

Crystallography News

British Crystallographic Association



Issue No. 161 June 2022

ISSN 1467-2790



BCA Spring Meeting 2022, University of Leeds

Spring Meeting Group & Session Reports

p6

Spring Meeting Bursary Reports

p21

BCA 2022 Poster Prizes

p25

Leeds & the Early Development of Crystallography

p27

ISIS Disordered Materials User Group Meeting

p28

Meetings of Interest

p30

*“Invaluable instrument
in pharmaceutical
process development”*



**DESIGNED BY SCIENTISTS
FOR SCIENTISTS**

Crystal
16

THE NEW INDUSTRY STANDARD

- Advanced temperature features
- Ground-breaking transmissivity technology
- State-of-the-art software
- Feedback control
- Overhead and bottom stirring

Please contact us for more information

info@crystallizationsystems.com

crystallizationsystems.com

Tel: +31 72 30 200 40

Pyrietstraat 2

1812 SC Alkmaar, The Netherlands

Follow us on  

Technobis

CRYSTALLIZATION SYSTEMS

Scientific Award 2022: Now Open!

Malvern Panalytical Scientific Award 2022



**Malvern
Panalytical**
a spectris company



Have you published outstanding research using a Malvern Panalytical solution? Send it in, and our scientists will select the best one to win **€5,000!**

Share your research publication



www.malvernpanalytical.com



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.

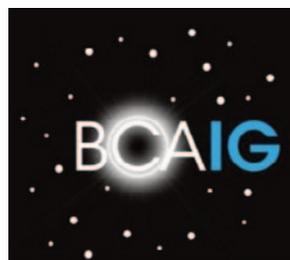
Apply early for in person attendance at international meetings.
Successful local/virtual meeting bursary winners are still eligible.

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/>



Contents

From the President	2
BCA Council 2022	3
From the Editor	4
Puzzle Corner	5
BCA Corporate Membership	5
BCA Spring Meeting Group & Session Reports	6
BCA Spring Meeting Bursary Reports	21
BCA 2022 Poster Prizes	25
Leeds & the Early Development of Crystallography . . .	27
ISIS Disordered Materials User Group Meeting	28
Meetings of Interest	30



BCA Administrative Office,

4 Dragon Road
Harrogate HG1 5DF
Tel: +44 (0)1423 529 333
e-mail: bca@hg3.co.uk

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 September 2022 issue are sent to the Editor to arrive before 25 July 2022.

Editor: John Finney
Department of Physics and Astronomy
and London Centre for Nanotechnology,
University College London, Gower Street,
London WC1E 6BT
e-mail: john.finney@ucl.ac.uk

Deputy Editor, Dave Allan
e-mail: dave.allan@diamond.ac.uk

The British Crystallographic Association is a Registered Charity (#284718)

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

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

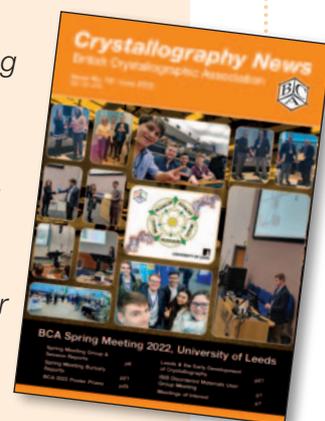
Printed by North Wolds Printers
83 Halifax Way, Pocklington Industrial Estate,
Pocklington, York, YO42 1NR
Tel: 01759 303944
Web: www.northwolds.co.uk

Honorary Life Membership of the BCA

Honorary Life Membership is the BCA's highest membership accolade. The award is made in recognition of significant contributions by the recipient to crystallographic science and to the work of the BCA. Recommendations of individuals deserving Honorary Life Membership may be made on an annual basis for consideration by Council. The President welcomes suggestions of esteemed colleagues to receive this award by the end of August, along with a short case for support of not more than 400 words.

This month's cover:

Top L-R: Natalie Pridmore presenting the Out-going Chair prize to Tom Roseveare; Hg3 staff Nicola Hardaker, Anna Whitelaw, Laura Gailuma; Bursary awardee Ben Coulson and Cardiff colleagues; Iain Oswald liberating a bottle of Tamdhu from Richard Cooper; Richard Cooper and new Honorary BCA Member Paul Raithby. Line 2 L-R: Alex Gibbs and Early Career Prizewinner Michael Cliffe; Early Career Prizewinner Hamish Yeung with CCDC sponsor Suzanna Ward; Bursary awardee Josh Morris in mid-talk. Line 3: Bursary holders Lee Birchall & Yichun Shen giving their talks. Bottom line L-R: Exhibitors, Posters and food!; the Kent delegation.



From the President



THE ship wherein Theseus and the youth of Athens returned from Crete had thirty oars, and was preserved by the Athenians down even to the time of Demetrius Phalereus, for they took away the old planks as they decayed, putting in new and stronger timber in their places, insomuch that this ship

became a standing example among the philosophers, for the logical question of things that grow; one side holding that the ship remained the same, and the other contending that it was not the same.
– Plutarch, ‘Theseus’

The British Crystallographic Association was established 1982 and – like this legendary ship of Theseus – many of its essential components have been replaced or strengthened since that time: some of our founders are no longer with us; new members have joined, organised and taken part in meetings; new groups and funds have been established to further the aims of the organisation; and, as exemplified in **Elsbeth Garman’s** BCA Hodgkin Lecture at the recent Spring Meeting, much of the technology of our crystallographic ‘pipelines’ has improved beyond what we could have predicted or imagined. Even the BCA Statutes, which ensure continuity in governance and aims of the organisation, have undergone steady clarification and improvement with the scrutiny of members at AGMs. Despite these changes, we still share an enduring belief in the value of bringing together practitioners of crystallographic science from across a range of disciplines. There are several reasons that this is important: sharing methods and practice to aid research; organizing UK and international initiatives; and education and networking for new members of the community. Each new generation of crystallographers (and users of crystallographic results) needs to learn the fundamentals of the subject and – in addition to sponsoring and organizing crystallography teaching schools – the BCA provides a network which can provide peer support to other members as they learn the ropes.

The recent BCA Spring Meeting at Leeds was the first to be held in person since 2019, and for many delegates including myself, it was our first in-person meeting since early 2020. Leeds is a distinguished location to hold the meeting, steeped in crystallographic history. William H. Bragg was Cavendish Professor of Physics at The University of Leeds in 1912 when he and his son, W. Lawrence Bragg, began interpreting X-ray diffraction patterns from sodium and potassium chloride. Later, William Astbury’s pioneering X-ray studies of proteins helped to establish the field of molecular biology as we know it today. Thank you to Programme Chair **Iain Oswald**, VP **Simon Parsons**, the Programme Committee and session chairs for organising and running an excellent programme, and thanks to Hg3 for managing the meeting and registration process with their customary proficiency. The commercial exhibition was very well attended and my thanks go to all those attending as well as to our corporate members for their continued support of the BCA. The prevailing mood amongst delegates seemed to be excitement at being back at a face to face event, while acknowledging that not everybody is ready or able to return due to differing personal circumstances. The Programme Committee were able to arrange remote video lectures for a small number of speakers who were unable to travel to Leeds,

and, as long as the right balance is achieved, and technical issues minimized, this could be replicated in future to assemble cutting-edge scientific programmes. We will continue to evaluate the possibility for future hybrid format meetings where the technology and costs allow in order to make these meetings more accessible.

I am delighted that **Helen Playford** has agreed to chair for the 2023 Spring Meeting Programme Committee, and, of course, planning is already underway. As usual, the programme will start to coalesce just as this edition of *Crystallography News* is distributed, so please send any ideas for sessions or workshops to helen.playford@stfc.ac.uk or to one of the Group representatives on the Programme Committee as soon as possible. Details of the 2023 Programme Committee are on the BCA website (<http://www.crystallography.org.uk>). The Spring Meeting will be held at the University of Sheffield from Monday 3rd until Thursday 6th April 2023, including the satellite organised and run by the YC Group on the Monday afternoon and Tuesday morning. I would strongly encourage everyone to take a few minutes to invite a few non-BCA (or lapsed BCA) colleagues or contacts to the meeting once the website and abstract submission goes live later this year. Don’t forget that bursaries are available to BCA members, so please spread the word.

During the latest AGM, there was very strong support for the idea of bidding to host a future IUCr in the UK. As I explained at the meeting, there is a long lead-time for this process, and with this mandate from the BCA we can start preparations for a bid to host a meeting in 2038 – still 16 years away! An early decision in the process is to work with our conference organisers to identify a suitable venue, but I am also open to any brilliant suggestions, so please get in touch if you would like to propose a site.

Thanks to **Elizabeth Shotton** (ex-BCA Treasurer) for passing on a box of BCA artefacts to add to our collection, including the hefty hardbound minutes of early Council meetings and AGMs. These have been reunited with a second minute book, early correspondence and copies of *Crystallography News* on a shelf in my office. There is a plan to digitize as much of this content as possible, which may begin this summer if various children don’t have alternative gainful employment. If you have any unwanted bits of BCA history (whatever happened to the famous BCA ties?) that are taking up space in your attic or office, please feel free to send them across for safe keeping.

Finally, I would like to use this column to reiterate my sincere thanks to members of BCA Council whose terms ended at the recent AGM, in particular for helping to guide the organisation through uncertain times. **Anna Warren** completed her second term as a member of Council, **Simon Parsons** reached the end of a three-year stint as Vice President and **Alex Stanley** completed a second term as BCA Secretary. I am also grateful to the newly elected members of Council for standing for election and volunteering their time and efforts: **Suzanna Ward** is our new VP, **Lauren Hatcher** takes over as Secretary and **Lucy Saunders** joins as a Council member. Turning back for a moment to my laboured Ship of Theseus analogy, the crystallographers may be replaced – but it remains the BCA Council. Let us hope that the next three years will be slightly less worrisome than the previous three.

Richard Cooper

BCA Council 2022

COUNCIL OFFICERS



President (2024)
Prof Richard Cooper
Chemistry Research
Laboratory, Mansfield Road,
Oxford, OX1 3TA
president@crystallography.org.uk



Vice President (2025)
Suzanna Ward
The CCDC,
12 Union Road,
Cambridge, CB2 1EZ
ward@ccdc.cam.ac.uk



Secretary (2025)
Dr Lauren Hatcher
School of Chemistry,
Cardiff University Main
Building, Park Place,
Cardiff, CF10 3AT
secretary@crystallography.org.uk



Treasurer (2023)
Dr Claire Naylor
SPT Labtech Ltd
treasurer@crystallography.org.uk

ORDINARY MEMBERS



Dr Lucy Saunders (2025)
Diamond Light Source,
Harwell Science and
Innovation Campus,
Didcot,
Oxford, OX11 0DE
lucy.saunders@diamond.ac.uk



Dr Cheryl Doherty (2024)
Bursary Officer (2019-present)
GSK
Stevenage
Herts, SG1 2NY
cheryl.x.doherty@gsk.com



Dr Hazel Sparkes (2023)
Department of Chemistry,
University of Bristol,
Cantock's Close,
Bristol, BS8 1TS
Tel: 0117 331 8298
hazel.sparkes@bristol.ac.uk

Elections to BCA Council

There will be elections this year for:

- **BCA Treasurer**
- **Ordinary Member**

Any two Members may make nominations, and such nominations should be accompanied by the written consent of the candidate to serve if elected. These must be received by the Secretary by 30th September 2022.

GROUP REPRESENTATIVES



Biological Structures
Dr Mark Roe
School of Life Sciences,
University of Sussex,
Falmer,
East Sussex, BN1 9RQ
Tel. 01273 678863 (Office)
Tel. 01273 872896 (X-Ray Lab)
M.Roe@sussex.ac.uk



Chemical Crystallography
Dr Gary Nichol
University of Edinburgh,
Joseph Black Building,
Edinburgh, EH9 3FJ
Tel: 0131 650 4806
g.s.nichol@ed.ac.uk



Industrial
Dr Helen Blade
AstraZeneca,
Macclesfield Campus,
Macclesfield,
Cheshire, SK10 2NA
Helen.Blade@astrazeneca.com



Physical Crystallography
Dr Helen Playford
Building R3, Room 1.22
STFC ISIS Facility,
Rutherford Appleton
Laboratory,
Didcot, OX11 0QX
Tel: 01235 446890
helen.playford@stfc.ac.uk



Young Crystallographers
Dr Anthony Blue Carter
School of Chemistry,
Science Centre South,
University College Dublin
(UCD), Belfield, Dublin 4,
Ireland
Anthony.Carter@ucd.ie

CO-OPTED MEMBERS



Programme Chair (2023)
Dr Helen Playford
Building R3, Room 1.22
STFC ISIS Facility,
Rutherford Appleton
Laboratory,
Didcot, OX11 0QX
Tel: 01235 446890
helen.playford@stfc.ac.uk



Dr Christine Beavers
Diamond House,
Harwell Science and
Innovation Campus,
Didcot,
Oxford, OX11 0DE
Tel: 01235 394038
christine.beavers@diamond.ac.uk

EDUCATION & OUTREACH

GROUP CHAIRS



Biological Structures
Dr Katherine Brown
Cavendish Laboratory,
Department of Physics,
University of Cambridge,
J J Thomson Avenue,
Cambridge, CB3 0HE
kb518@cam.ac.uk



Chemical Crystallography
Dr Michael Probert
School of Natural and
Environmental Sciences,
Newcastle University,
Bedson Building, Newcastle
upon Tyne, NE1 7RU
Tel: 0191 208 6641
Michael.Probert@newcastle.ac.uk



Industrial
Dr Helen Blade
AstraZeneca,
Macclesfield Campus,
Macclesfield,
Cheshire, SK10 2NA
Helen.Blade@astrazeneca.com



Physical Crystallography
Dr Alexandra Gibbs
School of Chemistry,
University of St Andrews,
North Haugh, St Andrews,
Fife, KY16 9ST
Tel: 01334 464212
a.gibbs@st-andrews.ac.uk



Young Crystallographers
Dr Anthony Blue Carter
School of Chemistry,
Science Centre South,
University College Dublin
(UCD), Belfield, Dublin 4,
Ireland
Anthony.Carter@ucd.ie

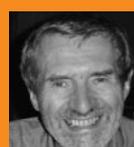
EX-OFFICIO MEMBERS



Past President
Prof Simon E V Phillips
Department of Biochemistry,
University of Oxford,
South Parks Road,
Oxford OX1 3QU
Simon.Phillips@rc-harwell.ac.uk



Webmaster
Dr Claire Hobday
University of Edinburgh,
Joseph Black Building,
David Brewster Road,
Edinburgh, EH9 3FJ
Claire.Hobday@ed.ac.uk



Editor "Crystallography News"
Prof John Finney
Department of Physics
and Astronomy and
London Centre for
Nanotechnology,
University College London,
Gower Street, London,
WC1E 6BT
john.finney@ucl.ac.uk

(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



I HOPE you agree that it's highly appropriate to celebrate the first in-person BCA Spring Meeting since 2019 with a bumper issue (and forget that the real reason might be my continuing inability to estimate space requirements...). So in this issue you will find reports of the invited and plenary lectures, the group sessions, and the various prize winners. And in

addition, the reports of the nine young scientists who were awarded bursaries.

I found these bursary reports particularly inspiring. In addition to their quality, I took particular note of the comments they made that underlined the importance of in-person conferences. This was the first in-person conference many had attended, and they emphasised the importance to them of not only the obvious point of networking, but also how it enabled them to put out their wares, and learn from others in ways that would be less effective online. As Rhona Lonergan puts it in her report: *"This gap in conferences created quite a nice level playing field as most people had either never presented a poster/talk or needed to relearn a touch as they went.... Old friends caught up on research and life side by side with the forging of new friendships as I experienced my first chance to forge academic friendships outside of my own university."* Putting these reports together made me even sadder about my having to miss both the meeting and the opportunity to meet some of these inspiring young scientists!

These comments reminded me of a recent article in *Nature*¹ that compared the relative effectiveness of virtual meetings and in-person ones in generating ideas. This study suggested that videoconferencing inhibits the production of creative ideas, and argued that "the effects are driven by differences in the physical nature of videoconferencing and in-person interactions" – for example, it focuses communicators on a screen, which prompts a narrower cognitive focus. Thus the authors conclude that virtual interaction comes with a cognitive cost for creative idea generation. I doubt this will surprise any of us, but it's good to see it confirmed by a serious study. Roll on the next in-person conference!

What you won't find in this issue in the following pages are any obituaries. Unfortunately, this is not because there have been no sad losses to crystallography in recent months – there have indeed been a number of eminent colleagues who have left us.

Two of these losses – Ken Holmes and Don Caspar – hit home particularly to me partly because they had preceded me at Birkbeck, but also because they had both made major contributions to our understanding of virus structure. Ken worked with Rosalind Franklin and Aaron Klug at Birkbeck, where he was awarded his Ph.D. for work on the structure of Tobacco Mosaic Virus (TMV). He moved on to the LMB in Cambridge where he advanced X-ray fibre diffraction in the study of muscle. Following a move to Heidelberg in 1968, he began to pioneer the use of synchrotron radiation as an X-ray source, founding with Gerd Rosenbaum the EMBL site at DESY Hamburg, where they built the first DESY X-ray beamline. As the obituary on the EMBL website says²: "His seminal visions opened a completely new field in the life sciences and

has become a main driver to build most powerful synchrotrons around the world, allowing to determine hundred thousands of structures of biological samples at atomic resolution".

Don Caspar also did early work on virus structures, with his Ph.D. also being on the structure of TMV. He then also spent some time at the LMB where he showed that the protein coat of spherical viruses was made up of identical subunits arranged in equivalent ways. He demonstrated that tomato bushy stunt virus had icosahedral symmetry (it soon becoming clear that so did many other viruses), and working with Aaron Klug at Birkbeck resolved an apparent conflict with biochemical data, through introducing the idea of quasi-equivalence – the concept that equivalent protein subunits could vary slightly in order to tightly seal the viral shells. In 1956 he and Rosalind Franklin published back-to-back papers³ on the location of viral RNA, so marking a friendship with Franklin during her last two years.



Ned in a comfortable environment.
Credit: Bill Duax.

The third scientist I'd like to remember was a very different person. I first met Ned Seeman in 1970 when I spent a year in George Jeffrey's Pittsburgh lab. (who also, incidentally, spent some time in Leeds with Gordon Cox). Ned was not your 'normal'

scientist, as Phil Ball's *Nature* obituary⁴ strongly hints (on his time spent at SUNY Albany, he is quoted as saying "The only thing worse than looking for a job was finding this one"). I'll leave it to Phil Ball's article to set out his ground-breaking work on designing and building programmable DNA nanostructures and nanomachines (an idea typically that came to him while sitting in a bar) and for which he was awarded the 2010 Kavli Prize in nanoscience. I'd like just to relate a couple of personal notes from my friendship with him. Brought up in the city of Chicago, Ned was very much a city kid, only comfortable in an urban environment. So when he stayed with us for a few days following the 1975 IUCr Congress in Amsterdam, he was very noticeably highly uncomfortable in the rural Berkshire environment where I then lived. Waking up one morning there was a clip-clopping on the lane. Ned, in unbelieving tones in a strong Chicago accent: "Is that a *real live horse*?!" He really was out of his comfort zone – until we took advantage of the three pubs within walking distance.

He has left us too early. He may have been called contradictory things like gruff and caring, vulgar and articulate, stubborn and visionary. But he was indeed a visionary whose presence I'll miss.

John Finney

References:

1. M.S. Brooks & J. Levav: 'Virtual communication curbs creative idea generation'. *Nature* **605**, 108 (2022). <https://www.nature.com/articles/s41586-022-04643-y>.
2. <https://www.embl.org/news/alumni/ken-holmes/>.
3. D.L.D. Caspar. *Nature* **177**, 928 (1956); R.E. Franklin. *Nature* **177**, 928 (1956).
4. P. Ball. *Nature* **600**, 605 (2021).



Puzzle Corner

THIS month's puzzle is based on the "connecting wall" in the TV quiz show "Only Connect". The objective is to find four groups of four, with something connecting those in each group.

SEVEN	SYNTHESIS	TRI	SHEEP
MONO	DENTAL	JAIL	MONASTIC
BIOLOGICAL	TRANSFORM	SERIES	FIVE
OUT-PATIENT	BLIND	UNIT	ANALYSIS

Answer to March's puzzle:

1. In Schoenflies: I_h . Possible Hermann-Mauguin symbols are: $m35$, $m5$, $m5m$, $53m$.
2. R3m with hexagonal closest packing and a hexagon normal to the z-axis.
3. Since 1970, when the design was officially approved for the World Cup.
4. This work is often known as the 'Great Mass in C'. Work it out from that!

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.

Corporate Members:

Bruker: <https://www.bruker.com/>

CCDC: <https://www.ccdc.cam.ac.uk/>

Douglas Instruments: <https://www.douglas.co.uk/>

International Centre for Diffraction Data: <https://www.icdd.com/>

Malvern Panalytical: <https://www.malvernpanalytical.com/en/>

Molecular Dimensions: <https://www.moleculardimensions.com/>

Oxford Cryosystems: <https://www.oxcryo.com/>

Rigaku Europe: <https://www.rigaku.com/division/rigaku-europe-se>

SciMed: <https://www.scimed.co.uk/>



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 Group and Session Reports



AT LAST! We met in person at Leeds – where much early crystallography was done (see the two articles on page 27).

As usual, the report of the meeting starts with the Young Crystallographers' Satellite Meeting, leading via the Lonsdale Lecture to the Main Meeting, where, following the Hodgkin Lecture, the reports are arranged by BCA group in random order. Prize lectures follow, before the reports of bursary holders and the poster prizewinners.

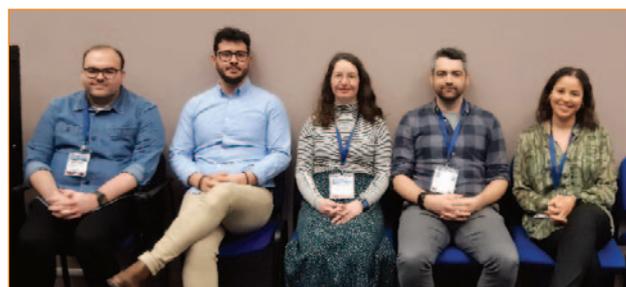
Enjoy!

YCG Satellite Meeting

Following two years of disruption, the YCG Satellite Meeting was held at the University of Leeds. As a member of the 2019 planning meeting, it was strange to be returning to a venue much later than the schedule on-site meeting in 2019. Nevertheless, it was good to have the opportunity to host an in-person meeting and great to be able to talk about science without too many technical issues.

The first day's sessions started with our first plenary speaker of the day **Claire Hobday** (University of Edinburgh) who spoke about some recent work focusing on materials with a barocaloric response and the use of the CSD to identify previously reported materials of interest. This session then featured four oral contributions from YCG members starting with **Emily Meekel** (University of Oxford) who has been exploring the use of 1,3-benzenedicarboxylic acid in the construction of Zn-based metal-organic frameworks. The second talk was from **Martin Ward** (University of Strathclyde) who highlighted ways that mechanochemical screening can be used to further understand the structural properties of multi-component forms of an anti-inflammatory drug. This talk was followed by a presentation from **Mario Falsaperna** (University of Kent) who spoke about some recent neutron diffraction studies of a 2D layered material which is of interest due to its magnetic properties. The session was concluded with a talk from **James Osbourne** (University of Liverpool) who spoke about using machine learning as a tool in processing powder diffraction data, a method which will be crucial when tackling the data generated through the use

of automation within solid form reactions such as mechanochemical screening.



Session 1 speakers (L-R): James Osbourne, Mario Falsaperna, Claire Hobday, Martin Ward and Emily Meekel.

The second session featured four early-stage crystallographers presenting their recent work. The first talk was presented by **Atika Al Hasaini** (University of Edinburgh) who spoke about her recent work on applying electric fields during crystallisation of proteins and how this effects the crystal growth. The second presenter (**Josh Morris**, Cardiff University) spoke about his recent interest in photoactive materials and how using a recently developed *in situ* stage at I19 (Diamond Light Source) can be used to further understand these materials. This talk was followed by **Cameron Wilson** (University of Edinburgh) presenting some work, in collaboration with the Cambridge Crystallographic Data Centre, developing a program which, through a more detailed analysis, allows for better characterisation of pressure-dependent transitions that may

have been previously overlooked during high pressure studies. The final speaker in this session was **Muzi Chen** (ICL) who presented some recent *in situ* temperature and pressure neutron diffraction studies on a series of rutile analogues which display both negative thermal expansion and negative linear compressibility.



Session 2 speakers (L-R): Cameron Wilson, Atika Al Hasaini and Josh Morris.

The final speaker session of the day started with an interesting talk on post-perovskite frameworks and their magnetic properties presented by **Madeleine Geers** (University of Nottingham). The magnetic properties were, in part, explored using both single crystal and powder neutron diffraction experiments. The second speaker was **Rhona Lonergan** (University of Kent) who spoke about developing accelerated contact ageing and the importance humidity played in these contact reactions. This presentation was accompanied by highlighting the similarities between the final products and the shapes observed in popcorn. The final speaker in this session was **Lewis Clough** (University of Edinburgh) who spoke about exploring the properties of a Blatter Radical as well as performing high pressure diamond anvil cell experiments on beamline I15 at Diamond Light Source.



Session 3 speakers (L-R): Lewis Clough, Rhona Lonergan and Madeleine Geers.

This session was followed by a series of flash presentations from conference attendees who were presenting posters. The day's sessions were concluded with a poster session where attendees could discuss their recent work.

Day two commenced with the Parkin Prize Lecture, a prize lecture awarded to a member of the community who has been actively involved in public engagement. This year's lecture was awarded to **Alex Tansell** (University of Warwick). Alex, who has a background in crystallography, spoke about his deviation from active research and pursuing a career in engagement and outreach. He spoke about the importance of engaging in outreach and provided some advice for getting involved both locally and nationally. This advice included not being shy to ask around your institution to see what you can get involved in.

Alex also discussed the need to take activities to the public rather than waiting for them to come to you, as well as highlighting some national organisation that you can get involved with.

The Prize Lecture was followed by four oral contributions from early career researchers. The first of these speakers was **Peter Smyth** (University of Kent) who spoke about work, in collaboration with beamline I24 (Diamond Light Source), on developing and performing laser-initiated time-resolved serial crystallography as a means of exploring NO binding within cytochrome $c'-\beta$. In the following talk, **Yitian Xiao** (University of Manchester) spoke about using both computation and neutron total scattering to understand hydrate formation of an antihistamine drug within a solution mixture. This was followed by a talk by **Elizabeth Galtry** (University of Nottingham) who has been developing, in collaboration with beamlines I11 and I19 (Diamond Light Source), a segmented flow continuous crystalliser. This plans to use temperature controls as a means of optimising crystallisation, but also to probe the segments crystallographically while running in flow. The next talk from **Arianna Minelli** (University of Oxford) discussed her recent work on a charge density wave phase of a Krogmann's salt. This session, and the overall meeting, was concluded with the second plenary talk presented by **Sam Horrell** (Diamond Light Source). Sam started with a crowdsourced (via Twitter) '10 things your Beamline Scientist wished you knew', including Diamond's recent revision of their Covid snack policy. The second half of Sam's talk involved demonstrating some of the recent developments on beamline I24, including some recent developments in exploring photoactivity.



Final Session speakers (L-R): Yitian Xiao, Elizabeth Galtry, Alex Tansell, Sam Horrell, Arianna Minelli and Peter Smyth.

All in all, the YCG Satellite Meeting was a good demonstration of the broad research interests of the early career researchers within the BCA. Being fortunate to meet in person following two years of largely virtual attendance was a great opportunity to discuss a wide variety of research topics, and the group looks forward to welcoming attendees to the 2023 meeting in Sheffield.

Tom Roseveare
University of Sheffield

Continued overleaf.

YCG+ Careers Session



Claire Hobday, Andrew Goodwin, Sam Horrell, Chris Frampton. Helen Blade appeared on the big screen above the group!

The session started with each of the five panellists: **Sam Horrell** (Diamond Light Source), **Claire Hobday** (University of Edinburgh), **Andrew Goodwin** (University of Oxford), **Helen Blade** (AstraZeneca – appearing remotely) and **Chris Frampton** (Rbar3 Ltd) giving an overview of their career paths to date before an open Q&A with the audience. This highlighted that there is no one route that has to be followed and that rejection/things not working out as you expected is part of life and should be seen as an opportunity to reassess, rather than a negative to be dwelled on. For example, Claire and Sam discovered they had both applied for things that the other had been the successful candidate for; Andrew changed his Ph.D. after realising novel synthesis was not the right fit for his skills; Helen now works in pharmaceuticals, despite her Ph.D. being in batteries science and Chris highlighted that even if you are in the fortunate position of having multiple job offers, it still may not work out as you expected but taking a new route can be beneficial.

During the session, a wide range of topics were discussed, including the benefits of taking advantage of opportunities to branch out into different areas and how the multidisciplinary nature of crystallography can help facilitate this. For example, BCA meetings provide opportunities to go to talks and chat to people from different areas to help improve your knowledge and make contacts outside of your area of expertise. The importance of making contacts, having good support, making yourself visible and collaborating, were all strong themes that came out of the discussion.

Another key theme was the importance of being happy overall in your job and that if you are not, you should not be afraid to seek a positive change and if necessary go elsewhere. While it may not always seem like it is that simple, the panel all strongly emphasised how much of a difference being happy in your job makes to your overall wellbeing and how important that is.

Many other topics, including misconceptions about your amount of freedom in industry, the positives of academia and the difficulties and impact on relationships/family of potentially having to move every few years were all also discussed.

Overall, the session was a very useful opportunity to hear the experiences and resulting advice from crystallographers in a range of fields, roles and career stages.

The following key tips and advice came out of the discussions:

- Go to conferences, network, give talks, get involved in committees/chairing sessions – it is good experience and gets your face known.
- Use mentoring schemes available and discuss with your supervisor whether there are opportunities to do extra activities to develop skills relevant to your next career step.

- The area of your Ph.D. does not have to determine the field you end up in; the building of scientific/research skills is the most important part and is transferable.
- Don't stay in a job/career if you are unhappy with it – no job is for everyone.
- Collaborate whenever you can (both within your institution and externally).
- Take advantage of opportunities to learn new skills, especially earlier in your career.
- It is important to have frank discussions with your partner about career decisions and moving. Draw clear lines together and weigh up the importance of each opportunity as it arises.

Natalie Pridmore
University of Bristol

Lonsdale Lecture

The Lonsdale Lecture celebrates the work of the late Dame Kathleen Lonsdale. It is awarded by the BCA on the advice of the YCG. Typically, this prize lecture is presented at the start of the Spring Meeting following the YCG Satellite Meeting. The presentation is an opportunity for the speaker to present on a range of topics with an educational perspective in mind.

It is particularly appropriate to give the Lonsdale Lecture in Leeds, as Kathleen spent some of her early years there, and it was where she settled the long-standing argument about the planarity of the benzene ring (see later article on page 27).



Andrew Goodwin (right) receiving the Lonsdale Prize Lecture certificate from Tom Roseveare (left).

This year's Lonsdale Lecture 'Disorder By Design: from form to function' was presented by **Andrew Goodwin** (University of Oxford) who discussed a variety of ways that disorder can be explored and applied in order to control a material's property. First, Andrew briefly commented on Kathleen Lonsdale's career and her broad interest in crystallography, allowing a range of topics to be covered in a prize lecture such as this. One aspect of Kathleen's career that Andrew focused on was her awareness of the aesthetic quality of the repeating patterns in crystallography which surpass its primary audience. This was demonstrated by her involvement in the 1951 Festival of Britain Pattern Group, which produced a range of textiles, wallpaper and ceramics inspired by diffraction data resolved by crystallographers based in the U.K. It is this aesthetic link that has often led to the collaboration between art and science. The connection between art and crystallography was also highlighted later in the Hodgkin Lecture by **Elsbeth Garman** (University of Oxford), who spoke briefly about Angela Palmer's sculpture '2020: The Sphere that Changed the World' that was on display at the Oxford University Museum of Natural History.

Following a brief discussion of Kathleen's career, Andrew spoke about a series of key research works that explore designing disorder. The first considers shape, and how the simple 3D building block pre-determines the type of a material that shape would produce. The second is a simpler example where the target shape is a tile that has functional groups on its edges that form intermolecular interactions. This then led to considering those shapes with favourable interactions on specific edges. The type of functional group and intermolecular interaction on each edge can, in turn, result in multiple possible tile orientations relative to neighbouring tiles. Ultimately, the degeneracy in tile orientation results in disorder by design. This work echoed the aesthetics observed in the patterns produced by the Festival of Britain Pattern Group.

Following the demonstration of using shape and function as a means of controlling disorder, Andrew went on to demonstrate how these features can be linked to properties of the material. His talk nicely echoed Kathleen's own comments in Chapter 14 of 'Fifty Years of X-ray Diffraction' (P.P. Ewald, 1962):

"Nowadays X-ray crystallographers, particularly if their basic training is in chemistry, study the dynamics of crystals; but only because they must. In order to refine the structure of an organic compound to the point where accurate bond lengths and angles are obtainable it is necessary to find and to make allowance for the anisotropic atomic thermal vibrations. To the early research workers, as also to the crystallographer-physicist of today, the interest is in the dynamics itself, and in its relation to a host of independent physical properties."

Andrew's talk demonstrated that understanding and controlling dynamics and disorder within crystalline materials can lead to a variety of properties. Andrew also discussed some practical ways in which it is possible to record and characterise disorder within a crystalline lattice.

Tom Roseveare
University of Sheffield

Hodgkin Lecture



President Richard Cooper with Elspeth Garman.

Elspeth Garman (University of Oxford) delivered the 10th BCA Hodgkin Lecture: 'Macromolecular Crystallography 112 Years A.D. (After Dorothy)' on the Wednesday afternoon. The Dorothy Hodgkin Prize was established by the BCA to celebrate Dorothy's 80th birthday and to recognise her contributions to crystallography and science. Awardees generally 'work in an area of crystallography in which Dorothy had an interest'.

Prof. Garman's lecture was organized around five stages of the macromolecular crystallography pipeline and contrasted the latest methods with those that Dorothy Hodgkin would have used. The first step in the modern pipeline, just as it was then, was to obtain sufficient protein to study. Modern protein expression and purification technology produce concentrated pure protein ready for crystallisation, but in earlier times this had to be obtained and extracted from heaps of animal and vegetable matter. The crystal growth step is now managed by automated pipetting, crystal hotels and imagers, and in much smaller volumes than previously possible. Elspeth noted a 1934 paper (Bernal & Crowfoot, *Nature* **133**, 794, 1934) which reported the benefits of maintaining crystals in contact with the mother liquor from which they were grown, which was essential to maintain crystal quality before low temperature data collection was possible, and without which the whole field of macromolecular crystallography would not have taken off as it did. The progress in X-ray sources for data collection was illustrated with photos of Dorothy's lab. in 1941 where datasets would take 3 weeks to collect, via Elspeth's rotating anode at LMB Oxford, to synchrotrons and XFELs.

Accompanying these steps forward has been a considerable increase in damage to samples by the X-ray photons and Elspeth discussed her wide-ranging research on radiation damage to samples, which includes quantifying radiation dose, modelling data collection strategies, and understanding radiation damage mechanisms. The increase in computational resources since Dorothy's early work has also had a profound impact on solution, modelling, refinement and visualisation of structures.

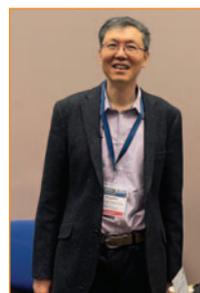
Finally, Elspeth introduced the B_{damage} and B_{net} metrics based on analysis of B factors corrected for local packing density. For any PDB structure, B_{net} can indicate the extent of radiation damage that has occurred during an X-ray data collection, and structures with high B_{net} show clear signs of radiation damage in their electron density (Shelley & Garman, *Nature Comms* **13**, 1314, 2022).

Elspeth concluded the Hodgkin Lecture by arguing that there are undoubtedly more changes ahead for macromolecular crystallography, with developments in serial X-ray crystallography, cryo-electron microscopy, and improvements in protein structure prediction all feeding complementary information into the evolving MX pipeline.

Richard Cooper
University of Oxford

Industrial Group

This year the Industrial group organised two sessions and one plenary lecture.



Plenary speaker Ping Xiao

IG Plenary

Professor Ping Xiao from the University of Manchester gave an excellent Plenary Lecture on the 'Measurements of Residual Stresses in Thermal Barrier Coatings'. He first introduced the concept of Thermal Barrier Coatings (TBCs), which are coatings that are applied to turbine blades in aeroplane engines and provide a protective coating that allows the engines to operate at higher temperatures, increasing their efficiency.

Repeated heating and cooling of the engines during normal flight operations creates stress, which can cause the coating to crack or fracture; therefore the coating needs to be monitored to prevent failures. Professor Xiao then described how he has used X-ray diffraction (amongst other techniques) to examine stress in thermal barrier coatings to ensure they never fail.

Parallel session 1. Metallurgical and other Applications (Chair **Judith Shackleton**).



Session 1 speakers (L-R): Judith Shackleton, Tony Fry, David Asquith, Joe Kelleher.

Dr Joe Kelleher (Rutherford Appleton Laboratory): ‘Engin-X Particle size effects in engineering diffraction spectra: mitigation and exploitation’. Time-of-flight neutron diffraction is a very useful technique to determine size and strain and broadening from diffraction data, which is not always possible from other diffraction experiments. This was illustrated by diffraction spectra collected on graphite. **Dr David Asquith** (Sheffield Hallam University): ‘Residual stress, preferential orientation, and cyclic loading in shot-peened aluminium’. Cold work induced residual stresses are used to influence the fatigue life of strain hardening metals. Dr Asquith discussed two different aluminium alloys that were studied to enable a mechanism for this process to be proposed. **Tony Fry** (National Physical Laboratory): ‘Measurements of Residual Stresses in Industrial Applications’. Advances in residual stress measurements have now made this technique increasingly useful. Examples were given of how this technique was used in industrial applications.

Parallel session 2. Industrial Crystallography: Changes and Challenges (Chair **Tony Bell**).



Session 2 speakers (L-R): Tony Bell, Jeremy Cockcroft, Robert Carroll, Simon Coles.

Prof. Jeremy Cockcroft (UCL): ‘The changing face of X-ray crystallography, are we keeping up-to-date?’. Professor Cockcroft talked about how advances in crystallographic

technology are not being kept up with in the way the subject is taught. The pitfalls and errors in this process were illustrated with examples from industrial patent litigation. **Prof. Perumala Venkata Sunder Raju** (CSIR, NGRI, Hyderabad, India): ‘Comparisons of Powder X-ray Diffraction patterns using NIST Standard Reference Materials (SRMs) vis-à-vis Natural Samples – Pros and Cons’ (virtual presentation). XRD data were collected on NIST SRMs 660 (LaB₆) and 675 (Mica) and were compared with XRD data from natural mineral samples from India. **Robert Carroll** (University of Southampton): ‘Developing the application of the Crystalline Sponge Method’. The Crystalline Sponge method is a great help in determining crystal structures as it removes the need for crystallisation. Instead, a porous crystalline MOF is used to capture the material of interest. Standard single-crystal XRD is then used to determine crystal structures. Robert showed how this method has been extended, giving examples of crystal structures of novel biaryl molecules. **Prof. Simon Coles** (University of Southampton): ‘Advanced crystallographic techniques for the UK research community’. The National Crystallography Service has been operating for over 40 years. It has recently been expanded with Newcastle University joining the service with Southampton University. Professor Coles talked on how this service, originally intended for academia, is now being expanded to include industrial customers.

This year’s Industrial Group Poster Prize went to **Jessica Metherall** (University of Newcastle) for her excellent poster on ‘High-Throughput Crystallisation of Organic Acids’. Thanks to *Natalie Johnson* for the photographs.

Tony Bell, Sheffield Hallam University
Natalie Johnson, CCDC
Judith Shackleton, ex Rolls-Royce; now retired

Biological Structures Group

The **BSG Plenary** (Chair **Kate Brown**, University of Cambridge) was given by **Randy Read** (University of Cambridge) on ‘Structural biology in a post-AlphaFold2 world’. Randy started by introducing protein structure prediction and then showed how there was a leap in performance with the introduction of AlphaFold (AF1) in 2018 and then a second leap with AlphaFold2 (AF2). The performance of these programs can be measured by the CASP tests (Critical Assessment of Structural Prediction), now in their 14th iteration. CASP14 ranked by reLLG score shows that AF2 is 15x better than every other technique. Almost all tests that had diffraction data could be solved by using the AF2 model in molecular replacement. RoseTTAFold also implemented ideas from AF1 and was able to solve three out of three structures that could not be solved by any other methods.

So how does the deep learning work? Neural networks are good at finding hidden patterns in data and we now have a massive amount of data to train on. First, a deep multiple sequence alignment is carried out to infer contacts from evolutionary covariance. Next, a model is built that uses this information. These two steps are then iterated to learn which covariances deserve the most attention. AF2 and RoseTTAFold are available for use free of charge, so anyone can now do protein structure prediction. The AF2 database at the EBI covers 90% of all proteins that have been sequenced. The remaining limitations of these programs are now being addressed (multimers, RNA structures, carbohydrates and

ligands). There will still be limitations: for instance AF2 knows nothing explicitly about physics and chemistry (no way to account for pH, ions, ligands, disease mutations, no insight into the folding process itself). But it is still good for other things – one can use AF2 for informing construct design or one can use the AF2 model to check that the sequence assignment in structures in the PDB is correct. AF2 can still be made better by retraining with quality-filtered data, generating more robust multimer models and running new tracks in the machine learning modes.



BSG Plenary Speaker Randy Read (right) with Session Chair Kate Brown.

The keynote for the **RNA-Protein Interactions** session (Chair **Fred Antson**, University of York) was given by **Max Wilkinson** (LMB, Cambridge) with a talk entitled 'A movie of splicing from Cryo-EM snapshots of the spliceosome'. Max started his talk by giving a tribute to Kiyoshi Nagai who passed away in 2019. He went on to show a full movie of the pre-mRNA splicing process. Splicing is the removal of non-coding region of exons. The group managed to make Cryo-EM structures for each step. The first step after the whole complex is assembled is to rearrange to bring the branch point Adenosine near the 5' splice site and create the active site. Once the 5' splice has occurred, several proteins leave to allow the 3' site to enter the active site and the Adenosine can attack to release the intron and splice together the exon (for a movie search 'nagai group splicing'). He finished by showing in detail how they solved each structure with an example of the C-complex. The C-complex seems to be a stable intermediate as it often accumulates in preparations of other states. Merging many datasets and by using focussed refinements on each subunit improved the resolution from 3.8Å to 2.8Å. They found two subunits that hadn't been discovered before – these were subunits used later in the cycle. He explained that they are probably pre-bound to speed up the exon ligation process.

The next talk was given by **De-Sheng Ker** (University of York) on 'The CryoEM structure of the Nipah virus nucleocapsid assembly'. Nipah virus was first discovered in 1999 and has a fatality rate of 40-75%. Currently there is no effective treatment. It is an ssRNA virus, the RNA being wrapped in a helical nucleocapsid protein at all times to protect it. The structure of the RNA-free nucleocapsid monomer is known, but not that of the full virus. After purifying the virus through SEC from *E.coli*, the EM data separates into two assemblies, spiral and clamshell. After much post-processing a 3.8Å structure of the spiral form was obtained. The RNA was found to bind between N- and C-term domains of the nucleocapsid protein, each monomer binding six bases, three binding inwards to the protein and then three out into solvent. Comparison of RNA free and bound structures show a nearly 30° relative rotation of C-term

to N-term of the protein. The '3in-3out' is a conserved binding mode in negative strand RNA viruses. The clamshells (35% of particles) proved to be RNA free and have a slightly different assembly to the published RNA free structure.

The third talk was from **Atlanta Cook** (University of Edinburgh) on 'Understanding RNA-protein interactions of SSD1, a pseudonuclease important in fungal virulence'. SSD1 is a known virulence factor for pathogenic fungi, which kill 1.6M people a year. It is required for tissue invasion by fungal hyphae and loss of SSD1 makes cells susceptible to cell wall stress. SSD1 is related to RNases, but is not itself an active nuclease. Analysis shows SSD1 binds to 5' UTRs of mainly cell wall biogenesis factor transcripts on specific, conserved bipartite sequences. The group managed to solve the structure to better than 2Å. The ancestor protein is a 3' nuclease, requiring the RNA to enter into the centre of the protein. In SSD1, this channel is blocked by loops. Surface analysis showed a large conserved region with a positive patch and mutations in this region showed large effects on binding and this loss of RNA binding equates to loss of SSD1 function in cells.

The last talk was by **Chris Hill** (University of Cambridge) entitled 'Structural and molecular basis for Coronavirus 2A protein as a viral gene expression switch'. Viruses can code more than one protein from the same strand of RNA, by frameshifting. In coronaviruses there is a frameshift site between proteins 2A and 2B, which switches protein production as the 2A protein concentration increases. Analysis showed that the spacing of the sequences is not quite correct for frameshifting and the 2A protein is required also for this process to occur. 2A had no known structure and no homology to anything known. The structure was finally solved from SeMet data to 2.5Å, revealing a novel fold (seven stranded curved beta sheet, supported by an alpha helix either side). Conservation analysis highlighted an Arg loop in 2A which proved to be important for binding to RNA. The protein binding adds extra stability, allowing the frameshifting that would otherwise not happen by pausing the ribosome long enough for the shift to occur.



RNA-Protein Interactions session speakers (L-R): Atlanta Cook, De-Sheng Ker, Fred Anston, Chris Hill.

The keynote for the **Correlative Tomography** session (Chair **Maria Harkiolaki**, Diamond Light Source) was given by **Peter Sadler** (Warwick) on 'Correlative synchrotron X-ray imaging of metal anticancer complexes in cancer cells'. Around 50% of chemotherapies use Pt drugs – we would like to find other metals that may be better and can circumvent resistance. Peter was looking at Os²⁺, Ir³⁺, Pt⁴⁺ which are all low spin d6, so kinetically inert, thus likely to get to the cancer sites before being broken down. He showed an example of an organo-osmium azopyridine iodide (FY26) which was highly active against cancer cells, but the molecule should be inert – so

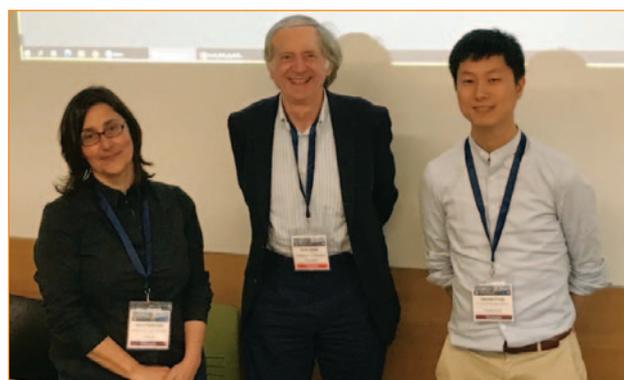
how was it working? By using radioactive Iodine, it can be shown that the Iodine comes off the complex very quickly in the cell, probably due to attack by glutathione on the organo-ligand, which then rearranges and loses the Iodine. A second example used nano-focus X-ray fluorescence to locate metal ions in the cell – Os is seen to be located in the mitochondria, while Zn is in the nucleus. He showed a chiral Os catalyst which could reduce pyruvate to the unnatural D-lactate, which killed the cancer cell. The stability of the catalyst could be studied by adding a Br to the ligand and using the X-rays to see if the metal and ligand stayed together in the cell. Lastly, he showed examples of photoactivatable chemotherapy (PACT) which use cell sensitisers. These are Ir compounds. They enter the mitochondria and after illumination with blue light the mitochondria are 10 times smaller (damaged), thus killing the cell.

Next was **Herman Fung** (EMBL, Heidelberg) with a talk on 'Cellular imaging by cryo 3D correlative light and electron tomography: advances in automation and in-cell labelling strategies'. Cryo-ET imaging can be done but only if the sample is thin enough (<200nm) – usually focussed ion beam milling of frozen samples needs to be used to get thin enough samples. To make sure that the molecule of interest is still in the part of the cell that is left after the milling, one needs to use fluorescent beads to delineate the correct milling procedure. This used to be done manually but this is slow – therefore Herman has automated much of the work to make it faster. The current limitations are mainly deformations of the grid itself (up to 2.5µm) which lead to localisation errors. He showed that labelling the molecules of interest directly with ferritin or GEM (genetically encoded multimeric) allows them to be seen in the Cryo-ET data.

Lastly **Ramona Duman** (Diamond Light Source) gave a talk on 'Using tomography for absorption corrections of long wavelength X-ray diffraction experiments'. Ramona first showed the I23 beamline, an *in vacuo* long wavelength beamline (1.5-5Å), which is used for SAD/MAD phasing based on S/P/Ca/K/Cl and also for element identification of ions in structures. Long wavelengths are needed to access the K edges of these light atoms and absorption of X-rays is wavelength dependent (increasing with λ^3), so for long wavelengths this is a problem. The experiments are done in vacuum to avoid air absorption, but the crystal needs a proper analytical absorption correction. On I23 they use tomography to give accurate measurements of the crystal with which the absorption for every diffracted beam can be calculated and these are then applied to the collected data. She showed an example of a low symmetry membrane protein (low symmetry means the empirical methods don't work so well) and showed that this was very important for data collected beyond 2.75Å.

The scheduled talk from **Paul Verkade** (University of Bristol): 'What? Actin inside microtubules?', was unfortunately not possible due to technical problems.

The **Electron Diffraction** session (Chair **Peijun Zhang**, Diamond Light Source) started with **Tim Gruene** (Vienna, Austria) with his talk 'Instrumental requirements for electron crystallography are less demanding than you might think'. Tim started by showing that a diffractometer for ED is very similar to that for XRD – the only difference being wavelength (0.5-1.5Å X-ray, 0.01-0.03Å ED). Data are collected in rotation mode on an area detector with the crystal mounted on a goniometer. The method requires a stable rotation range of 150° or so with a 0.5µm beam. In diffraction mode the beam movement is much less than for imaging mode – thus requirements are not



Correlative Tomography session speakers (L-R): Maria Harkiolarki, Peter Sadler, Herman Fung.

so stringent as manufacturers stipulate for EM. The source doesn't need to be too strong – a LaB6 source is fine. The best detector is a Jungfrau (charge integrating, not photon counting) made for FELs, but suitable for ED – very good for very strong spots and very low noise. Electrons interact very strongly with matter, thus the crystals must be very thin ($\leq 1\mu\text{m}$) and one must remember that the ionic scattering factors are very different due to the charge on the electron. He showed that ED can do everything SXR can do and that ED is more powerful for determination of absolute chirality and oxidation states. Also, with very small crystals ED will give more data than even the strongest synchrotron sources can and it is possible to collect many datasets from the crystals on the grid very quickly and then choose the best.

Next **Tarik Drevon** (Research Complex at Harwell) gave a talk on 'Dynamical Diffraction of High Energy Electrons by Light Atom Structures'. In ED, you often get multiple scattering. If inelastic scattering is considered, the order of scattering events is very important. If one could model these better, this should lower the high R-factors seen in ED. He used the T-matrix to solve Schrödinger's equation for the diffraction. To do this he had to make a few assumptions – e.g. atoms are spheres. The T-matrix is a representation of all the interactions between pairs of atoms. Further work still needs to be done to include inelastic scattering and functions more suited to the atomic electrostatic potential.

Next, **Fraser White** (Rigaku) introduced 'The XtaLAB Synergy-ED' and showed some results. The software running the ED machine is very similar to the X-ray software and so familiar to everyone. As of April 2022, 160 structures have been determined in-house from a wide variety of samples.

Courtney Lendon (University of Exeter) then gave a talk on 'The experience of using Micro-ED as non-experts'. She showed that one can use crystals that would otherwise be ignored as failed experiments. The data collection is done in minutes, with a small amount of sample, and can be performed on a standard Cryo-EM. The problems encountered were mainly sample preparation and vitrification. They used standard crystal screens to start, but optimised to make crystals smaller rather than bigger. They then used a vitrobot to freeze samples – changing the blotting time, force and humidity – and checking the grids on TEM to get best grids.

The last talk in the session was given by **Huw Jenkins** (University of York) on '3DED/microED at YSBL: progress and latest results'. Huw showed the system set-up at York for ED, a 200kV Glacios, with autoloader and many detectors: STEM detectors, Falcon 4 camera for cryo-EM and Ceta-D detector for ED. They have mainly collected data on small molecules so

far (26 real samples, 18 collected (350 datasets)). He finished showing a precursor to sigma-alkane complex that was then reacted on-grid with hydrogen to give a single crystal (C2/c) to single crystal (P2₁/c) transition reaction.



Electron Diffraction session speakers (L-R): Tim Gruene, Tarik Devon, Fraser White, Huw Jenkins, Courtney Lendon, Peijun Zhang.

The **Membrane Proteins** session (Chair **Julien Bergeron**, KCL) keynote was given by **Jamie Blaza** (University of York) on 'Understanding the mechanism of the bifurcating hydrogenase from *T.maritima* through the application of cryo-EM and symmetry expansion'. *T.maritima* is a hyperthermophilic anaerobic bacterium. During its metabolism of glucose, both NADH and ferredoxin are reduced. TmHydABC (150kDa) is a bifurcating enzyme to produce H₂ from these reduced entities and there is lots of interest to use this enzyme to make reduced ferredoxin to drive energy transfer in other (synthesised) enzymes. The group could make the enzyme in *E.coli* and add the Fe-Fe centre after purification under N₂, but the [Fe-Fe] site is very sensitive to O₂ and they were unable to make grids with the holo-enzyme. Thus, all work has been done with the apo-enzyme which is structurally isomorphous. EM showed the protein exists as a tetramer with a core made of HydA and lobes made from HydBC. There are two electronically connected halves in the tetramer. The problem with having a symmetric particle is that it obscures any non-symmetric interactions. Therefore, they needed to do symmetry expansion and then classify on different masks to see the real differences. This shows a bridge at the top of the enzyme from the C-terms of HydA and HydB. This must be important as only the bifurcating enzymes have the C-term HydB extension. The bridge may be the point at which ferredoxin binds.

Soi Bui (KCL) then gave a talk entitled 'Structural basis for the lipid transfer mechanism in the maintenance of lipid asymmetry system'. The MLA (maintenance of lipid asymmetry) system shuttles lipids from the outer membrane to the inner. MlaA is in the outer membrane and binds the lipids and passes them to MlaC which shuttles the lipid across the periplasm to the MlaFEDB complex. MlaD lies in the periplasm, MlaE in the inner membrane, MlaF is an ATPase. The group were able to reconstitute the whole MlaFEDB complex and reconstruct it with cryo-EM. They are also collaborating on the *E.coli* homologue, where they were able to trap the complex of MlaD/C. Initial maps show there are two classes, with one or two MlaC molecules bound. No lipid was observed in MlaC – this is consistent with reports that MlaC exists in a closed conformation when not bound to another Mla component, so none would have been trapped in the purification. The binding of the two molecules appears to be largely driven by electrostatics.

The last talk was given by **Satomi Inaba-Inoue** (ICL) on 'The Molecular Mechanism of Antimicrobial Peptide Transporter

SbmA'. Bacteria spend a lot of time trying to kill their neighbours and many things (peptides, molecules) are passed through the outer membrane into the periplasm. SbmA then can transport these through the inner membrane into the cell, where they can block enzymes. The SbmA dimer is ~90kDa, so it was complexed with a Fab to increase the molecular mass to ~200kDa and the whole system was reconstituted in nanodiscs. Data were collected to a resolution of 3.2Å showing SbmA has eight transmembrane helices per protomer and is a novel fold for a secondary transporter. Two gates can be determined, one in the centre of the protein and one at the cytoplasmic end. They could also see a Glu ladder, which if mutated, stops activity, so it is probably important for proton movement.



Membrane Protein session speakers (L-R): Soi Bui, Satomi Inaba-Inoue, Jamie Blaza, Julien Bergeron.

The session on **Room Temperature Data Collection** (Chair **Allen Orville**, Diamond Light Source) started with a keynote by **Arwen Pearson** (Hamburg, Germany) on 'Time-resolved crystallographic studies of protein function'. Arwen started by explaining that we need to do time resolved experiments to provide a detailed understanding of structure-function relationships of enzymes. The interesting biological processes are often on the ms-μs timescales. To do this we need to stop reaction at specific points, often mechanically trapped (freeze-quench), with coloured co-factors to follow spectroscopically if possible. If we can't do this, then the best way is to do pump-probe experiments collected using SFX – i.e. each 'shot' is taken from a new sample, so it doesn't matter if reaction is reversible or not as a new crystal is used every time. She stated that these are not easy experiments – a lot of work has to be done up front to make sure they will work. Reproducible, well diffracting crystals. Reaction initiation has to be worked out (chemical/light), sample delivery has to be decided and a good reference resting state structure is required to subtract from collected structures. To make this more accessible to the community, the synchrotrons need to make everything standardised and easy to use. This is being implemented on the T-REXX beamline at Petra III, which has been open to users since 2019. The majority of data are collected on fixed target chips, which allow several data collection modes – burst, serial or hit-and-return. They have an easy user interface in MxCUBE, automated data processing, electron density maps calculated in one hour and all uploaded to ISpyB automatically.

Pierre Aller (Diamond Light Source DLS) then spoke on 'Enabling time resolved experiments at DLS and other facilities'. The XFEL-Hub at Diamond allows travel grants for UK researchers using XFELs and they also have a Dynamic Structural Biology BAG for SSX at DLS. The lab. at DLS has equipment for offline testing, anaerobic chambers and a Hirox microscope (for looking at crystal size and density). There are two delivery systems available – high viscosity extruder or fixed

target. They can do either an eject dose series (add ligand, then take a shot every 10ms for 100ms (10 datasets, but may have radiation damage)) or eject and revisit (time delay 540ms – 5s). He showed examples from both for ligand binding. Currently under construction is a drop-on-drop-on-tape – this allows for time-resolved mixing experiments using PolyPico to acoustically dispense reactants, where one can do several measurements on the tape before the X-ray hits (i.e. spectroscopic).

The third talk was from **Catherine Tooke** (University of Bristol) on 'Following antibiotic and inhibitor degradation by the CTX-M-15 beta lactamase'. It is predicted in 2050 there will be 10M deaths directly attributable to AMR (antimicrobial resistance). Beta-lactams are the most prescribed antibiotics worldwide, their resistance mediated by beta-lactamases. CTX-M-15 is a class A serine beta-lactamase, which can hydrolyse penicillins and cephalosporins, but not yet carbapenems. CTX-M-15 is found worldwide and so is an interesting target. It crystallises easily and diffracts very well ($<1.5\text{\AA}$). They collected data with fixed targets and drop-on-tape methods to try to understand how the beta-lactamases might hydrolyse carbapenems. The study used ertapenem which is readily soluble to 1M in water. The results showed the ligand can get into the active site on a relatively long timescale, $\sim 2\text{s}$. Longer timepoints ($>15\text{min}$) showed multiple tautomers bound.

The last talk was given by **Christopher Hutchinson** (ICL) on 'Ultrafast time-resolved serial femtosecond crystallography practical methodology'. Chris explained that to do time-resolved SFX experiments at XFELs you need to pump with an optical laser, before collecting with an X-ray probe. At ultrafast (fs-ps) timescales a very high energy laser is required to illuminate everything at the same time, but proteins are not designed to function properly under this load. The reaction pathways are limited by the quantum yield – you need at least 10% of states to be in the excited mode. Thus it is better if the crystals are small and have low absorption: otherwise the light is mostly absorbed on one side of the crystal. He showed examples of a pump-probe and a pump-dump-probe experiment that showed interesting effects. He also showed that the optical pumping can depend on the crystal orientation, if the crystal has preferred orientations.



Room Temperature Data Collection session speakers (L-R): Allen Orville, Pierre Aller, Catherine Tooke.

The keynote for the **Covid Drug Discovery** session (Chair **Daren Fearon**, Diamond Light Source) was given by **Marion Schuller** (University of Oxford) with a talk entitled 'ADP-ribosylation signalling and coronavirus infection'. ADP-ribosylation is catalysed by ADP-ribotransferases and can transfer one or more ADPs to proteins or RNA. PARPs are also active in antiviral defences, for instance PARP9 targets 3C protease for degradation. In the case of coronavirus infection

there is an accumulation of PARP14 which suppresses viral replication. Viruses have evolved ways of evading PARP14 suppression though. NSP3 MacroDomain (Mac1) protein (a PARP binding protein) in SARS-Cov-2 is essential for replication and is seen as a good target for inhibitors. The team carried out a powerful screening approach combining *in silico* and XChem fragment screening. The protein has two obvious interaction sites – the active site and the adenosine site. They found 234 fragments bound, mostly in the adenine site, but some across the surface and a few in the catalytic site. The XChem results were confirmed by ITC, DSF and also a ADP-ribose-peptide displacement assay. Four hits were confirmed at around 1-10mM Kd. Fragment linking and fragment merging were then used to expand the fragments to larger molecules. They are currently trying to create leads that will cover other viral MacroDomains with selectivity over the human analogues.

The second talk was from **Wiebke Ewert** (DESY, Germany) on 'X-Ray screening of SARS-Cov-2 proteases for effective structure-based drug design'. The coronavirus genome is quite large with a lot of non-structural proteins; these are mainly organised on one ORF and need to be separated by a protease, Mpro. Fragment screening has limitations because the compounds are small, hit rates are low and the hits need to be turned to leads. Instead, the group tried to repurpose already available drugs. Two libraries were available (~ 6000 compounds) and these compounds already have a lot of information known about them. Crystals of Mpro were first made in late March. Up to 600 datasets/day and full screen was completed by end of April. 43 hits were found in 29 structures, 11 of which proved to have antiviral activity in cell assays and one was so promising it is in preclinical tests. The team then took all the lessons learned from this and applied them to the next target: Papain-like protease (PLpro). A screen was set up with a large natural compound library and a small targeted library of metal binding compounds. Overlapping binding sites from both libraries will serve as new lead structures.

Next **Halina Mikolajek** (Diamond Light Source) told us about their research into 'Nanobodies against Covid-19'. Nanobodies are the VHH domain of a Fab antibody and, because they are small, they are easily designed and synthesised in the lab. They have three variable CDRs that form the binding site. Nanobodies were made to target the spike protein of SARS-Cov-2 (specifically the RBD protein) to stop it binding to the ACE2 receptor, thus stopping the virus from entering the cell. Hamster models proved that the nanobodies completely neutralised Cov-2. By changing the CDRs the group can get binding to different parts of the target molecule. It is expected that several nanobodies would be given as a cocktail to overcome new variants. They characterised the complexes by X-ray crystallography and cryo-EM.

The last talk was given by **Andreas Lutten** (Uppsala, Sweden) on 'Ultralarge Virtual Screening Identifies SARS-CoV-2 Main Protease Inhibitors with Broad-Spectrum Activity against Coronaviruses'. The group started with the X-ray structure of Mpro with a known inhibitor (X77) from the PDB and used this as a start point for screening. They carried out *in silico* docking with the ZINC15 library (235M compounds – one day on a supercomputer). After removal of difficult molecules, clustering similar compounds and visual inspection, this led to 100 candidates. Also, in parallel, they carried out fragment elaboration on a hit determined from DLS XChem screen and used the fragment to generate 2M compounds available from Enamine, which after analysis was trimmed to 96 compounds.

When both routes were tested in an Mpro activity screen, hits were 3% from ultra large screen and 5% from fragment elaboration screen. Hits were determined to have binding constants in the 20-80 μ m range and further elaboration now has the best inhibitor as a 50nM binder. This inhibitor also inhibits SARS-Cov-1 and MERS-1, though no human proteases. All the current known mutations in MPro do not block binding of this inhibitor (*in silico*).



Covid Drug Discovery session speakers (L-R): Weibke Everitt, Daren Fearon, Marion Schuller.

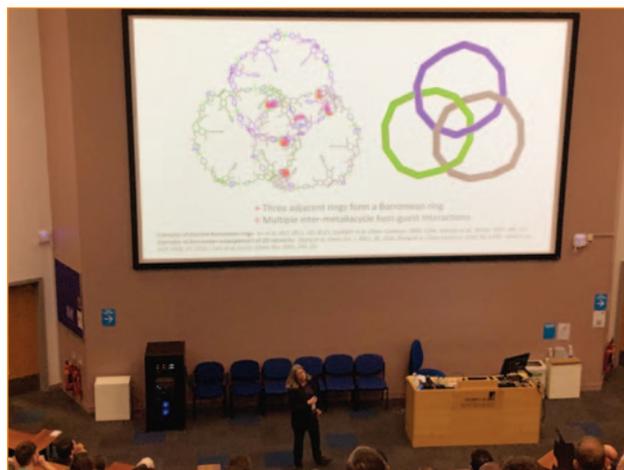
Mark Roe
University of Sussex

Chemical Crystallography Group

CCG Plenary

Prof. Michaele Hardie from the University of Leeds gave this year's CCG plenary lecture and used her home advantage to great effect with a true tour de force of supramolecular cage system and networks with pyramidal ligands. Michaele walked us through metallo-supramolecular chemistry and the self-assembly of discrete nano-scale metallo-supramolecular cages. She started with the cyclotrimeratylene (CTV) system, a pyramidal shaped molecule that can host a range of molecules within its intrinsic pore. These systems can be synthesised with a wide range of 'side arms' attached to central pyramids to give a range of functionality and variation in the packing for self-assembly. Michaele went on to describe a luminescent cage $\text{Ir(III)}_2\text{L}_2$ that can be synthesised as a chiral mixture of different cages. These will exhibit homochiral self-sorting over the course of several months but in this case, crystallisation was the most efficient route to separation. Many of the systems shown by Michaele had been determined from spectroscopic techniques; however, many had also been characterised with single crystal X-ray diffraction. For these structures, I tip my hat to the crystallographer to keep on top of such large and complex structures! Almost as impressive as some of the ChemDraw! One system described was a $\text{Pd}_3(\text{bis-nap})$ capsule crystal that is full of voids and remarkably robust. These systems should not be porous as there are no solvent accessible channels; however the solvent can be removed, and the single crystals can be shown to irreversibly uptake I_2 . This leads to a distinct colour change of the single crystal showing the flexibility of the cages to accept large guests and reinforcing the notion of porosity without solvent-accessible channels. The avalanche of different systems and new structures kept coming. A parting shot of a Cu_6L_6 chainmail of Borromean rings that crystallises as hollow straws (see image above right) wrapped up a truly excellent plenary and Michaele left us with her conclusion that

the assembly of cages are predictable, but the assembly of networks is not.



Charlie McMonagle
ESRF

Extreme Conditions



L-R: Charlie McMonagle, Rebecca Scatena, Christine Beavers, Nick Funnell, Craig Bull.

The session on Crystallography at Extreme Conditions will always peak my interest and this session did not disappoint. I should point out that the extreme on this occasion was pressure. We had four speakers whose subject areas spanned chemical space even if their job location was centred around the Oxford site; pressure of research condensing to one location?!?. **Dr Christine Beavers** (Diamond Light Source) provided the keynote lecture in this session and gave a great overview of high-pressure including comparisons including multiple elephants standing on a single tack to visualise the extreme pressures of deep earth research. Getting the elephant off its tack and into high heels Christine showed a range of examples of molecular systems at high pressure. Some are remarkably resistant to pressure with examples of Threonine up to over 20 GPa – the highest pressure molecular structure in the CCDC. Standard processes such as spin coating can induce significant strain in the system; this is the case for lead halide perovskites that have pressure-induced tilting that can be replicated at 0.7 GPa in a pressure cell. Christine urged all to consider high-pressure experiments and the possibility of performing these at I15 regardless of system or pressure range.

Next up was Dr Roy Funnell... sorry, I mean, **Dr Nick Funnell** (ISIS) talking about ROY. He loves this molecule and his insights over the last few years and publications has really changed the way we look at the polymorphs and their different colours. Formerly, changes to intramolecular torsional angles have been cited as the rationale for the changes to the colour. However,

his high-pressure studies have been able to question that basis with respect to the ON (orange needle) form of ROY and instead have been able to indicate the role of intermolecular interactions in these colour changes using a combination of high-pressure crystallography and electronic band structure calculations.

Prof. Craig Bull (ISIS) was next to speak. He always has a few slides on Pearl in his back pocket for such occasions! Unfortunately for you (the reader), the deadline for the April beamtime applications is past now but there will be a further one later in the year. In terms of science, Craig focussed on the polymorphism of Barium titanate as the compound has favourable ferroelectric properties which are key to capacitors and transducers. Showing off the potential of Pearl for phase diagram studies, Craig discussed how they were able to map out the temperature/pressure phase diagram and provide clearer indications of the boundaries between the various cubic, tetragonal, and rhombohedral phases.

Finally, **Dr Rebecca Scatena** (Diamond Light Source) introduced us to the world of Jahn-Teller distortions in hybrid perovskite materials. She discussed the Prussian blue materials that undergo changes to the Jahn-Teller directions under pressure conditions that impact on the antiferromagnetic directions. She was able to show how the network itself, and the tilts of the octahedral, are the primary driver for the phase transition.

Thank you to **Dr Charlie McMonagle** (ESRF) for chairing this very well attended session where the newly furnished tutorial-type lecture theatre was used. I was a little disappointed that the beautiful mossy wall had disappeared since our first visit. In any case, I hope that this arrangement was not too left field, but I guess the proof is in the post-conference questionnaire!

Iain Oswald
University of Strathclyde

Nucleation & Phase Changes

The second CCG Tuesday afternoon session focused on nucleation & phase changes of both organic and inorganic molecules. This session looked both at the discrepancies in phase based on the crystallisation, but also was an opportunity for researchers to discuss the transformations that can occur when crystalline materials are perturbed by an external stimulus.

The session started with a virtual keynote presentation from **G rard Coquerel** (Universit  de Rouen, Normandie) entitled 'Polymorphic transitions in organic solid state. Two complex cases with simple molecules'. G rard reported two examples of organic crystalline solids (ciclopirox and phenanthrene) that display temperature-dependent phase transformation. Interestingly, in the latter case, the phase transformation was also dependent on the purity of the material being studied.

The second speaker of the session was **Bhaskar Tiwari** (DESY), who presented work, in collaboration with Edinburgh University, entitled 'Polymorphism of ribavirin at high pressure'. This presentation discussed work completed at the Extreme Conditions beamline at DESY, and focussed on the high-pressure phase transformation of Ribavirin, an antiviral agent, using a diamond anvil cell and a neon pressure-transmitting medium.

The next oral contribution was delivered by **Lee Birchall** (University of Kent) entitled 'Exploring phase changes,

polymorphism and structure-property relationships in spin-crossover co-crystals'. Lee discussed his recent work on using organic hydrogen bond acceptors to affect the phases obtained of an inorganic spin-crossover (SCO) complex. Following the crystallisation of a series of different SCO co-crystals, Lee discussed how these different phases affected the SCO properties of the complex. This work, in part, involved monitoring the co-crystals using variable temperature single crystal X-ray diffraction.

The final speaker of the session was **Lucy Saunders** (Diamond Light Source) who presented a talk entitled 'Utilising proton transfer in molecular crystals for electric field applications'. Lucy discussed the development of an *in situ* electric field (ELF) set up on beamline I19 at Diamond Light Source. Her presentation demonstrated the major iterations of the set up as well as the challenges encountered when mounting single crystals in the ELF cell. Lucy also presented some proof-of-concept work on a hydrogen bonded co-crystal when an electric field is applied.

Tom Roseveare
University of Sheffield

Tricks of the trade – From Crystallisation to Publication



L-R: Ton Spek, Gary Nicol, Natalie Johnson, Robert Bannister, Claire Wilson.

This session was opened by **Dr Ton Spek** (Utrecht) who gave the keynote 'PLATON tools to help with resolving cryptic checkCIF alerts', covering aspects of PLATON, the Structure Viewing and Analysis toolkit software. Ton started with a brief introduction to the software, including its origin in the National Single Crystal Service facility where it was first developed 40 years ago. Showing it is still relevant to crystallographers today, Ton highlighted some of its key components including checkCIF, which is entering its 25th year, and which he recommends using in the early stages of a crystallographic refinement to prevent any later trips during the publication stages. To round off the keynote, the audience was taken through a recently published example to highlight how CIF alerts still get missed and what the consequences of this can be. Following PLATON analysis of this particular entry, a suspect methanol solvent molecule was found to have its hydroxyl proton incorrectly located. A question from the audience led to the discussion of future developments of PLATON checkCIF, including towards more non-routine refinements such as Hirshfeld atom refinement. The answer is ... stayed tuned!

Next up was **Dr Robert Bannister** from the National Crystallographic Service presenting their solutions to crystallisation bottlenecks with a talk entitled 'A national service to address crystallisability challenges'. They are using a crystal sponge method which can capture otherwise inaccessible reaction products from solution and has applications in

separation chemistry. To the joy of Ph.D. students everywhere, Robert also presented an automated, high-throughput nanodroplet crystalliser, allowing a range of hits to be obtained at the press of button.

In his talk entitled 'The usefulness of rapid structure determination tools in a service crystallography laboratory; or, structure? Now? What is this?!', **Dr Gary Nichol** (University of Edinburgh) celebrated, with an opening song, two programs which help him out daily in his service role at the University of Edinburgh: 'Structure now' and 'What is this?!'. He discussed the pros and cons of each, raising how these programs address the fact that it now takes longer to make your post lunch time brew than it does to get a first picture of a crystal structure. Gary showed how he uses their output to inform his next experimental step, which might even mean a change in diffractometer.

To finish the session, the final talk was from **Dr Natalie Johnson** of the CCDC entitled 'Fantastic structures and where to find them', in which she shared the new and latest tips to interact with the CSD suite. We learnt of new searching methods including introducing specificity into your Conquest search such as focussing on a subunit or by functional group targeting, searching certain structure categories whether it be high pressure, electron diffraction or pesticides and a new structure search using a similarity scoring function.

Overall, it was an excellent session in which to learn about the old and the new tricks of the trade of crystallography.

Lucy Saunders
Diamond Light Source

Understanding Crystallization Through Diffraction and Complementary Methods (joint session with BSG)

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 well-attended session, chaired by **Prof. Joop H. ter Horst** (Université de Rouen, Normandie) discussed innovative diffraction and complementary methods that deliver breakthroughs both in the understanding as well as the control of crystallization processes of all types of solids.

First, **Prof. Sven Schroeder** of the University of Leeds discussed several advanced X-ray characterisation techniques to obtain information about the changes in local structure around solutes in supersaturated solutions. He argued that these studies provide increasing evidence that the critical step in nucleation of organic species from solution is the formation of clusters of solvated solute molecules.

Then, **Dr Mikkel Juelsholt** (University of Oxford) discussed the chemistry of nucleation of tungsten oxide. He used *in situ* total scattering with pair distribution analysis to show that the kind of nucleation precursor can directly determine the formation of metastable crystalline phases. This would allow chemists, using careful design of the precursor, to target specific metastable phases.

Following him, **Yichen Shen** (University of Manchester) discussed the solution aggregation in two carbamazepine co-crystal systems using NMR, among other techniques. She identified that depending on the aggregation in solution a classical or non-classical nucleation mechanism can occur.

Finally, **Amy Lunt** of the University of Liverpool discussed an automated robotic workflow to screen crystal forms using powder X-ray diffraction. She showed that the revolutionary acceleration of functional materials discovery is starting to be realised, following the exciting developments in the chemical science community.

Joop H. ter Horst
Université de Rouen, Normandie

Physical Crystallography Group

PCG Plenary

We were delighted to welcome **Prof. Xiaodong Zou** (Stockholm University) to give our PCG plenary this year. After giving us an accessible introduction to the fundamentals of electron crystallography Prof. Zou gave us a fascinating insight into the powerful capabilities of these techniques. She explained both the practicalities of undertaking the experiments and their impact in studying the structures of a wide variety of complex and highly topical materials. Prof. Zou has been at the forefront of developing both experimental methods and software throughout her career and gave some very thought-provoking examples of the problems that have recently been tackled by her group and others. Some key methods have been greatly simplified by, for example, the serial, continuous rotation and stepwise rotation electron diffraction software she has developed and she outlined the implementation of these.

Prof. Zou rounded up her lecture by encouraging us all to consider taking advantage of the possibilities of electron crystallography and highlighted the software that is now available to make this technique more accessible to all. The highly engaging question session at the end showed the success of the lecture on this front!

Alex Gibbs
University of St Andrews

Porous Materials



L-R: Tom Hitchings, Paul O'Meara, Samantha Chong.

The first PCG session focussed on the diverse functionality associated with the versatility of porous materials. Chaired by **Aly Abdeldaim** (ISIS/University of Birmingham), this session was commenced by **Dr Samantha Chong** (University of Liverpool) in a lecture focussed on the complementarity of molecular *ab initio* and *in situ* techniques in revealing the underlying dynamic nature of molecular cages. In her insightful talk, Dr Chong specifically focussed on illustrating how the

simple static structure of molecular cages cannot explain diffusion dynamics. Instead, she gave an excellent illustration of how the local flexibility of the cage architecture plays a crucial role in determining the permissible guest-host dynamics through the pores of the structure. The resulting conclusion created an interesting discussion throughout the following Q&A session.

The following talk, given by **Thomas Hitchings** (University of Kent), focussed on the functionality of metal organic frameworks (MOFs) as potential relaxor ferroelectrics. In his exciting talk, Tom aimed at identifying the origin of the observed ferroelectric properties in a formate-based MOF as a starting point for revealing global design rules for obtaining such functionality. Using a combination of diffraction, quasi-elastic scattering, and NMR techniques, he successfully elucidated the necessary interdisciplinary characterisation methods for identifying the underlying functionality observed.

Next, and in a change of pace, **Dr Paul O'Meara** (Malvern Panalytical) highlighted the power of powder X-ray diffraction techniques in revealing the water content of MOFs. Specifically, he focussed on investigating the extent of hydration in CAU-10-H and the associated structural phase transitions. Throughout the talk, Paul illustrated the meticulous care necessary for an accurate determination of the crystallographic structure.

Finally, **Dr Patrick W. Doheny** (University of Kent) gave an exciting online talk focussed on the design aspects necessary for emergence of magnetocaloric properties in MOFs. Using an adipate-based MOF as an example, he illustrated the potential of MOFs as magnetocaloric materials by using a combination of magnetic and single-crystal X-ray characterization techniques.

Aly Abdeldaim
ISIS/University of Birmingham

Structure-Property Relationships in Energy Storage



L-R: Karen Johnston, Tony Keane, John Cattermull.

This session, chaired by **Karen Johnston** (Durham University) was a hybrid session, featuring two in-person talks, two virtual talks – and an array of associated technical issues that were (thankfully) quickly resolved. The session touched upon some of the main areas within energy storage, including new materials for lithium- (Li-ion) and sodium-ion (Na-ion) batteries, waste recycling for batteries, new technologies beyond conventional Li-ion and hybrid perovskites.

The keynote lecture was given virtually (live) by **Prof. Laurence Croguennec** from the Institute of Chemistry of Condensed Matter (ICMCB-CNRS), University of Bordeaux. She provided a concise summary of her 20 year career in battery research at

the ICMCB. Laurence started by discussing layered Li-based oxides and her work on defects and substitutions within these systems and how this can lead to the successful tailoring of specific properties. She also discussed some of the challenges associated with practically using some of these systems in functioning batteries, including stabilisation of the layers and the need for composite-type materials in the development of all-solid-state batteries (ASSBs). Continuing along a similar line, she then discussed her work on the development of novel Na-based materials for use in Na-ion batteries, focussing on cationic and/or anionic substitutions within these systems and their resulting influence on the observed physical properties. Throughout her talk, Laurence demonstrated the importance of using multiple, complementary techniques in her research. In particular, she highlighted how diffraction-based methods can be successfully combined with spectroscopic methods such as solid-state NMR spectroscopy to extract as much structural information as possible.

Dr Tony Keene (University College Dublin) then discussed a possible avenue for dealing with battery waste, specifically treating 'battery ash' to produce a double layered hydroxide material, labelled 'PM1'. As Tony discussed, this is an important area that needs careful consideration as we endeavour to make our laboratory practices more environmentally conscious and sustainable.

John Cattermull from the University of Oxford then detailed some of his recent results regarding beyond Li-ion technology, specifically exploring structural complexities in Prussian Blue analogues (PBAs). John is exploring these materials for potential use in future K-ion batteries. In particular, he is trying to identify how the functionality and performance of PBAs might be controlled through judicious choice of composition.

The final speaker of the session was **Harry Lloyd** (University of Birmingham). Sadly, Harry was not able to attend the session in person so, instead, delivered a pre-recorded presentation on some of his recent Ph.D. work on hybrid perovskite systems. Although only in the early stages of his Ph.D., Harry discussed how he is exploring greener synthesis methods for hybrid perovskites and the feasibility of tuning the properties *via* clever compositional substitutions.

Karen Johnston
Durham University

Advances in Complementary Techniques and *In-Situ* Crystallography (joint with CCG)



L-R: Hamish Yeung, Fiona Meldrum, Tom Fellowes, Jan Gertenbach.

This joint PCG/CCG session, chaired by **Hamish Yeung** (University of Birmingham) began with a keynote lecture by **Prof. Fiona Meldrum** (University of Leeds), who described how coherent X-ray diffraction and super-resolution imaging has yielded fascinating new insights into bio-inspired crystals such as calcite during crystal growth and dissolution. Prof. Meldrum showed several beautiful 3-D images of the internal structure of crystals grown under meticulous control, which revealed the origins of screw dislocations and unconventional dislocation loops that govern their crystallisation. The impressive detail afforded by these cutting-edge methods inspired an engaged audience, and the discussion that followed was extremely thought-provoking.

The second talk came from **Dr Tom Fellowes** (University of Liverpool), who described an elegant combined single crystal X-ray diffraction and single-crystal solid-state NMR study into chalcogen bonding in ebselen co-crystals. The size of crystals Tom was able to grow was almost as impressive as the arising insights into the strong 'non-covalent' interactions within the crystal structure, which suggested that significant covalency underpins their formation.

The next talk was delivered by **Dr Jan Gertenbach** (Malvern Panalytical), who described how new phases can be accessed in $\text{MF}_3 \cdot n\text{H}_2\text{O}$ ($M = \text{Fe}, \text{Cr}$) metal fluorides using controlled atmospheres within the diffractometer. These materials, of great relevance to battery technology, could only be formed upon carefully controlled dehydration, and interesting structural insight could be gained by *in situ* X-ray diffraction and laboratory pair distribution function (PDF) measurements. Jan also highlighted the exciting potential for quantitative phase information from the PDF measurements.

The final talk of the session was delivered in virtual fashion by **Dr Mark Warren** (Diamond Light Source), who gave an exciting overview of the ever-developing *in situ* experimental capabilities at the chemical crystallography Beamline I19. His examples included state-of-the-art 'low' high-pressure, segmented flow, photocrystallography, time-resolved pump-probe experiments, electric fields and laser-induced nucleation. Despite the virtual format, Mark's talk provoked a great discussion and I'm certain that the beamline will be receiving plenty of new interest from the user community, new and old!

Hamish Yeung
University of Birmingham

Extracting Information from Disordered and Poorly Crystalline Materials



L-R: Arianna Minelli, Kirsten Marie Jensen, Johnathan Bulled, Nikolaj Roth, Jeremiah Tidey.

The session was chaired by **Arianna Minelli** (University of Oxford) and featured all kinds of structures that cannot be simply described by their average structures, but a degree of complexity should always be added.

Kirsten Marie Ørnsbjerg Jensen (University of Copenhagen) delivered a wonderful keynote on how to extract useful information about nanostructures using total scattering techniques. The problem of refining the atomic structure of nanoparticles is well known, since Bragg diffraction and regular crystallography methods rely on the existence of a long-range order that cannot exist with such small particles. Real space comes in to help with Pair Distribution Function (PDF) analysis, a Fourier transform of the total scattering data. Her work on tungsten oxide nanoparticles offered a beautiful example of what can be done and seen with this analysis. Finally, she showed her work on the study of the nucleation and growth during a solvothermal synthesis. Again, the total scattering results show the nanostructure clusters forming *in situ* and give insight into the influence of the solvent and synthesis conditions during the nucleation.

Nikolaj Roth (University of Oxford) showed how the study of diffuse scattering and correlated disorder can reveal the real structure of materials, and explain the difference between samples which apparently are the same. As an example, the defective half-Heusler compound $\text{Nb}_{5/6}\text{CoSb}$ was produced using different synthetic routes: a slow cooling and a quenching. Without the analysis of the diffuse scattering, the differences found in the samples were attributed to a variable vacancy number. The diffuse scattering showed that the vacancies correlation length is larger in the sample prepared with a slow cooling process with respect to the quenched one.

A talk that will get physicists to talk a lot was delivered by **Jeremiah Tidey** (University of Warwick) on phase coexistence in cuprates – especially considering that the various electronic phases such as superconductivity and charge density waves are considered as competitors. He revealed, thanks to diffraction studies, the coexistence of LTT and LTO, low temperature tetragonal and orthorhombic phases, for two cuprates. This work suggests again the importance of the real structure analysis. The take home message is: don't settle for the average structure!

The session was concluded by **Johnathan Bulled** (University of Oxford), where we followed his journey through the refinement of a Hamiltonian to explain a complicated system such as the magnetic metal-organic framework, $\text{NaMn}(\text{HCOO})_3$. In this structure, the manganese ions occupy a geometrically frustrated trillium net (have a look at the flower!). The talk was a very pedagogic explanation on how to build your Monte Carlo calculation for your needs. Starting from a simple nearest-neighbour Heisenberg antiferromagnet, he then added more and more interactions, for example the dipolar one. Thanks to this, the ground state and the broad phase transition were explained.

Arianna Minelli
University of Oxford

Continued overleaf.

Functional Materials



L-R: Aly Abdeldaim, Rebecca Clulow, Richard Dixey, Josh Makepeace.

The high-quality talks in the Functional Materials session, chaired by **Paul Saines** (University of Kent), gave an excellent overview of the key role structure-property relationships play in promising materials, including for energy storage, clean cooling and magnetic properties.

The session commenced with a keynote talk by **Josh Makepeace**, a UKRI Future Fellow at the University of Birmingham, who gave an overview of the importance of hydrogen storage using chemisorption to the clean energy economy of the future, and the role lithium imide and amide can play in this. This included an understanding of how increasing the lithium composition of a family of lithium-imide materials can be used to tune their structures and both thermal stability and ease of hydrogen release.

The next talk was by **Rebecca Clulow** from Uppsala University, who spoke about the synthesis of high entropy perovskite and Ruddlesden Popper phases that contained up to seven transition metals on their B-site. This highlighted that high entropy approaches for tuning the properties of alloys could also be achieved in magnetic oxides, clearly engaging the audience based on the high number of questions Rebecca fielded with significant expertise.

Richard Dixey (Queen Mary University of London) then highlighted that organic plastic crystals based on quinuclidinium cations make excellent barocalorics for high efficiency clean cooling via their high barocaloric entropy changes for moderate pressure changes. Their performance could be optimised by incorporating molecular anions, but it is clear there is significant scope to improve the materials further by more detailed understanding of their structure-property relationships.

Finally the session was concluded by **Aly Abdeldaim** from the University of Birmingham who highlighted $\text{RuP}_3\text{SiO}_{11}$ as a promising spin $\frac{1}{2}$ Kitaev candidate which he had analysed using neutron diffraction and spectroscopy. Although further analysis is required to confirm this, it is arguably the closest realisation of an undistorted Kitaev phase and may be difficult to improve upon given the weak Jahn-Teller distortion associated with low spin d5 metals.

Paul Saines
University of Kent

Early Career Prize Session

The Early Career Prize session lived up to my expectations and gave us all a brilliant look at the science of three very worthy winners. Congratulations to **Dr Andrea Thorn** (BCG), **Dr Hamish Yeung** (CCG) and **Dr Matthew Cliffe** (PCG)!

This hybrid session began with a virtual presentation by Andrea beaming in from Hamburg. After a few technical difficulties to begin with, Andrea gave a fantastic tour of the work of the COVID taskforce and their work linking into the lifecycle of SARS-COVID. In her talk, she focussed on particular areas of the lifecycle and provided us with the science performed on each of these areas. It was a very accessible talk on a subject that has been such a large part of our lives for the past two years. Next up was Hamish who teased us with the many areas of interest to him such as hybrid perovskites and molecular conductors before focussing on solvothermal synthesis and the developments on the I12 beamline at Diamond Light Source. He discussed particular systems such as lithium tartrate & ZIF-8 and showed how *in situ* measurements were invaluable in exploring the reaction pathway through the formation of intermediates. The final presentation was provided by Matthew who gave us an insight into the world of metal isocyanates to tackle the challenges of quantum materials. These unusual materials make use of their pseudo-halogen like properties to provide an extension of types of materials that could be used. His work to date has explored the substitution of metal centres to alter properties whilst maintaining isostructurality with the parent compounds. All in all, this was a really fantastic session that shows that the future of Crystallography is certainly bright!

Iain Oswald
University of Strathclyde

Spring Meeting Sponsors and Exhibitors

The BCA would like to thank the following organisations for their generous support of the Spring Meeting 2022:

- ACA AIPP
- Anton Paar Ltd
- Bruker UK Limited
- Calibre Scientific
- CCDC
- Constant Systems Ltd
- Crystal Growth and Design
- CrystEngComm
- Douglas Instruments Ltd
- ELDICO Scientific AG
- Formulatrix Inc
- Indicatix
- IUCr
- Malvern Panalytical
- Oxford Cryosystems
- PDBe
- PROTO / Hiltonbrooks
- Rigaku Europe SE
- Royal Society of Chemistry
- STOE & Cie GmbH
- Technobis Crystallization Systems

BCA Spring Meeting 2022 Bursary Reports

As BCA members will know, a condition of being awarded a BCA Bursary to attend the Spring Meeting is a report on the meeting for publication in Crystallography News. What struck me from these reports this year in addition to their general quality were the comments underlining the importance of in-person conferences (this was the first in-person conference many had attended) – networking, putting out their wares and learning from others in ways that would be less effective online. Putting these reports together for Crystallography News made me even sadder about my having to miss the meeting!

AS my colleagues and I set off to Leeds for the British Crystallography Association's Spring Meeting, we could all feel the atmosphere of anticipation on the drive north. Worldwide events had relegated our recent conference experiences to be delivered through a screen, and the shift back to in-person events felt auspicious. Although I had good memories from physical conferences from my postgraduate years, I had yet to attend one as a postdoc., and I was a relative newcomer to the BCA. I was excited to see what was in store for us.

The first event was the Young Crystallographers' Group Early Career Satellite Meeting, where **Claire Hobday** was the first to take the stage with her fascinating research towards solid-state refrigerants. What followed was an afternoon of talks from the early-stage research community, everybody keen to speak to the receptive audience. Many were speaking at the front of an auditorium for the first time, but every single talk was high quality and engaging. The evening session concluded as students and academics chatted about science over some excellent food and drink.

The next day, the general meeting began, and a wealth of expertise coalesced into a diverse series of talks over the next three days, the broadness of topics indicative of the versatility of crystallography in modern science. It was a particular pleasure to see the hard work of younger academics, **Andrea Thorn, Hamish Yeung** and **Matt Cliffe** get recognised in their awarded prize lectures from the BCG, CCG and PCC groups. I was also struck by the openness of the committees and took the opportunity to attend the general meetings and learn more about how the BCA manages itself.

The evening poster sessions were a personal highlight for me. I was lucky enough to be able to present my work, and I am grateful that I received genuine interest along with a host of useful feedback and ideas for me to take back to the lab. in Wales. It was a whirlwind event, but I used my few spare moments to circulate the room and learn some fascinating new science from some enthusiastic and knowledgeable researchers.

The peak of the conference was the evening dinner hosted at the Marriott Hotel, where we feasted and chatted. After dinner, several researchers were awarded poster prizes – I was honoured to be among them. The generosity of the sponsors and hard work of the committee had paid off and spirits were high. By the end of the evening, the dance floor was packed with students and academics alike, and the revelry continued into the wee hours of the morning.

After the final day of the conference had come to an end, I reflected on the week on my journey back to Cardiff. I am blown away by how welcoming and receptive the BCA was. The feeling of being a newcomer quickly dissipated and I felt immediately accepted as a member of the community. I greatly anticipate the next BCA event and I cannot wait to see everyone again.

Ben Coulson
Cardiff University

UNTIL the 2022 BCA spring meeting, I had only been able to attend one other in-person conference, with the rest being online due to the Covid-19 pandemic. Whilst the online conferences were fantastic for keeping up to date with new and exciting research, I didn't realize how much was missing from them in terms of the social aspects until I attended the Spring Meeting in Leeds. It was very nice to speak to so many other students throughout the conference who shared the same excitement around crystallography and their work.

The YCG Satellite Meeting included a broad range of talks, which I personally really enjoy. I think that a range of talks is especially important for early stage crystallographers like myself, as they provide exposure to different areas, which can really help with identifying future career interests. Some highlights from the YCG Satellite Meeting for me were the talks from **Emily Meekel, Cameron Wilson** and **Atika Al Hasaini**. Emily discussed the predictability of MOF topologies and it was fascinating to learn how important it is to think about torsion angles on the linkers when designing MOFs; something which can be easy to overlook. Cameron talked about the CellVol code and how it can be used to identify subtle crystallographic phase transitions. It amazes me how much information can be extracted from crystallographic measurements and talks like this inspire me to look at my structures from as many different perspectives as possible. The use of electric fields in crystallography was discussed at various points throughout the conference and the talk from Atika was focused on the use of electric fields in the crystallisation of proteins. The results were really interesting and showed that electric-field-assisted crystallisation can result in both increased crystal quantities and sizes. I look forward to seeing the future developments in electric-field crystallography.

The main meeting was brilliant, and I greatly appreciated and

enjoyed the opportunity to give a talk in the 'CCG: Nucleation & Phase Changes' session. It is impossible to highlight all the wonderful science from the conference in this short report so I will briefly discuss one thing that stood out to me, which is electron diffraction. I have attended online conferences where electron diffraction has been discussed but it always seemed a few years away and completely inaccessible to most. However, **Xiaodong Zou** gave a fascinating talk on electron diffraction, and I was particularly surprised by how many people I talked to were currently using it as part of their Ph.D. studies. It was also nice to talk to the exhibitors to learn a bit more about electron diffraction and its place amongst the other established analytical methods.

Overall, I had a fantastic time at the conference along with the rest of my group and I found the whole atmosphere throughout the week to be very welcoming, friendly and positive. Crystallography is in an extremely exciting time right now with so many new developments and I can't wait for the next meeting!

Lee Birchall
University of Kent

TRAVELLING from Canterbury to Leeds the night before, the conference started with the YCG Satellite Meeting with engaging talks from a breadth of early-stage crystallographers. The Satellite Meeting was a fantastic start to the first in-person conference for many new Ph.D. students, providing an opportunity to meet and talk about their work. The poster session encouraged this further, with many participants finishing the first day in the pub down the road from the conference venue.

The following day started with the Parkin Lecture, delivered by **Dr Alexander Tansell**, which highlighted the importance of science communication with the general public and their role in how they want science to be communicated, illustrated with insightful stats. At the closing plenary, **Dr Sam Horrell** highlighted some good tips on performing an experiment on a beamline, using Twitter as a resource. By this time, the exhibition hall was filling up for the main meeting, commencing with the Lonsdale Lecture given by **Prof. Andrew Goodwin**. The Lonsdale Lecture is awarded by the YCG committee and aims to include a strong teaching element. I really enjoyed the journey through geometry, into what constitutes a crystal, and finishing with interesting local orderings – described by a tiling method invented by a monk for information storage (Truchet tiling) – which gave effortless accessibility to these complex ideas.

After the PCG plenary, the parallel sessions began. As I was one of the speakers in the Porous Materials session, this was the one I went to. I then diverted from the PCG session to the next CCG session on Nucleation & Phase Changes. Tuesday concluded with the CCG plenary and poster session over dinner, and the pub down the road again became quite populated. Some delegates even took advantage of the open mic. night with performances ranging from electric guitar to traditional Irish folk.

After the IG plenary on the third day, the parallel sessions resumed, of which I attended the joint PCG and CCG sessions. A captivating talk from **Prof. Fiona Meldrum** was delivered on the dislocations found in calcite and how these are

observed in nature. Following lunch and the prize lectures, a new type of interactive session, the YCG+ careers panel, with the '+' suggesting that this was open to all groups but with a career focus. This gave perspective into the range of possible careers in the field.

One of the highlights of any meeting is the conference dinner, this year hosted by the Marriott, and after two years of online conferences, this was much anticipated. Once the food had been finished and prizes had been awarded, a pleasant buzz of networking ensued. The DJ did an excellent job, with one of my highlights being the macarena. I enjoyed describing this as an audibly driven self-assembly of crystallographers into a (heavily) disordered system, displaying some kind of collective dynamics.



The meeting concluded with another two sets of parallel sessions; I attended both PCG sessions. The image shows a group of crystallographers that sparked a brief Twitter discussion on the collective noun to describe such a group. My personal favourites were a packing, a centring, and an asymmetric unit. Overall, the first in-person conference for many attendees was thoroughly enjoyable and interesting; surely indicative of meetings to come.

Thomas Hitchings
University of Kent

11th to the 14th of April this year. This was the first time the British Crystallographic Association Spring Meeting had taken place in person since 2019 due to the pandemic and was much anticipated by all attendees. The warmth of the welcome on arrival in Leeds was noted by us all and the location/conference venue coupled with the programme and presentations for the week ahead looked enticing.

The conference started with the Young Crystallographers' Group Satellite Meeting which is aimed at students and researchers in the early stages of their careers. This meeting was well attended and succeeded in comprehensively covering many different areas of crystallography whilst still providing a relaxed and welcoming environment for the younger researchers to share their results. The programme also incorporated a careers session with crystallographers from several different fields and career paths, giving an insight into the different career options available and an opportunity to get advice from professionals in each of the specific fields.

The main meeting commenced the following day with the Lonsdale prize lecture which was given this year by **Prof. Andrew Goodwin** on the topic of 'Disorder by design: from form to function'. The next three days covered a wide range of

topics with plenaries from all of the four major groups (BSG, CCG, PCG and IG) and parallel sessions covering a more specialised range of topics. The early career prize lectures were a highlight and gave a valuable insight and introduction into some of the best work being carried out in the different areas of crystallography. The conference also provided plenty of time and opportunity to network with other researchers working within crystallography with poster sessions, lunches and coffee breaks allowing for a more relaxed social setting for discussions, and culminated in a conference dinner and party.

The whole conference was a great welcome back to in-person meetings and provided many opportunities to network with the crystallographic community and share our results. I hope to be back soon!

Rebecca Clulow
Uppsala University, Sweden

I ARRIVED in the University of Leeds for the BCA Spring Meeting 2022. It was my first time to attend a conference and I had fantastic experience there, not only because of the lovely birds and rabbits on campus, which we do not have in Manchester, but also the thrilling presentations of the cutting-edge science and technology.

The conference contained two meetings and the first is the YCG Early Career Satellite Meeting, starting on the afternoon of Monday 11th April. **Dr Claire Hobday** from the University of Edinburgh gave a wonderful talk on pressure-driven phase transitions and looked into the future of solid-state refrigeration as an opening. The YCG meeting closed on the noon of 12th April with an interesting and fun closing plenary talk on solid-state refrigeration given by **Dr Sam Horrell** from the Diamond Light Source. The YCG meeting provided an excellent opportunity for young crystallographers to give a presentation on their amazing work, and to communicate and make friends with each other freely.

The next three days followed with the Main Meeting Programme, with three parallel sessions at the same time. I was very honoured to give an oral presentation on the final day of the conference to introduce the work I am currently doing about solution phase aggregation. I was also pleased that many researchers were interested in my research and gave me their contact details after the meeting. The main conference gave me a good chance to know the inspirational work in other groups and make the field that I am working on known to others as well.

There was plenty of time for networking with well-scheduled networking events such as coffee breaks during each session, and also poster sessions with lunch, dinner and wine. There was also a grand conference dinner at a hotel on the last evening of the conference, providing a larger space and better atmosphere for building networks.

Additionally, the sponsor exhibition was great for talking with these companies about their new technologies and equipment, and for collecting stamps from the event as well as for picking up some freebies.

The conference closed on 14th April and it was a fabulous event to attend. It widened my research horizon especially on

inorganic and protein crystallization, which I would not have known about without attending the conference. Moreover, it built my confidence in my own research and improved my skills of giving presentations.

Yichun Shen
University of Manchester

WE arrived at Leeds for the BCA Spring Meeting 2022 on the afternoon of Sunday 10th April, which was one day before the conference. This gave us some time to walk around the city and the campus. The University of Leeds has an awesome view and environment. It was definitely a great experience for me to remember, not only because it was the first face-to-face conference I've been able to attend since the pandemic over the last two years, but also I was given the opportunity to present my work in the meeting.

The conference started on Monday afternoon with the YCG Early Career Satellite Meeting. Lots of young crystallographers from different areas were able to present their researches about crystallization of inorganic and protein materials and newly developed crystallization techniques and screening methods. I was able to give my presentation about linking solution structures to the final hydrate crystal form on Tuesday morning.

On the same day, the main meeting started at 11.30am with a fantastic talk from **Prof. Andrew Goodwin** about disordered materials, and he presented his recent work on the metal-organic frameworks. He talked about different techniques that have been used in the field to study disordered material structures.

During the following parallel sessions, researchers from different areas presented their work about crystallization under extreme conditions and their studies on polymorphic transforms, which definitely allowed me to learn a lot about crystals. There were other interesting sessions about protein crystallization and even studies on the Covid-19 virus.

On the last day, **Prof. Sven L.M. Schroeder** gave an incredible talk on classical nucleation theory and his studies using imidazole. It is such fascinating research and the methods they've used are very inspiring. There were also more studies on nucleation theories and pathways that were very interesting.

The poster sessions on every evening provided us a great opportunity to show people our work and also to look at other people's work. There was plenty of time and opportunities to network with people from all over the world and talk about research. It was a very friendly environment in which to talk about my own research and people were more than happy to give me feedback.

The conference included a wide range of topics from nucleation theories, disordered materials, inorganic and protein crystallization and different techniques. It was a great event as it helped me to widen my understanding of crystallization and to decide what I want to pursue in my future career.

Yitian Xiao
University of Manchester

THE 2020 Spring BCA Meeting in Leeds was supposed to be the first conference of my Ph.D. After its cancellation just as final preparations were being made, it was great to finally make it up to Leeds two years later for what was still my first (in-person) conference. An experience that I know I was not alone in. This gap in conferences created quite a nice level playing field as most people had either never presented a poster/talk or needed to relearn a touch as they went. Everything felt very fresh and new. The result was a lovely open and understanding atmosphere.

The meeting began with an engaging plenary talk from **Dr Claire Hobday**, and an amazing string of high quality presentations at the YCG Satellite Meeting. I felt honoured to share my work during one of these sessions, with so many of my talented peers in the welcoming environment that the YCG provided. The poster exhibition and wine that night gave us a great opportunity to properly mingle and start getting to know people.

Tuesday morning saw the end of the YCG meeting and the main meeting was kicked off in style with fascinating talks from **Professors Andrew Goodwin** and **Xiaodong Zou**. It was very interesting to see the recent developments in electron diffraction and I think I wasn't the only one who left that talk very excited about how useful it would be for my own work. With the afternoon came parallel sessions. Due to incredible talks taking place in every session concurrently, hard decisions often had to be made. If someone could prioritise researching a way for me to be in two places at once before the next BCA meeting, that would be much appreciated!

Wednesday started with more parallel sessions until the prize talks brought us all back together. It was fascinating to see **Andrea Thorn's** BSG prize talk about the Coronavirus Structural Task Force which gave some further insight on something that's been all around us for two years. I really liked the honesty of how much they still didn't know alongside all the incredible things they had discovered. The conference dinner on Thursday night provided an amazing opportunity to further get to know people in a more relaxed environment. I was honoured to receive one of the poster prizes, awarded after dinner, alongside some amazing crystallographers.

The meeting gave me the opportunity to learn about, discuss, and share in research on the cutting edge of crystallography but it also gave me so much more than that. From the first moment that we entered the exhibition hall, there was a hum in the air, a hum that was sustained the whole way through the week. Two years' worth of excitement and enthusiasm was in the air. Old friends caught up on research and life side by side with the forging of new friendships as I experienced my first chance to forge academic friendships outside of my own university. It was a feeling I won't soon forget, and one that made me excited for future conferences.

Rhona Lonergan
University of Kent

AFTER a long drive to Leeds for my first in-person conference as a Ph.D. student, I was excited to begin with the excellent plenary lecture covering solid-state refrigeration using pressure-induced phase transitions given by **Dr Claire Hobday**. Following several interesting talks across a range of topical crystallography, I was ready

to give my own talk about my recent work developing ferroelectric materials for solar energy capture, and studying these using dynamic X-ray diffraction techniques.

The evening of the first day of the YCG Satellite Meeting was concluded with some fascinating discussions with fellow Ph.D. students and postdocs over the poster session (made even better with the lovely dinner and wine available!).

The next morning was off to a good start with a great Parkin Lecture from an old colleague **Dr Alex Tansell**, which highlighted the importance of public engagement with our research. The YCG meeting then concluded that afternoon with a very insightful (and humorous) plenary talk by **Dr Sam Horrell**, a beamline scientist at the Diamond Light Source.

After a quick coffee break, the Lonsdale Lecture given by **Prof. Andrew Goodwin** (who I discovered during the conference had previously worked in the same University of Sydney lab. that I had!) began the BCA Main Meeting. I was able to hear a number of excellent talks during the parallel sessions, moving between the CCG, PCG, and BCG rooms to listen to those most relevant to my work. It was often very difficult to choose which talks to attend, as they were all interesting, although I generally stuck with the area I understood better, which was the CCG. This proceeded until the various AGMs, followed by a careers session for YCG members.

Prof. Elspeth Garman gave the Hodgkin Lecture which was terrifically interesting, and a fantastic tribute to Professor Dorothy Hodgkin. Wednesday was then concluded with the conference dinner, which everyone thoroughly enjoyed, and various prizes were awarded for some of the wonderful posters and presentations given throughout the week.

On the morning of the final day, we were all awake early to check out of the hotel and pack the car ready to head home to Cardiff. **Prof. Randy Read** started Thursday's lectures, discussing the field of structural biology following the advances made by AlphaFold. We all listened to a few more talks, learning some great 'Tricks of the Trade' from the CCG parallel session, before saying our goodbyes to old colleagues and new friends and departing from Leeds after an amazing conference.

Joshua J. Morris
Cardiff University

THIS year's BCA Spring Meeting was special for many of its attendees – the first in-person meeting since the pandemic hit, the first time seeing colleagues and friends over the last two/three years and, in my case, the first in-person conference I attended since starting my Ph.D. back in October 2020. The meeting was held in a modern venue at the University of Leeds and included a fantastic programme and list of speakers, which made the wait well worth it.

The main event was preceded by the YCG Satellite Meeting. This meeting offered a friendly environment for early career researchers to present and get feedback on their current work. In particular, it was great to hear about the incredibly interesting results obtained by students in the early stages of their Ph.Ds. From the event, I especially enjoyed **Emily Meekel's** talk on Zn-1,3-BDC MOFs, **Dr Sam Horrell's** light-hearted talk on

'10 things your Beamline Scientist wished you knew', and **James Osborne's** talk on a Python-based tool for the clustering of powder X-ray diffraction data, which is an exciting and solid step forward towards the automation of data analysis in crystallography.

The conference ran for three days and was divided into lectures, plenaries, and three sessions running parallel to one other, all covering the breadth of topics that fall under the umbrella of crystallography: from chemical to pharmaceutical and biological research, theoretical and practical studies, and both lab-based and computational work. A highlight for me was **Andrew Goodwin's** talk on designing disordered functional materials (the Lonsdale Lecture). Whilst it is not a topic close to my area of research, it is one of the best talks I have ever attended; he managed to grab the auditorium's attention and deliver information in a way that was easy to follow, whilst smoothly transitioning between the work carried out by his research group and the work and life of Kathleen Lonsdale.

It was also a pleasure to attend **Amy Lunt's** talk on an automated robotic workflow to screen crystal forms using powder X-ray diffraction. The incredible workflow she has developed during her Ph.D. is very impressive, and it is inspiring to see other Ph.D. students carrying out such amazing research.

In addition to the lecture sessions, plenty of time was given to network with companies and colleagues through scheduled networking events, for example the poster sessions and the trade exhibitions held during lunch and coffee breaks. Additionally, a wonderful conference dinner was held at the Marriott Hotel on the third night, and one or two trips to the pub also took place! I would like to thank the organisers within the BCA and Hg3 for putting together such an enjoyable and stimulating event. I am looking forward to seeing what next year's Spring Meeting holds.

Julia Gasol-Cardona
University of Strathclyde

BCA 2022 Poster Prizes



The **ACA/AIPP** poster prize was presented to **Catherine Tooke** by **John Helliwell** for her poster *Following antibiotic and inhibitor degradation by the CTX-M-15 β -lactamase using serial, room-temperature crystallography at synchrotron and XFEL sources.*



The **Oxford Cryosystems** CCG poster prize was presented to **Rhona Lonergan** by **Mike Probert** for her poster *Selective synthesis of polymorphs of [Fe(abpt)₂(NCS)₂] through mechanochemical control.*

The **Calibre Scientific** poster prize was awarded to **Anna Warren** for her poster *VMXm: A new micro/nanofocus protein crystallography beamline at Diamond.*

The **Technobis Crystallisation Systems** CCG poster prize was awarded to **Jake Weatherston** for his poster *High Pressure and Low Temperature in-situ Crystallisation of Methyl Anthralinate.*



The **Crystal Growth and Design** CCG poster prizes were presented by **Mike Probert** to **Ben Coulson** (*Towards Photoresponsive Metal-Organic Frameworks (MOF) Exhibiting Ferroelectricity*), **Lina Mardiana** (*High Throughput Crystallisation of Complex Natural Products for X-Ray Analysis*) and **Emily Thompson** (*Electron Diffraction: trials, tribulations, and small molecule success story*).



The **PDBe** BSG poster prize was presented by **Kate Brown** to **Satomi Inaba-Inoue** for her poster *Molecular mechanism of antimicrobial peptide transporter SbmA.*



The **Royal Society of Chemistry** CCG poster prizes were presented by **Mike Probert** to **Lewis Jackson** (*Co-crystallisation of Spin Crossover Active Complexes: [Fe(2-(2-Pyridyl)benzimidazole)₃][BF₄]₂ and [Fe(2,6-bis(pyrazol-3-yl)pyridine)₂][BF₄]₂*) and **Lucy Hunter** (*Reversible pressure-induced bond rearrangement in flexible lanthanide 2,5-bis(allyloxy)terephthalate coordination polymer networks*).



The **Institute of Physics** PCG poster prize was presented by **Lewis Owen** to **Mario Falsaperna** for his poster *Neutron diffraction study of the canted antiferromagnetic 2D layered framework: [Li(C₂O₄)₂][Co₅(OH)₈].*

Continued overleaf.



The **Solid State Chemistry** PCG poster prize was presented by **Lewis Owen** to **Stephen Brown** for his poster *Synthesis, Structural Determination, and Photochemical Properties of Cerium-oxo Clusters*.



The **STOE & Cie** PCG poster prize was presented by **Lewis Owen** to **Ben Tragheim** for his poster *Interplay of Jahn-Teller distortions, orbital order and structural degrees of freedom in LaMn1-xGaxO3*.



The **Industrial Group** poster prize was presented by **Judith Shackleton** to **Jessica Metherall** for her poster *High-Throughput Crystallisation of Organic Acids*.



The **Rigaku** YCG poster prize was presented by **Tom Roseveare** to **Phillippa Partridge** for her poster *The Phase Behaviour of Organic Ionic Plastic Crystals*.



The **Cruickshank** YCG poster prize was presented by **Tom Roseveare** to **Lee Birchall** for his poster *Exploring Phase Changes, Polymorphism and Structure-Property Relationships in Spin-Crossover Co-Crystals*.



The **Best Flash Presentation** prize was presented by **Tom Roseveare** to **Chloe Seddon** for her poster presentation *Deciphering the role of the outer membrane porin OmpW during bacterial conjugation*.



The **IUCr** poster prizes were presented by **John Helliwell** to **Dashnor Beqiri** (pictured left) (*Engineering soft modes in Layered Perovskites*) and **Cameron Wilson** (pictured right) (*High Pressure Phase Transitions in Glyphosate Identified Using the CellVol Code*).



The **Indicatrix** Prize was presented by **Mike Hall** to **Robert Carroll** for his poster *Developing the Application of the Crystalline Sponge Method*.

Thank you to Alex Stanley for the presentation images.

Second Intensive Summer School in Physical Crystallography

11-14 July at Cosener's House, Abingdon, UK.

A line-up of expert lecturers will teach an interdisciplinary course spanning the breadth of principles and approaches essential to contemporary physical crystallography:

1. *Foundations of crystallography* – Dr Emma McCabe (University of Durham).
2. *Phonons* – Professor Andrew Goodwin (University of Oxford).
3. *Irreducible representations, magnetic space group* – Dr Fabio Orlando (ISIS Neutron and Muon Source).
4. *Landau theory and phase transitions* – Dr Roger Johnson (UCL).
5. *Symmetry and physical properties* – Dr Alex Gibbs (University of St Andrews).

Full details and application form are at:
<https://sites.google.com/sheffield.ac.uk/pgc-summer-school-2022/home>.

Leeds & the Early Development of Crystallography

ALL the crystallographic work the BCA does now and has done in the past is built upon what others have done before us. We do need to realise this, and to feel we are not alone but are supported by those who have contributed in the past.

For all of us this starts with the Braggs, father and son, William Henry (1862-1942) and William Lawrence (1890-1971). The father brought the family to England in 1908. William Henry accepted the Cavendish Chair in Physics at the University of Leeds. William Lawrence entered Trinity College Cambridge in 1909. It is reputed that he worked out the basis of Bragg's Law whilst strolling by the river Cam. World War I intervened, involving them both, but in 1915 they were jointly awarded the Nobel Prize for Physics 'for their services in the analysis of crystal structure by means of X-rays'. In recent times, in Leeds, in the Parkinson building, a blue plaque celebrating the Braggs' achievement was installed. After the war, William Henry moved variously to University College (UCL) and the Royal Institution (RI). If readers use their computer search engines to search for 'Leeds Crystallography' and click on 'The birth of crystallography – Leeds Alumni Online' and/or similar sites, they will find the Braggs' story at length.

Having excelled in her University of London B.Sc. in 1922 at Bedford College and her M.Sc. at UCL in 1924, Kathleen Yardley (Lonsdale) (1903-1971) was asked by Henry to join his research team at the RI. Following her marriage in 1927 to her husband who worked at the Silk Research Association, she moved on to Leeds, in the Physics Department, Henry's previous laboratory. At Leeds in 1928, she determined the structure of hexamethylbenzene and proved conclusively that its benzene ring was hexagonal and planar, a fundamental result that settled an age-old debate in chemistry. Furthermore, in 1931, she was the first to use Fourier methods while solving the structure of hexachlorobenzene. In 1934, Kathleen returned to work with Bragg at the RI, moving to UCL after World War II to become Reader in Crystallography, then Professor of Chemistry, then Head of UCL's crystallography unit within Chemistry from 1949 to 1968. She was one of the first two women to be elected FRS, and is commemorated in Leeds with a lecture theatre (situated in the Sir William Henry Bragg Building) named after her.

At the RI in 1927, Henry set Ernest Gordon Cox (1906-1996), newly graduated in physics from Bristol University, the task of determining the crystal structure of benzene. With a special rotation camera built by C.J. Jenkinson, which kept benzene crystals at 251K long enough for X-ray photographs to be taken, Cox obtained results favouring a flat six-membered ring with the C-C bond length of about 1.42Å. He moved to Birmingham in 1929 to join W.N. Haworth's department and worked on structures such as sugars and vitamin C. After the war he became a professor of chemistry at Leeds in 1945, where he encouraged advances in instrumentation, theoretical and computational methods. He led the Leeds chemical crystallography group until 1960.

In 1946, Cox welcomed to Leeds the talented Durward W.J. Cruickshank (1924-2007) as a temporary research assistant. Durward stayed in Cox's group until 1962. Cox encouraged Durward to take the undergraduate course for the Mathematical Tripos at Cambridge, where, he later wrote, "I learnt some mathematics, at the feet of Herman Bondi, Fred Hoyle, S.E. Boys, Paul Dirac *et al.*" He returned to Leeds in 1950 to a Lectureship in Mathematical Chemistry. During his time in Cambridge, he followed the development at that time of stored-program computers and attended the 1950 Cambridge Summer School, which introduced him, he said, to the principles of computer programming, machine order codes, binary arithmetic, conditional jumps, etc. He returned to Cox's Leeds group well equipped for a decade of developing advanced X-ray crystallographic methods and carrying out high quality structural studies.

Written in memory of Durward Cruickshank, who taught me the importance of Crystallographic Heritage.

Dr Brian Beagley – a BCA Founder Member

Leeds and the development of crystallography – the biological strand

AS Brian Beagley discusses in his article above, the University of Leeds has played a major role in the early development of crystallography. Parallel to the small molecule strand that he focusses on, Leeds has also been very important in crystallographic developments on the biological front.

As with the small molecule work at Leeds, W.H. Bragg was instrumental in getting a biological strand going. Regretting that, while in Leeds he had been unable to apply his research to help the local textile industry, he supported the application of Bill Astbury – then with Bragg at the RI – for the post of Lecturer in Textile Physics at Leeds. Starting by working on wool fibres, Astbury pioneered the use of X-rays in fibre diffraction, developing his laboratory into what Max Perutz hailed as "the X-ray Vatican". It was in his laboratory that the first X-ray pictures of DNA were taken with Florence Bell in 1938. Astbury also coined the terms 'Alpha' and 'Beta' for the diffraction patterns of major forms of protein structure.

Astbury's vision to establish Leeds as the national centre for molecular biology (he published the first definition of the term) led to the university establishing its Department of Biomolecular Structure soon after World War II. Following Astbury's premature death in 1961, the Astbury Department of Biophysics was formed by joining up with the Plant Biophysics unit under R.D. Preston. He took advantage of the favourable university

funding environment of the 1960s, resulting in a new building (designed by the architects of the Barbican in London*) that was equipped to world class standards. One particularly important outcome of this period was the solution and publication in 1968 of the 'Cross-beta' protein structure by Sandy Geddes and colleagues. This is now all the rage as beta-amyloid implicated in Alzheimer's disease.

When Preston retired in the early 1970s, Tony North took over the Department as Professor of Molecular Biophysics, expanding the department's work into protein crystallography. This was consolidated with the appointment of Simon Phillips in 1985 (as a 'new Blood' lecturer – the oldies among us will remember those!). And the rest – as they say – is history, with

the Astbury Centre for Structural Molecular Biology in Leeds now a multidisciplinary research centre with an international research reputation.

John Finney – with acknowledgment to Simon Phillips

**As an aside, the Barbican concert hall doesn't have a central aisle but doors at the ends of the seating rows – an 'innovation' that was carried over to the new building's lecture theatre in Leeds. Not good for getting mikes to those asking questions after a talk, but great for latecomers...*

Disordered Materials User Group Meeting

THE Disordered Materials Group at the ISIS Neutron and Muon Source held a virtual group meeting, over Zoom, on the afternoon of 8th January 2022. The meeting kicked off with a facility update from new ISIS Director, **Roger Eccleston**. He discussed the progress of various facility-wide projects, including the update to the first target station, the planned 'Endeavour' project of new instruments and instrument upgrades (see *Crystallography News* December 2021), and longer-term feasibility studies for a next generation 'ISIS-II' neutron source. The Disordered Materials Group leader, **Daniel Bowron**, then gave an update from the group. He highlighted instrument upgrades including the installation of a 'pop-up' neutron camera in NIMROD to check sample positioning and homogeneity, and an upgrade to the SANDALS incident beamline: with square collimation and a frame overlap chopper that will increase flux to sample and decrease backgrounds. An update on the ISIS deuteration lab. was then given by its operations manager, **Sarah Youngs**, who presented the range of deuterated chemicals that can be produced by the lab. to support user experiments.

There followed a series of software updates: **Tristan Youngs** provided a summary of the *Dissolve* software that is being developed in the group to provide the future simulation-based analysis tools for the group's instruments.¹ The software can replicate the results of the Empirical Potential Structure Refinement (EPSR) code and has been extended allowing, for example, analysis of adsorbates contained within metal-organic frameworks (MOFs). The user-friendly graphical user interface was demonstrated as part of the meeting, with a complete MOF simulation set up during the talk. A second key software development for the group has been the development of a new Python GUI for the Gudrun data reduction software, led by industrial placement student **Jared Swift**. Jared gave an overview of the GUI which reproduces the existing capability of the Java GUI and extends it to allow, for instance, easier assignment of sample composition and automatic reporting and plotting of results. Thirdly, industrial placement student

Ethan Devlin is leading development of new *JournalViewer* software used throughout ISIS, and he gave a thorough overview of current features and improvements, illustrating plotting of sample environment data and grouping on similar sample data in a live demo.

The majority of the meeting was a long overdue chance for disordered materials neutron users to share their new results. These covered areas of glass science, liquid structure and chemistry, materials science and geochemistry. In the field of glass science, **Gavin Mountjoy** (University of Kent) gave a talk on 'The effect of fluorine on calcium silicate glass structure from neutron diffraction, X-ray absorption spectroscopy, NMR, and molecular dynamics'. The direct application of this work is to fluoride release from toothpastes, with CaO-SiO₂-CaF₂ as model system. Successful analysis required use of neutron scattering on GEM, NMR and X-ray spectroscopy to guide fitting for structural changes upon changes in fluoride content². **Stephen Wilke** from Materials Development Inc. then presented 'Octahedral oxide glass networks at ambient pressure: Structure of neodymium titanate glass'. Stephen showed how containerless sample techniques were used to study small samples of these glasses, allowing the use of isotopic substitution and EPSR methods to understand the structure. The final talk on glasses was from **Alfred Amon** (UCL) on 'Structure of the mixed-molecular inorganic glass Ga₂l₃.17'. Neutron diffraction on the GEM instrument was used to characterise local structure in this novel ion-conducting mixed molecular glass.³

Talks on liquid structure determination included a presentation by **Johanna Busch** (University of Rostock) on 'When Like-Charged Ions Attract: The Influence of Hydroxyl Defects on the Size and Distribution of Cation Clusters in Ionic Liquids'. Molecular dynamics simulation and neutron diffraction on NIMROD with analysis using *Dissolve* were used to uncover changes in cluster structures with the removal of some hydroxyl groups. **Anita Zeidler** (University of Bath) gave a talk on 'Structure and dynamics of aqueous NaCl solutions at high

temperatures and pressures'. The study was conducted on D4c at the ILL, with the talk highlighting the critical importance of careful sample synthesis ensuring sufficiently pure samples for successful isotopic substitution measurements on the chloride.⁴ The final liquid structure talk was from **Bob Baker** (Trinity College Dublin) entitled 'Can neutrons help actinide science? A case study of aqueous thorium and uranium compounds'. Aqueous Uranyl Chloride structure was studied using neutron scattering measurements on SANDALS, allowing a full understanding of these important model systems for nuclear material storage assessments.

Talks on more applied systems included a presentation from **Maria Diaz-Lopez** (Diamond Light Source) on 'Effect of short-range order in the Li-diffusion of 'disordered' rock-salt cathodes'. This presented *operando* X-ray total scattering allowing an analysis of diffuse scattering peaks during cycling to reveal local structure changes in nanoscale Li_2MnO_3 .⁵

Leslie Ruppert (US Geological Survey) gave the presentation 'Understanding energy resources with total neutron scattering: Porosity and CO_2 and CH_4 behaviour in shales revealed using the NIMROD'. Here reservoir shale samples were studied, with the wide Q-range of NIMROD allowing a simultaneous determination of pore filling, liquid structure and mineralogy of the samples under geological pressures of methane and carbon dioxide. The results of this study are expected to help steer our understanding and approaches to gas extraction and geological carbon dioxide sequestration.^{6,7}

Lastly, it is worth noting that the postponed in-person version of the meeting, allowing for more talks and time for active discussion, is due to take place at The Cosener's House, Abingdon from 14th-17th June 2022. You can find them and the registration information at:

<https://www.isis.stfc.ac.uk/Pages/DMUGM2022.aspx>

Tom Headen
ISIS Neutron and Muon Source, Rutherford Appleton Laboratory

References:

1. T. Youngs. *Mol. Phys.* **117**, 3464 (2019).
<https://doi.org/10.1080/00268976.2019.1651918>.
2. L. F. Chungong *et al.* *Biomedical Glasses* **5**, 112 (2019).
<https://doi.org/10.1515/bglass-2019-0010>.
3. A. Amon *et al.* *Inorganic Chemistry* **60**, 6319 (2021).
<https://doi.org/10.1021/acs.inorgchem.1c00049>.
4. A. Polidori *et al.* *J. Chem. Phys.* **155**, 194506 (2021).
<https://doi.org/10.1063/5.0067166>.
5. M. Diaz-Lopez *et al.* *J. Mater. Chem. A* **8**, 10998 (2020).
6. L. F. Ruppert *et al.* *Energy & Fuels* **34**, 2765 (2020).
7. A. M. Jubb *et al.* *Energy & Fuels* **34**, 10926 (2020).

BCA Statement on Ukraine

The BCA Council has issued the following statement on behalf of the British Crystallographic Association.

• Statement of Support for Ukraine •

The British Crystallographic Association condemns the terrible attacks on Ukraine by Russian armed forces which have precipitated a rapid and enduring humanitarian crisis. We are deeply concerned about the lives and wellbeing of our fellow Ukrainian crystallographers, scientists and citizens, and the future of crystallographic science in the country.

In common with many scientific fields, crystallography has thrived and progressed through international co-operation and sharing of knowledge. We add this appeal for a rapid end to the hostilities to those of many scientific organisations, communities and scientists around the world, including many Russians who have spoken out against the war.

The BCA will endeavour to assist Ukrainian colleagues displaced by war by offering to share information for those seeking temporary positions in the UK.

• How to help •

Support the Ukraine Humanitarian Appeal by donating to or fundraising for the Disasters Emergency Committee:

<https://www.dec.org.uk/>

The Council for At Risk Academics offers support to academics who have been forced to flee their homes due to violence or conflict. You can support them by donating or by volunteering in some of their programmes in the UK:

<https://www.cara.ngo/how-to-help/>

Please direct any enquiries to BCA President Richard Cooper

president@crystallography.org.uk

Meetings of interest

WITH a little less concern about the virus, the conference scene seems to have been significantly revitalised, with quite a lot of new meetings being organised – so you might find something new and interesting in this list. 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, john.finney@ucl.ac.uk.

5th Jun 2022 - 10th June 2022

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

<https://euchemsil2022.org/>

9th Jun 2022 - 10th June 2022

Assembling Matter at all Scales
Dresden, Germany.

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

14th Jun 2022 - 17th June 2022

Cryo-EM Course
Online

<https://www.bnl.gov/cryoemcourse/>

19th Jun 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 Jun 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>

28th Jun 2022 - 1st July 2022

14th International Conference on Biology and Synchrotron Radiation
Lund, Sweden.

<https://www.bsr14.com/>

3rd Jul 2022 - 9th Jul 2022

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

<https://wp.nyu.edu/abudhabi-iccoss2021/>

4th Jul 2022 - 6th Jul 2022

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

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

4th Jul 2022 - 8th Jul 2022

Combined Analysis using X-ray Scattering
Caen, France.

<https://www.ecole.ensicaen.fr/~chateign/formation/agendas/Flyer-workshop-CA-2022.pdf>

10th Jul 2022 - 15th Jul 2022

XAFS 2022
Sydney, Australia and online.

<https://xrayabsorption.org/xafs2022/>

10th Jul 2022 - 15th Jul 2022

ECS7. 7th European Crystallographic School
Lisbon, Portugal.

<https://ecs7.events.chemistry.pt/>

10th Jul 2022 - 16th Jul 2022

16th International Conference on the Physics of Non-Crystalline
Solids
Canterbury, U.K.

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

13th Jul 2022 - 15th Jul 2022

Challenges in Biological Cryo-electron Microscopy: Faraday
Discussion
Sheffield, U.K. and online.

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

18th Jul 2022 - 22nd Jul 2022

2nd International Conference on Noncovalent Interactions
Strasbourg, France.

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

20th Jul 2022 - 23rd Jul 2022

3rd European School on Crystal Growth
Paris, France.

<https://www.escg3-eccg7-paris2022.insight-outside.fr/>

25th Jul 2022 - 27th Jul 2022

7th European Conference on Crystal Growth
Paris, France.

<https://www.escg3-eccg7-paris2022.insight-outside.fr/>

29th Jul 2022 - 3rd Aug 2022

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

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

1st Aug 2022 - 5th Aug 2022

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

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

7th Aug 2022 - 12th Aug 2022

Bioinspired Materials
Andermatt, Switzerland.

<https://bioinspired2022.ch/>

21st Aug 2022 - 26th Aug 2022

CMD29 (Condensed Matter Division of the European Physical
Society)
Manchester, U.K.

<https://cmd29.iopconfs.org/>

21st Aug 2022 - 25th Aug 2022

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

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

21st Aug 2022 - 26th Aug 2022

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

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

22nd Aug 2022 - 25th Aug 2022

15th International School and Symposium on Synchrotron
Radiation in Natural Sciences
Przegorzały (near Krakow), Poland.

<https://www.issrns2022.synchrotron.org.pl/>

22nd Aug 2022 - 25th Aug 2022

International Cryo-EM Workshop for Advanced Materials
Albuquerque, NM, U.S.A.

watt@lanl.gov

23rd Aug 2022 - 27th Aug 2022

33rd European Crystallographic Meeting (ECM33)
Versailles, France.

<https://www.ecm33.fr/>

29th Aug 2022 - 1st Sep 2022

Electron Crystallography School
Paris, France.

<https://ecs2022.sciencesconf.org/>

8th Sep 2022 - 9th Sep 2022

STOE User Meeting
Darmstadt, Germany and online.

<https://www.stoe.com/meeting/>

11th Sep 2022 - 16th Sep 2022

XVIII International Small Angle Scattering Conference
Campinas-SP, Brazil. Hybrid.

<https://pages.cnpem.br/sas2022/>



Chilled Out

This is how we want you to feel when using an Oxford Cryosystems cooling device. You already know that our products are the highest quality, designed by experts with over 30 years' experience in manufacturing coolers optimised for X-ray crystallography. You probably know that our technical support team are consistently praised for their friendly, fast and efficient approach.

You may not know, however, that our Cryoconnector software is available for all of our devices, and allows you to monitor and control your system remotely. It will even send you an email if your device status changes.

So you can just relax and let us do the work...

For further information visit
www.oxcryo.com



Cobra



Helix



PheniX



Chimera



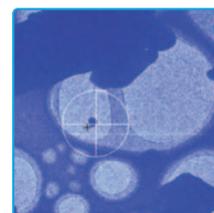
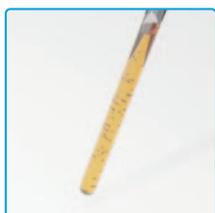
Cryostream



OxfordCryosystems

WHATEVER THE SIZE OF YOUR CRYSTALS, WE HAVE A DIFFRACTOMETER FOR YOU

- A full range of diffractometers in every performance class
- HyPix technology for noise-free direct detection
- CrysAlis^{Pro} software powers all of our diffractometers



As a researcher, you might not be able to choose the size of crystals you can grow, but you can choose the diffractometer you use to study them. At Rigaku Oxford Diffraction, we have developed a diffractometer in every performance class, from the XtaLAB mini II, the world's most compact diffractometer, to the XtaLAB Synergy-ED, the world's first commercially available electron diffractometer. Choose your diffractometer to fit your research. Choose Rigaku.

