraction techniques, which were considered for many years only able to show perfectly periodic arrangements. In reality, this perfect periodicity simply describes an average reconstruction of the structure and the disorder adds a supplementary signal, normally found as diffuse scattering. This session looks at all degrees of complexity in disordered materials; from correlated disorder in a single crystal to poorly crystalline materials and all the way to amorphous phases.

BSG: Room Temperature Data Collection

Session Chair: **Dr Allen Orville** (Diamond Light Source)

Keynote: **Prof. Arwen Pearson** (Centre for Free-Electron Laser Science, Hamburg)

Life is dynamic and room temperature crystallographic studies are providing important new functional, structural, and mechanistic insights into many biological systems. This session will include speakers highlighting serial and time resolved experiments, *in situ* room temperature data collection, and other room temperature approaches.

CCG: Tricks of the Trade – From Crystallisation to Publication

Session Chair: **Dr Claire Wilson** (University of Glasgow)

Keynote: **Prof. Ton Spek** (Utrecht University)

PLATON tools to help with resolving cryptic checkCIF ALERTS

This session is an opportunity to share tricks of the trade, to highlight tools or methods of interest to many in the chemical crystallography community but which are not currently as widely used as they could and should be. These could be software, practical or analytical tools or methods which have been newly developed or older ones which have fallen out of

use and been rediscovered or repurposed to provide a valuable option for current chemical crystallographers at any stage from crystallisation to publication.

12:00 – 13:30 Parallel Sessions

PCG: Functional Materials

Session Chair: **Dr Paul Saines** (University of Kent)

Keynote: **Dr Josh Makepeace** (University of Birmingham)

The role of compositional flexibility in energy storage applications of lithium imide-based materials

Functional materials are critical to underpinning the technologies needed for modern society, including, for example, clean energy generation, medical sensing and quantum technologies. This session will focus on understanding the structure-property relationships in functional materials and how this enables materials to be optimised for application. Studies using experimental approaches that extend conventional approaches, including those combining computational methods, are of particular interest for this session.

BSG: Covid Drug Discovery

Session Chair: **Dr Daren Fearon** (Diamond Light Source)

Keynote: **Dr Ivan Ahel** (William Dunn School of Pathology, University of Oxford)

ADP-ribosylation signalling and coronavirus infection

The outbreak of Covid-19 has inspired international efforts to develop novel antiviral agents to help address both the current pandemic and any future pandemics caused by coronaviruses. Fragment-based drug discovery and structure-based drug design have made significant contributions to the development of these much needed antivirals with over 1500 X-ray crystal structures deposited in the PDB to date. This session will focus on structural methods used to identify ligands which bind to coronavirus proteins and how these methods have been applied to further develop these ligands into promising leads and drugs.

CCG/BSG: Understanding Crystallization Through Diffraction and Complementary Methods

Session Chair: **Prof. Joop ter Horst** (University of Rouen)

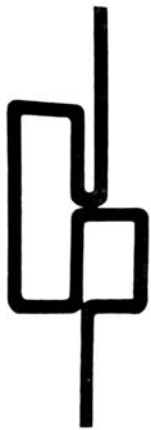
Keynote: **Prof. Sven L.M. Schroeder** (University of Leeds)

Beyond CNT: Kinetics of Homogeneous Crystal Nucleation from Molecular Structure and Thermodynamic Parameters

Crystallization is the process of forming crystal solid particles, preferably of a certain structure, size, shape, and purity. This process is governed by the sub-processes of, among others, crystal nucleation and growth which are still not completely understood. This session will discuss innovative diffraction and complementary methods that deliver breakthroughs both in the understanding as well as control of crystallization processes of all types of solids.

CLOSE OF CONFERENCE





CRYSTALLOGRAPHY NEWS



BRITISH
CRYSTALLOGRAPHIC
ASSOCIATION

No. 1 JUNE 1982

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Front cover and contents of the first edition of Crystallography News following the setup of the BCA in 1982.

Keep in touch with crystallography today! Join the

British Crystallographic Association

Subject groups : PHYSICAL CRYSTALLOGRAPHY : jointly with I.O.P.
CHEMICAL CRYSTALLOGRAPHY : jointly with R.S.C.
INDUSTRIAL CRYSTALLOGRAPHY *
BIOLOGICAL STRUCTURES *

* To be inaugurated at the BCA Spring Meeting, 28-31 March 1983
at Royal Holloway College, Egham, Surrey.

Newsletter: The quarterly "Crystallography News".

Meetings: BCA Spring Meeting, subject groups, special topics.

Membership: The BCA is the second largest crystallographic
society in the world. Membership fee: £10 per annum.

Student & Retired Rate: £5 p.a. Membership of one
subject group is free to BCA members: £1 p.a. for each
additional subject group.

FURTHER DETAILS FROM

Hon. Treasurer: Prof. C.A. Taylor,
Department of Physics,
University College, P.O. Box 78,
Cardiff CF1 1XL (0222-44211 X 2060)

Hon. Sec: Dr. A.C. Skapski,
Department of Chemistry,
Imperial College, London,
SW7 2AY (01-589-5111 X1212)

BCA 2021 AGM Minutes

Draft minutes of the 2021 Annual General Meeting of the British Crystallographic Association Zoom Webinar 17:30, Wednesday 31st March 2021

1. **Approval of Agenda**

The agenda was approved; proposer: Claire Hobday, seconder: Mark Roe.

2. **Apologies for Absence**

Adrian Whitwood and Philip Duke.

3. **Minutes of the previous AGM 2020**

Hazel Sparkes identified that the Treasurer should be Claire Naylor in section 9 (Elections to Council). Elizabeth Shotton noted that Crystallography Times was mentioned instead of the correct News in section 4. With the above correction noted, minutes were approved by Elspeth Garman and Mike Probert.

4. **President's report**

The President, Simon Phillips, started with the sad report of the loss of a BCA Founder member (1927-2021) Judith Milledge. Judith was a Ph.D. student with Kathleen Lonsdale and assisted with the preparation of the first edition of the International Tables. Her expertise was on diamond structures and she was also a committed teacher. Congratulations were given to Elspeth Garman for the award of the 2020 Suffrage Science Award in Life Sciences. This scheme celebrates women in science for their scientific achievements and for their ability to inspire others. Thanks and congratulations were given to Tom 'Ed' Edwards, Simon Parsons, Hg3 and teams for dealing with rescheduling the Spring Meeting, and also for joining together with the BACG to convert it to a joint meeting in a virtual format. The 2022 Spring Meeting will be held in Leeds, 11th – 14th April, with the Programme Chair being taken up by Iain Oswald from the University of Strathclyde. The President thanked the BCA Officers: Simon Parsons, Alex Stanley and Claire Naylor. The Education and Outreach Coordinator, Simon Coles, who is retiring this year, was thanked, especially for his recent work on Crystallography News. The members of the BCA Council were thanked for their input, enthusiasm and willingness to endure long Council Meetings on Zoom. Thanks were also given to John Finney, the editor of Crystallography News, Nicola Hardaker and all the team at Hg3 and to all the BCA members for their continued support of the Association in a difficult time.

Simon Coles presented the slides of the EOC for an update on education and outreach activities: He noted that no major organisational changes had been made in terms of group reps although he was to stand down and wished Christine Beavers (DLS) well after having been elected to the role. Simon highlighted that the EOC were looking to migrate learn.crystallography.org.uk/learningresources/ to github. One bursary application for the outreach bursary (<£2500) and grant (<£500) scheme had been made from

the CCG group. The proposal was to build a series of core educational, animated videos to support learning of diffraction with the target audience of Ph.D. students. Ten of these have been proposed with the first funded by the EOC bursary and this has now been storyboarded and handed over to an animation company. The remaining series still needs to be funded depending on feedback on this pilot episode. Digital and online activities in the field of crystallography were mentioned including the CCDC educational resources and webinar series, NCS support for undergraduates and the Rigaku virtual summer schools.

5. **Secretary's report**

The Secretary, Alex Stanley, reported that all Officers' and Council meetings had been held virtually which proved to be very successful and as a bonus reduces any expenses for travel. Nominations for elections and the election process continue to run smoothly. Thanks were given to the Nominating Committee.

6. **Hg3 Report**

Simon Phillips, on behalf of the Hg3 representative, Nicola Hardaker, reported that the total BCA membership as of 18th March 2021 was 489 which is slightly down on previous years but was following the trend of other organisations which Hg3 manage. The names of the eight Corporate Members were given and remain the same as last year. Crystallography News has the following current advertisers: Bruker, Malvern Panalytical, Oxford Cryosystems and Rigaku Oxford Diffraction (all issues). This current meeting has had admirable support from exhibitors and sponsors given the circumstances. The attendance figures as of last week are 285, comprised of 159 delegate registrations, 76 rolled over from 2020, 34 invited speakers booked and 16 exhibitors/sponsors. It was noted that this total figure was reported to have exceeded 300 at the start of the meeting. Simon Parsons reiterated the thanks to the sponsors and to remind delegates to visit the exhibition as he had heard that contact with the exhibitors was a bit thin. Iain Oswald mentioned that with respect to poster prizes, CrystEngComm had sponsored two prizes. John Helliwell said that there are poster prizes from the IUCr and the ACA/AIPP. Nicola Hardaker mentioned that those poster prizes listed above were ones that were sponsored this year. The RSC ones were rolled over from last year. Anonymous: Was there an agreement with the ACA that they could attend this meeting virtually from the US? Simon Phillips said that there was a discussion underway but that no decision had been finalised. The President of the ACA changed hands in January, hence delaying the conversation.

7. Report of the Treasurer including presentation of the Accounts for 2020 and Examining Accountant's Report

The Treasurer, Claire Naylor, reported that a copy of the account summary for the period from Jan. 1st to Dec. 31st, 2020, had been circulated and a full breakdown of the accounts was included in the BCA annual accounts available by email, or online at the Charity Commission website. Summaries of the income, Spring Meeting finances and outgoings (governance and charitable expenditure) were circulated before this AGM began and presented. The main point to note for 2020 income is that it is much smaller than previous years since there have been fewer meetings held. Membership subs are slightly down and advertising revenue for Crystallography News is slightly up. The Spring Meeting finances for 2020 were presented. There were some unavoidable expenses for the cancelled meeting primarily due to management and bank charges. A large thank you was given to Hg3 and the entire Council for keeping our losses as small as possible. Expenditure on governance is always kept to a minimum where possible. Expenses are substantially lower due to the absence of the Spring Meeting. Overall, the net loss for the year was just over £20,000 and this included not only losses on the Spring Meeting but also investments took a hit with the pandemic. Thanks were given to Hg3, Council members, BCA group Treasurers, Charles Stanley Bank and UHY Hacker Young accountants. In response to a query asked at the last AGM in regard to the increase in the fees for printing and stationery, the Treasurer noted that this was purely a change in the way that expenses were coded and in fact, these costs had remained stable. Accounts were accepted; proposer: Kirsten Christensen; seconder: Helen Playford.

8. Appointment of the Examining Accountant for 2021

The proposal was to appoint the Young Company. This was approved; proposer Sandy Blake, seconder: Simon Coles.

9. Elections to Council

The President reported that elections had been carried out by electronic ballot. BCA members were notified by email that voting had opened and provided with a personal link to the voting site. The results were as follows:

President:

Richard Cooper (2021-2024).

BCA Council Ordinary Member:

Cheryl Doherty (2021-2024).

Education and Outreach Coordinator:

Christine Beavers (2021-2024).

It was highlighted that in 2022 there would be elections for Vice President, Secretary, and an Ordinary Member. Candidates are identified by the Nominating Committee or by BCA members and nominations are made to the Secretary, with a deadline of 30th September 2021. For 2021-2022 the Nominating Committee is Chris Frampton* (Chair), Phil Lightfoot*, Elspeth Garman, Lee Brammer and Chick Wilson.

*retiring in 2021 – positions yet to be filled.

10. Honorary Members

Honorary Members are chosen for their contributions to both crystallography and to the BCA. There are no new Honorary Life Members for 2021. The nomination deadline for 2022 Honorary Members was given: August 31st,

2021. Nominations should be sent to the BCA President with a brief case for support of not more than 400 words. Nominations will be considered at the September Council Meeting. New Honorary Members may not be awarded every year and there is a maximum of two in any calendar year.

11. Membership, annual subscriptions and subventions

Membership figures were presented showing a high of over 800 members in 2003, a low of less than 400 in 2012 and a slight decline of recent years from 552 members at 31st December 2019, 566 at September 2020 to 489 at March 2021. The President encouraged members to encourage colleagues to join. Elspeth Garman commented that the membership figures were slightly skewed in 2012 as there were over 200 lapsed members who were still being accounted for and a huge effort went into reviewing the membership figures. Simon Phillips acknowledged this comment and thanked Elspeth for her efforts. Lee Brammer supported Elspeth's statement and suggested that we try to standardise the dates to compare membership numbers more easily.

12. Equality, Diversity and Inclusivity report

The BCA EDI policy was adopted in March 2018 and the President restated the policy on a slide and that the intention is to ensure quality and equality. Programme Committee members for 2022 were also encouraged to be mindful of this and invited feedback to the President. The figures for the Spring Meeting 2021 were reported for 2021 with student members 49% female, Young Crystallographers not including students 43% female and standard members 31% female (73 female, 160 male). Programme Committee members and speakers at the current (and previous) Spring Meetings were also given; for 2021 the main meeting figures were as follows: (percentages given are female; YCG in parentheses): Programme Committee 44%, plenary speakers 29 (100) %, keynotes 25%, speakers 38 (50)% and chairs 36 (50)%. These numbers reflect our membership gender distribution.

13. AOB

Simon Parsons thanked Simon Phillips very much for his tenure as President especially given the challenging times. He noted that Simon made well informed and reasoned decisions which turned out in hindsight to be the very best course of action with respect to cancelling the Spring Meeting in 2020 and the 2021 Spring Meeting becoming virtual. A bottle of whisky was virtually presented as a thanks from the committee. Simon Phillips gave his thanks to all and wished the incoming President, Richard Cooper, the best of luck. Richard Cooper reiterated the praise given by both Simon Phillips and Simon Parsons and to the delegates for attending the first online Spring Meeting. He encouraged everyone to send any suggestions or ideas in via the Programme Committee. He reminded us that the BCA, as a charity, is to uphold its remit for outreach and education and that both support and the receipt of membership dues from the delegation make this entirely possible. Sharing news stories or materials related to outreach and education is encouraged and he welcomed the election of Christine Beavers to Council to support these activities.

The meeting closed at 18:10.

BCA Industrial Group XRF Meeting 2021



AFTER no meeting in 2020, for obvious reasons, the annual Industrial Group X-Ray Fluorescence (XRF) meeting returned as a Zoom meeting on 10th November 2021.

45 delegates, from six different countries, registered for this meeting. Six speakers gave presentations from all over the world.

Mike Dobby (Consultant, Dronfield UK) gave a talk entitled 'What has changed in XRF technology in the last 20 years'. He talked about how advances in XRF detectors had changed XRF analyses. He also talked about the challenges of doing XRF at home with a hand-held spectrometer.

Tanya Norris (Wagners Cement, Pinkeba, Queensland, Australia) gave a talk entitled 'The importance of XRF analysis in a cement plant'. She talked on how fused beads are made of cement samples to make sure that the cement follows Australian composition standards.

Michael McKee (University of Leicester, UK) gave a talk entitled 'How can we use x-ray fluorescence to solve 'The Mercury Mystery'?'. This fascinating talk was about the planet, not the element! His Ph.D. thesis work concerns an XRF detector on the BepiColombo spacecraft currently en route to the planet. XRF will be used to help to find out how the planet formed.

Alex Husbands (Aqua Force Recycling, Wolverhampton, UK) gave a talk entitled 'Using XRF for industrial waste analysis'. This was about how XRF is used to characterise unknown waste samples so that waste materials can be safely disposed of or recycled.

Konstantin Brendgens (Fluxana, Bedberg-Hau, Germany) gave a talk entitled 'Sulfuric Ores: Fusion with gas and electrical machines'. Preparing fused bead samples for XRF with metal sulfide samples can be challenging as these sulfides can damage platinumware. Pre-oxidation of sulfide to sulfate with a metal nitrate means that fused beads can be safely prepared without having to replace expensive platinum crucibles.

Zach Dismukes (Bowman Analytics, Schaumburg, IL, USA) gave a talk entitled 'Using XRF for plating thickness analysis on a wide variety of materials.' XRF can be used to determine the thickness of metals coated on substrates from the relative intensities of XRF lines for the different elements involved.

As usual there was also the sponsor session where representatives of six different sponsors gave short talks on their XRF instruments and materials.

In spite of some hiccups with Zoom the meeting was a success. The provisional date for the next meeting is 15th June 2022, when it is hoped that a face to face meeting (with a possible Zoom component) will take place at Sheffield Hallam University.

A.M.T. Bell
Sheffield Hallam University

PCG Intensive School in Physical Crystallography

THE next PCG Intensive School in Physical Crystallography will be held in the summer of 2022 – dates tbc.

This school is aimed at anyone who is interested in learning about advanced topics in physical crystallography from experts in the field. Information about the previous school, held in 2018, can be found here: <https://pcgschool2018.wordpress.com/> and the 2022 school is likely to follow a similar format.

Further information will be circulated in due course. In the meantime, please contact **Alex Gibbs** (a.gibbs@st-andrews.ac.uk) with any questions, comments or suggestions.



CCG 2021 Autumn Meeting

THE 2021 CCG Autumn Meeting took place online on the 24th November. The theme of the meeting was *'Crystals out of Equilibrium'* and showcased work from a diverse line-up of speakers looking at dynamic crystals and processes, functional properties and metastability of crystalline materials. A small registration fee of £10 was requested to cover the costs of technical aspects of the meeting as well as to contribute to the ongoing scientific endeavours of the CCG, including supporting attendance at the Durham Crystallography School. The CCG committee were delighted to welcome more than sixty participants from all over the world.

The first session was chaired by **Dr Helena J. Shepherd** (University of Kent), and began with the Plenary speaker, **Professor Panče Naumov** from NYU Abu Dhabi. Panče took us on a tour of some truly fascinating responsive crystals that he and his research group have investigated in recent years. Crystals were seen jumping, bending, exploding and deforming as a result of numerous different stimuli. Many of the underlying phenomena that cause these surprising events were clearly explained using a combination of experimental and theoretical methods, including some very impressive structural data. The importance of quantifying anisotropic mechanical properties for understanding the behaviour of dynamic crystals was also discussed, and potential applications for crystalline molecular materials were highlighted. Panče's account of *'The Rise of the Dynamic Crystals'* set the stage for the rest of the meeting looking at out-of-equilibrium processes in the solid state.

The session continued with a talk from **Dr Hamish Yeung** from the University of Birmingham entitled *'Buckling under pressure: mechanical control over conducting molecular crystals'*. Hamish presented a high pressure investigation of the single-component molecular conductor [Pd(dddt)₂] (dddt = 5,6-dihydro-1,4-dithiin-2,3-dithiolate), using structural studies to rationalise the almost temperature-independent resistivity of the material under high pressure. *In situ* studies of single crystals under high pressure revealed buckling of the otherwise flat molecules as pressure increases as well as a shortening of the intermetallic distances.

The final talk of the morning session was delivered by **Dr Asel Sartbaeva** from the University of Bath. Asel described her work on ordered aluminosilicate zeolites and their compressibility under pressure. She introduced the *'flexibility window'*, a range of densities within which the tetrahedra making up the

framework can appear ordered. This is a geometric property of framework materials, and simulations can be used to model amorphization behaviour of known frameworks, and also to gain insight into materials that have been predicted to exist but which so far have not been synthesised.

After the lunch break, the second session of the day was chaired by **Lucy Hunter** (Newcastle University). The first speaker of this session was **Professor Fiona Meldrum** from the University of Leeds, whose work presented some interesting and striking research involving the Bio-Inspired Assembly of Single Crystal Nanocomposites. The work showed how calcite (CaCO₃) can be used as inspiration for creating a plethora of materials which show enhanced combined properties such as high thermal and electrical conductivity. These materials were created by embedding nanoparticles within single crystals. Several techniques, including atomic force microscopy, were used to give a great insight into how and where particles embed themselves, particularly regarding the pathway from adsorption on crystal surfaces to occlusion.

The second talk of the session was delivered by **Dr Enrico Da Como** from the University of Bath. It was based around the interesting phenomena of memory and hysteresis in TaS₂-xSex crystals grown out of equilibrium. Here Enrico's work showed us how the research group used novel quench cooling-synthesis methods to grow charge density wave materials, such as transition metal chalcogenides. The bulk electronic structures of these crystals were analysed using laser spectroscopy, to reveal that such compounds can show Peierls distortions as a result of the charge transfer across the material. This work has the potential to be used for advanced technological applications, for example in quantum memory devices.

The final talk of this session was presented by **Dr Claire Hobday** from the University of Edinburgh, whose work was entitled *'Exploring solid-state materials for pressure induced refrigeration'*. Claire's work focused on the investigation of fascinating materials that show a barocaloric effect, a highly desirable property in the synthesis of solid-state refrigerants. The research incorporated the use of the Crystallographic Structural Database to probe and collect data on the property-design relationships of such crystalline materials. Furthermore, she showed results probing unique barocaloric effects through the use of extreme pressures as a stimulant, with particular focus on the properties shown by DABCO BF₄.



Speakers from session 1, L – R: Panče Naumov, Hamish Yeung, Asel Sartbaeva.



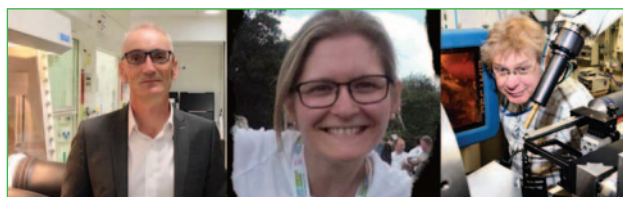
Speakers from session 2, L – R: Fiona Meldrum, Enrico Da Como, Claire Hobday.

After a short tea break, the final session of the day began with **Professor Andrew Weller** from the University of York. Andy presented his group's recent work developing functional Solid-State Molecular Organometallic Framework Molecule (SMOM) materials for various applications including photoswitching and guest encapsulation. He showed how the formation and resulting structure of these SMOM materials is driven by the templating of large, bulky anions, e.g. BArF, and, by using a combination of advanced synthetic methods, crystallography and complementary analytical techniques, how the key structure-property relationships in these materials can be used to rationalise their useful physical properties.

The second presentation of the session was given by **Dr Andrea Laybourn** from the University of Nottingham. Andrea's group is pioneering the use of microwaves in the study of metal organic frameworks (MOFs), which has many potential benefits including reducing the cost and environmental impact of their synthesis. Her talk discussed many aspects of her work, including how microwaves can selectively control the temperature experienced by the MOFs, leading to control of the product materials.

The final talk of the day was given by **Dr Dave Allan**, Principal Beamline Scientist on Beamline I19 at Diamond Light Source. Dave presented a detailed overview of I19's equipment and capabilities, with particular focus on the many exciting set-ups available for *in situ* experiments, including high-pressure, environmental gas cell, photocrystallography and time-resolved methods, as well as electric field cell studies. Dave's talk highlighted some of the recent developments on the beamline,

particularly for the latter two techniques, and gave us all food for thought about the exciting experiments we could do with our own samples on I19 in the near future.



Speakers from session 3, L – R: Andrew Weller, Andrea Laybourn, Dave Allen.

At the end of the scientific session, participants were able to meet in a virtual bar to keep the discussion going and catch up with friends, colleagues and collaborators. This was the second CCG Autumn Meeting to take place virtually, and was a success both in terms of the scientific content, the number of attendees and the diverse locations of audience members. While many of us would like to be able to meet in person again, discussions were had with members of the community as to whether these shorter one-day meetings may be better held online – even once all pandemic-related difficulties have been overcome. While no decisions have been made regarding the CCG Autumn Meeting yet, it is certainly a question that many from right across the scientific spectrum will be asking.

Lucy Hunter, Newcastle University
Lauren Hatcher, Cardiff University
Helena Shepherd, University of Kent

ACA Awards

THE American Crystallographic Association recognizes distinguished achievement in the field of crystallography by both mature and early career crystallographers through the presentation of various annual awards and prizes (you may have noticed – page 18 of the December 2021 *Crystallography News* – that **Jacqui Cole** from Cambridge won last year's Warren Award). Perhaps you know someone who would be a worthy winner of one of the 2023 Awards for which nominations are now open:



David G. Rognlie Award (recognizes 'an exceptional discovery or technical development of particularly high impact in any area of structural science');

A.L. Patterson Award (recognises 'outstanding research in the structure of matter by diffraction methods');

Elizabeth A. Wood Science Writing Award (recognises 'persons who have written books or articles that bring science to the attention of a wider audience');

Margaret C. Etter Early Career Award (recognises 'outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career').

Full details of the Awards and how to nominate are available at <https://www.amercrystalassn.org/awards>.

The deadline for submission of nominations is April 1st 2022.

A Journey into Reciprocal Space. A crystallographer's perspective (second edition)

Mike Glazer

Hardback ISBN: 9780750338738

Ebook ISBN: 9780750338752

DOI: 10.1088/978-0-7503-3875-2

Publisher: Institute of Physics Publishing

WE are led on “A Journey into Reciprocal Space” by someone who has a keen interest in the rich history of crystallography, and who has actively developed the understanding of the structure-property relationship in functional materials over the last five decades. The book draws on Mike Glazer's broad experiences in crystallography taking us all the way from the description of a crystal to an understanding of physical processes which involve the scattering of electrons and phonons, in under 100 pages. The book is nicely peppered with anecdotes, such as the controversy regarding the ionic nature of salt, and Mike's pedagogical style, as well as an occasional hobby horse, that those of us who have seen him lecture will be familiar with, are rendered well in written form. While the later chapters are probably not for the faint hearted, there is plenty here for those just embarking on a career in crystallography, as well as more seasoned practitioners like myself who will learn and re-learn many things through studying this book.

Chapter 1 gives a nice description of crystal structure and crystallographic symmetry illustrated with inorganic examples. It includes a whistle-stop tour on how to read the International Tables for Crystallography which is not commonly found in other textbooks on this subject. The treatment in this chapter is also much more comprehensive and rigorous than found elsewhere in textbooks aimed at both physicists and chemists. However, the core concepts in this and the following two chapters would still be well suited for the basis of an undergraduate course on crystallography. There is also a wealth of information in Chapter 1 for more experienced practitioners to help keep them honest, such as when to refer to Crystal Family or Crystal Class, the difference between space groups and space group types and the meaning of obverse and reverse setting of the rhombohedral unit cell. ‘Government health warnings’ about the correct use of the word lattice are also issued – Twitter users, for your own sakes, please take note!

After a concise introduction to the reciprocal lattice in Chapter 2, Chapter 3 goes into kinematic diffraction theory. This follows a historical perspective, initially giving the Laue equations and then Bragg's law. The Ewald sphere construction is developed, which is used to explain single crystal, Laue, and powder diffraction. Fourier transforms and convolution theory follow and are used to link back to chapter 1, explaining how the diffraction pattern of crystals can be built up from their constituent parts. Form factors are derived in the same vein, after which, all the parts are in place to develop the well-known

structure factor equation. While this approach is certainly very satisfying for those who manage to assimilate the abstract concepts required to reach this point, others will prefer to skip straight to the structure factor equation where the relationship between this and systematic absences are explored. The chapter also includes sections on structure solution and refinement and total scattering, which give a flavour of the processes involved in modelling diffraction data. More advanced topics of aperiodic and disordered crystals are also covered briefly.

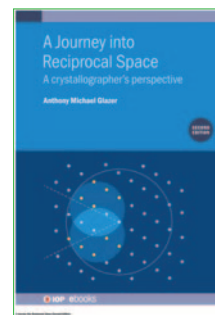
Chapter 4 takes us beyond kinematical to dynamical diffraction theory, where my own understanding stops at the Renninger effect but I'm sure that, as structure determination by electron diffraction (3D ED) becomes more mainstream, many of us may end up reaching for this section of the book.

The last three chapters cover topics particularly close to my heart and provide the link between crystal structure and physical properties via the developed understanding of reciprocal space and diffraction. Chapters describing what the 1st Brillouin zone is and how to make sense of electronic and phonon dispersion curves will be a valuable resource to point my research students to, and these chapters should also feature on the reading list for any graduate level course on solid state physics.

The last chapter called ‘Distortion modes’ is new to the second edition of the book and seems at first sight a bit out of place. However, it provides the link for how phonons or electrons in a periodic crystal can order, causing an associated distortion of a ‘parent’ structure. The natural language to describe these phase transitions is then using irreducible representations of the parent. Mike Glazer illustrates this nicely with some classic examples on perovskites (of course!), detailing how the ferroelectric and tilt instabilities can be understood in the language of irreducible representations. While a flavour of what irreducible representations are is given in this chapter, greater emphasis is rightly placed on how distortion mode analysis can be used to understand phase transitions and symmetry breaking. This includes a nice walk-through example on how to use the web-based program ISODISTORT to perform distortion mode analysis. This chapter will be particularly invaluable to researchers working on studying solid state phase transitions.

The 2nd addition of ‘A Journey into Reciprocal Space, A crystallographer's perspective’ is published by the IOP and is currently available as a hardback or ebook (£32). I read my copy on my phone via the Bookshelf app. It was easy to browse and search through the chapters. Figures and equations were clearly rendered, with just the occasional larger table being incompatible with this viewing format.

Mark Senn
University of Warwick



News from the Cambridge Crystallographic Data Centre (CCDC)

CSD Communications help the scientific community access unpublished crystallography data

In 2021 over 5,000 new structures were published as *CSD Communications*, taking the total number since 1976 to over 43,500. We have BCA members to thank for a significant proportion of these.

CSD Communications are a way to publish structures in the Cambridge Structural Database (CSD) without an associated scientific article. The goal is to help you share your research and make more crystallographic data available to the community.

They provide:

- **Recognition:** A citable DOI allows you to receive credit for your structures and add the data to your ORCID record;
- **Discoverability:** Automatic linking via CCDC DOI from third-party repositories, such as DataCite, the Web of Science Data Citation Index;
- **Ease:** Publish data through the deposition process and update details via the "MyStructures" User Portal;
- **Integrity:** resulting CSD entry curated and enhanced by our scientific editors;
- **Cost-free:** both free to publish and free to access through our Access Structures service.

In 2021 the UK was the 4th highest country publishing *CSD Communications* and **Bill Clegg**, from Newcastle University, was one of our top depositors. A huge thank you from the CCDC to both Bill and the UK crystallography community for your contributions.

2021.3 CSD release out now

The latest CSD release, 2021.3, was launched in December 2021. It brings new features, changes to subsets, SMARTS, and SMILES, structure editing, licence management, and brand-new functionality for CSD-Theory users.

Note that this release requires a full uninstall and re-install; you cannot apply an auto-update through the software. Go to www.ccdc.cam.ac.uk/solutions/whats-new to learn more.

The CSD Data release contains 1,161,919 entries and 1,138,368 unique structures. This is an increase of over 63,000 entries in 2021, including over 400 historical entries converted from hardcopy data. Alongside all this new data, over 25,000 existing CSD entries have been improved and enhanced through our annual CSD Improvements programme, and a series of new CSD subsets included with your CSD Software Portfolio. Read the blog to learn more: www.ccdc.cam.ac.uk/Community/blog/CSD-data-update-december-2021.

Registrations are open for CCDC's 2022 webinars

Registrations are open for CCDC's 2022 What's Up Webinars which include live demonstrations of CSD software functionality and time to ask our scientists your questions. Everyone is welcome to join and learn tips, tricks and new developments in the CSD database and software - whether you're a Mercury pro or just starting out.

Learn more and register at www.ccdc.cam.ac.uk/News/Events.

Work at a non-profit, advancing science for the public benefit – now hiring!

CCDC is growing and therefore hiring for many different roles. At CCDC, we create and supply the CSD – the database system storing the world's published 3D small-molecule crystal structures. This is used by thousands of organisations in over 70 countries. We're a professional organisation, established as a not-for-profit company and registered charity. Although independent, we are a University of Cambridge Partner Institute. Roles in our science, commercial, software and support teams all offer competitive benefits and a flexible working environment which promotes collaboration and innovation.

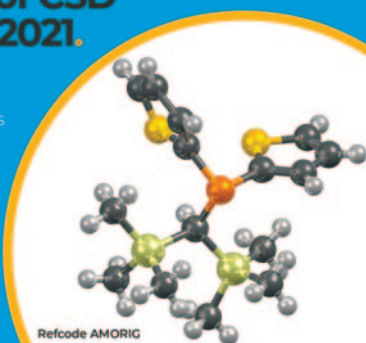
Join our enthusiastic teams and help to advance structural science. Learn more about career opportunities and apply at www.ccdc.cam.ac.uk/theccdcprofile/careers.

CCDC
Cambridge

Top BCA publishers of CSD Communications in 2021.

1. **Bill Clegg**, Newcastle University
2. **Malcolm Halcrow**, University of Leeds
3. **Paul Waddell**, Newcastle University
4. **Adrian Whitwood**, University of York
5. **Andrei Batsanov**, Durham University

CCDC



Want to share your research this way with the global community? Then go to www.ccdc.cam.ac.uk/Community/csd-communications/CSDCommunicationsInformation which includes videos and links to get started, plus more about how publishing this way can impact the wider scientific effort.



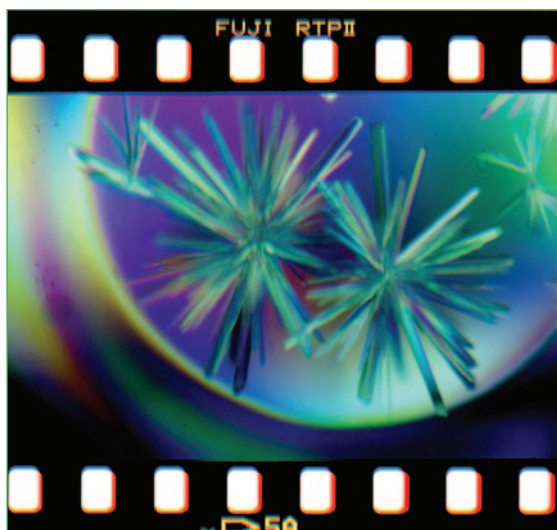
Bernard O'Hara



I first met Bernard as a newly started Ph.D. student at Birkbeck College (University of London) in 1985. He was often to be found in the evening using the precession cameras in the basement of the Crystallography Department. Upon breaking the ice (not that there ever was any with Bernard), it turned out that he was a part-time Ph.D. student who had

completed the M.Sc. in Biomolecular Organisation at Birkbeck while working full-time at the London Hospital in Whitechapel in a rheumatology laboratory. His Ph.D. project at Birkbeck involved screening for heavy atom derivatives of human serum amyloid P-component (or SAP, for short) and this meant working at weekends, in addition to weekday evenings. He impressed his supervisors (Prof. Sir Tom Blundell, Prof. Steve Wood and Prof. Sir Mark Pepys) to the extent that they offered him funding to continue his work full-time, which ultimately led to successful structure determination of this pentameric protein in the early nineties. As this was the first pentraxin protein to be solved, a major publication in *Nature* ensued (Emsley et al., 1994).

Bernard received his Ph.D. in 1992, having transferred to Prof. Laurence Pearl's group at UCL where he worked as a post doctoral research fellow on structural studies of various enzymes and transcriptional regulators, including AmiC. Bernard moved back to Birkbeck in 1999 to work with Dr Renos Savva in the newly opened Rosalind Franklin Laboratory. During work on that project he took a rather famous photograph of crystals of a DNA glycosylase bound to an oligonucleotide (see image). This image was acquired by the Wellcome Trust science images library and graced the tarpaulins over building sites at the Wellcome Trust building refurbishment and also the new entrance at Euston Square station, each several meters high.



Bernard continued his research at the Birkbeck/UCL campus well into the 2000s, working on a range of structure-based drug design projects, including one with Profs Neil MacDonald and Patrick Vallance targeting nitric oxide synthase (NOS), and gaining more publications in really top-notch journals. Bernard then accepted a managerial position at Molecular Dimensions Limited in East Anglia until family health issues led him to concentrate on being a full-time carer. I was shocked to receive the following from him in 2016: *"I should let you know that I have been unwell the past 18 months. I developed a form of facial motor neurone disease. So, life is a bit tough for me at the moment. On the positive side I have lost a lot of weight because I can't eat but I can still enjoy a beer."* It was great to see him again a few months later at the BCA Winter Meeting in 2016 held, befittingly, in the basement at Birkbeck. Alas, that was the last time we met, and I was saddened to hear that he had passed away just before Christmas in 2020, aged only 63.

This from Prof. Laurence Pearl (Sussex): *"Very sorry to hear this – Bernard was a lovely gentle and generous man with a huge passion for science. He did some great work on the AmiC-AmiR complex, which was something of a milestone at the time"*. And this from Dr Tracey Barrett (Birkbeck): *"I'm really sorry to hear this news too. I'll always remember our data collection trips to Daresbury in the late nineties"*. And from Dr Peter Rehse: *"He was one of the nicest men I knew"*.

Prof. Tom Blundell (Cambridge) recalls: *"Bernard O'Hara worked with my group in Birkbeck from 1985. He was initially a part-time student studying in the evenings for the M.Sc. in Biomolecular Organisation on which I lectured but was also Head of Department of Crystallography. He then moved to work for his Ph.D., initially part time, but then full time in a collaboration with Mark Pepys in the late 80s. We published two papers on the pentameric form of human serum amyloid P component. Initially we reported the crystallization, X-ray diffraction and neutron scattering studies (Wood et al., 1988) followed by the 3D structure defined at 2Å resolution, with Bernard's involvement (Emsley et al., 1994). It revealed a lectin-like fold and calcium-mediated ligand binding. I enjoyed having Bernard with us – he was a great member of the team. I had not realised that he had been so unwell over the past six years. I was very sad to hear of his death. I send my love and condolences to his family."*

From Prof. Mark Pepys (UCL): *"Bernard was an intelligent, charming and industrious colleague, a much-valued member of the team that solved the crystal structure of serum amyloid P component (SAP), the first member of the important pentraxin family of plasma proteins to be thus characterized. It was a seminal step towards design and development of drugs targeting SAP and the closely related C-reactive protein, clinical trials of which are ongoing. Bernard was there at the start and will always be fondly remembered for his engaging personality"*

as well as his scientific contributions. Sincere and affectionate condolences to his family.”

And finally some comments sent to one of us (JC) from Glaucius Oliva: “He was a fantastic character, highly creative and skilled in the lab., genuinely attentive and caring to his friends, always cheerful and positive about life and his work, and priceless fun when we were gathered around a few beers. During my years at Birkbeck College, Bernard, together with Richard (Garratt) and you were the mainstays of support for me, a foreign student, initially lost in London and having serious difficulties with the language. Recorded in my mind are the memorable 5-a-side football sessions at ULU, followed by cheerful stops at the ULU pub or the 5th floor bar at Birkbeck, often filled with discussions about science, politics and football. Bernard was a central character in our initial structural work with the human protein Serum Amyloid P-component, from crystallization experiments to the preparation of isomorphous derivatives of heavy atoms. After my return to Brazil, over the years, our contacts became scarcer, and I did not follow his final years with health problems in the family and his tragic passing now. I was really very sad and dismayed to learn of his death.”

Bernard was an exceptionally competent and dedicated experimentalist as well as a very active participant in the many laboratory meetings that were an important part of our formative

years. Many ex-colleagues have enduring and endearing memories of the gentle giant in the lab. and in the Birkbeck, or ULU (University of London Union), bars. He was a really nice person to know who took a serious interest in everyone’s well-being, had a charming sense of humour and remained completely amicable, both in times of genuine stress and in the good-humoured ribbing from colleagues, which he always endured with characteristic ebullience.

Above all, our thoughts are with his family at this sad time.

Jon Cooper and Renos Savva (UCL/Birkbeck)

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Graham Fisher



Credit: Barbara Fisher.

Dr Graham Richard Fisher passed away peacefully but unexpectedly on 6th December 2021, aged 70.

Graham first ventured into the world of crystallography while working at the General Electric Company (GEC) at Borehamwood, Herts/Hirst Research (HRC) at Wembley, London. He was happy with this position but desired a more challenging role so set his eyes on doing a part-time Ph.D.

course alongside his ‘day job’. Birkbeck College specialised in part-time education with the distinction of housing a self-contained Department of Crystallography which already had strong links with GEC/HRC as a user of X-ray equipment. So Graham eventually found his way to my office to enquire about starting part-time research on the X-ray topography of silicon carbide polytypic crystals which were vapour-grown by GEC/HRC.

The X-ray topographs he collected were taken on the first purpose-built synchrotron topography station at Daresbury just as it was being installed, and so Graham’s expertise in X-ray optics proved to be invaluable at this early stage of Daresbury development. He collected about 100 topographs which formed a unique database on polytypism, not to mention a clutch of publications one of which (in *Philosophical Magazine* in 1990*) has become a landmark in the field. Some Ph.D.! Yet not only did Graham achieve all of this entirely on a part-time basis: he somehow also managed to find time to give lectures on the Crystallography M.Sc. course and help students with their X-ray diffraction projects.

Graham then made a life-changing move from GEC/HRC to join Monsanto (which eventually became MEMC Electronic Materials Inc.), initially at its Milton Keynes facility as a Senior Research Scientist. This move was accompanied by a change of research direction to the production of high quality silicon wafers for the semi-conductor industry. Inevitably this required Graham to later uproot from the UK to MEMC (later SunEdison), first to the company’s Novara branch in Italy and later to its main site in Missouri in the USA. Here Graham quickly made a very positive impression for both the success of his projects and the manner in which he inspired his workforce. He rose through the ranks at MEMC, holding several positions of increasing responsibility in manufacturing and R&D, and eventually retiring as Chief Scientist and acting Deputy Director, as well as Director of Intellectual property and Director of Emerging Technologies. In addition to his ‘core’ work, he was dedicated to and promoted the company’s technical ladder program. Moreover, not only was he a Trustee of the Academy of Science of St Louis, but was also instrumental in SunEdison and MEMC sponsoring the St Louis Science Fair – one of the largest science fairs in the U.S.

He was an excellent scientist, an exceptional student, a close friend and trusty colleague and simply a great guy. I will miss him greatly.

He is survived by his wife Barbara A. Fisher.

Paul Barnes Birkbeck College

* G. R. Fisher and P. Barnes. ‘Towards a unified view of polytypism in silicon carbide’. *Phil. Mag. B*, **61**, 217-236 (1990).

Ron Patrick



I first met Ron Patrick in 1967 at Birkbeck College, London, where we shared an office in the Crystallography Department. He was studying for a Masters in Crystallography and I was beginning my Ph.D. studies.

Ron was born on 29th December 1931 in West Ham, the only child of George and Ivy. He was

educated locally and on leaving school he joined the Merchant Navy for a short period before doing his National Service as a storeman in the Army, based in Brentwood in the Essex Regiment. He always spoke of this experience very amusingly for the rest of his life.

After his National Service he studied for a B.Sc. in Physics at West Ham College, completing the course in 1959. He then worked as a lecturer in Physics and Mathematics at East Ham College, later moving to Hackney Technical College. Ron began his M.Sc. in Crystallography as a part-time student during the first year of study, but obtained sabbatical leave in order to complete the course. His classmates included John Lee, John Mason, Chris Peers and Peter Timmins and Ron's group all successfully completed their M.Sc. in July 1968.

Ron loved crystallography and stayed on at Birkbeck College to study part-time for a Ph.D., working with David Moss and

Rex Palmer, with whom he published several papers. During this period he got to know John Painter, who was in charge of maintaining the departmental X-ray sets, and learned how to repair X-ray cables. This led him to start up a company to manufacture X-ray sets for medical purposes with his wife Dorothy. The company, called Essex X-Ray and Medical Equipment Ltd, supplied high voltage cables to universities and hospitals and became very successful both here and in the U.S.A. As the business grew, Ron gave up his lecturing job and research studies in order to concentrate on his new career, in which he was very successful.

In his spare time Ron was a great fan of football, supporting West Ham throughout his life. He also loved the sound of the big band orchestras and in particular the songs of Ella Fitzgerald. I remember him walking down the corridor in the Crystallography Department humming his favourite songs by imitating the big band sound of a trumpet. He was certainly a very special person, full of energy and a great zest for life.

He died on 27 October 2021, just two months short of his 90th birthday. He is survived by Dorothy, his children Andrew and Clare and his three grandsons, Alex, Elliott and Benjamin.

Colin Reynolds
Liverpool John Moores University

Ian Forster Ferguson 1931-2022



Dr. Ian Ferguson, formerly of the United Kingdom Atomic Energy Authority (UKAEA) and one of the more prominent members of the BCA Industrial Group in its early years, died on 2nd January 2022 aged 90.

Ian was born in Liverpool in 1931 but was brought up in Southampton. He did his first

degree in chemistry at the University of Southampton before starting his work with UKAEA, where he spent his whole career. Initially Ian worked at Harwell. He then moved north to Capenhurst in Cheshire and then to Springfields in Lancashire where he spent the rest of his career.

At Springfields he was head of the Microstructural Studies Section, which used X-ray Powder Diffraction and Electron Microscope based techniques to analyse many different nuclear and non-nuclear materials. Ian contributed to 80 scientific papers on materials analysis and on computer programs for X-ray powder diffraction data analysis. He also wrote a book on 'Auger Micro Probe Analysis' which was published in 1989.

Whilst Ian was employed at UKAEA he was an external student at the University of London where he was awarded a Ph.D. in 1961. One his Ph.D. examiners was Dame Kathleen Lonsdale. His Ph.D. thesis was entitled 'The derivation of crystallite size

and shape from diffraction line profiles.' Most people will know about using the Scherrer equation to estimate the crystallite size of a material from the breadth of Bragg reflections in a powder diffraction pattern. It is also possible to determine the crystallite *shape* of a material by looking at the breadths of Bragg reflections in different crystallographic directions.

Ian retired from UKAEA in 1990 but continued to attend BCA meetings for many years afterwards, and in 1995 he won the BCA Industrial Group award.

I did my first degree in chemistry at the University of Sheffield 1981-1984. In my final year I did a single-crystal crystallography project with Dr Arnold Smith, a former secretary of the BCA. On my graduation day Dr Smith gave me a letter from Dr Ferguson who was looking for a keen young person to do some X-ray powder diffraction in his laboratory at Springfields. So in 1985 I started work with Ian: he was my first boss from 1985-1990 before I left the UKAEA to return to academia. 37 years later I am still doing X-ray powder diffraction.

I kept in contact with Ian for the rest of his life. His wife Margot predeceased him in 2017. He had 2 daughters and 3 grandchildren.

Tony Bell
Sheffield Hallam University

Meetings of interest

BECAUSE of the continued presence of the virus, some meetings may still be cancelled or postponed. At the time of writing, all the meetings listed here were scheduled to go ahead, but there may have been further changes since going to press. Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

Note that many online meetings charge little or no registration, so if there's a topic that's of particular interest but you'd rather not travel, you might check it out. Also, some meetings listed with a location may be running a mixed in-person/online format.

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

6th April 2022 - 8th April 2022

Advances in Protein Folding, Evolution and Design
Bayreuth, Germany and online.

<https://apfed22.uni-bayreuth.de/>

11th April 2022 - 14th April 2022

BCA Spring Meeting 2022

University of Leeds, U.K.

<https://registrations.hg3conferences.co.uk/bca2022>

24th April 2022 - 26th April 2022

Neutron & Muon Science User Meeting

Warwick Conference Centre.

<https://www.isis.stfc.ac.uk/Pages/NMSUM2022.aspx>

9th May 2022 - 15th May 2022

FEBS2022 Advanced Course: Probing Biomolecules with
Electrons, Phonons, Neutrons and Magnetic Spins
Spetses Island, Greece.

<https://probingbiomolecules2022.febsevents.org/tentative-programme>

31st May 2022 - 3rd June 2022

17th European Powder Diffraction Conference – EPDIC17
Šibenik, Croatia.

<https://www.epdic17.org/>

3rd June 2022 - 11th June 2022

Erice School: Crystallography under Extreme Conditions
Erice, Italy.

<https://crystalalice.org/2022/>

3rd June 2022 - 11th June 2022

Erice School: Diffuse Scattering
Erice, Italy.

<https://crystalalice.org/2022/>

5th June 2022 - 10th June 2022

28th EUACHEM Conference on Molten Salts and Ionic Liquids
Patras, Greece.

<https://euchemsil2022.org/>

9th June 2022 - 10th June 2022

Assembling Matter at all Scales
Dresden, Germany.

<https://www.max-bergmann-symposium-2022.de/>

19th June 2022 - 30th June 2022

Zürich School of Crystallography 2022: Bring Your Own Crystals
Zürich, Switzerland.

<https://www.chem.uzh.ch/linden/zsc/index.html>

26th June 2022 - 30th June 2022

FASEB Virus Structure and Assembly Conference
Southbridge, MA, U.S.A.

<https://www.faseb.org/meetings-and-events/src-events/the-virus-structure-and-assembly-conference>

3rd July 2022 - 9th July 2022

Chemistry of the Organic Solid State (ICOSS XXV)
Ohrid, North Macedonia.

<https://wp.nyu.edu/abudhabi-icoss2021/>

4th July 2022 - 6th July 2022

Emerging Inorganic Materials in Thin-film Photovoltaics. Faraday
Discussion
Bath, U.K.

<https://rsc.li/photovoltaics-fd2022>

10th July 2022 - 15th July 2022

XAFS 2022

Sydney, Australia and online.

<https://xafs2021.org/>

10th July 2022 - 16th July 2022

16th International Conference on the Physics of Non-Crystalline
Solids

Canterbury, U.K.

<https://sgt.org/mpage/PNCS16>

13th July 2022 - 15th July 2022

Challenges in Biological Cryo-electron Microscopy: Faraday
Discussion

Sheffield, U.K. and online.

<https://rsc.li/bio-cryo-electro-fd2022>

18th July 2022 - 22nd July 2022

2nd International Conference on Noncovalent Interactions
Strasbourg, France.

<https://icni2021.unistra.fr/>

29th July 2022 - 3rd August 2022

72nd ACA Annual Meeting
Portland, OR, U.S.A.

<https://www.amercrystalassn.org/future-meetings>

1st August 2022 - 5th August 2022

Denver X-ray Conference
Rockville, MD, U.S.A.

<https://www.dxcicdd.com/>

21st August 2022 - 26th August 2022

CMD29 (Condensed Matter Division of the European Physical
Society)

Manchester, U.K.

<http://cmd29.iopconfs.org/Home>

21st August 2022 - 25th August 2022

International Conference on Neutron Scattering (ICNS 2022)
Buenos Aires, Argentina.

<https://www.sni-portal.de/en/files/FlyerICNS2022B.pdf>

21st August 2022 - 26th August 2022

12th International Conference on Inelastic X-ray Scattering
Oxford, U.K.

<https://www.diamond.ac.uk/Conference/IXS2022>



Chilled Out

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Just like crystals, not all diffractometers are created equal. Whether you are interested in large or small; protein, small molecule, or materials, Rigaku has a diffractometer for you. Our lineup now includes the XtaLAB Synergy-ED, the world's first commercially available electron diffractometer giving you access to the incredibly small.

Welcome to the nano-crystallography revolution.

