# Crystallography News

## British Crystallographic Association

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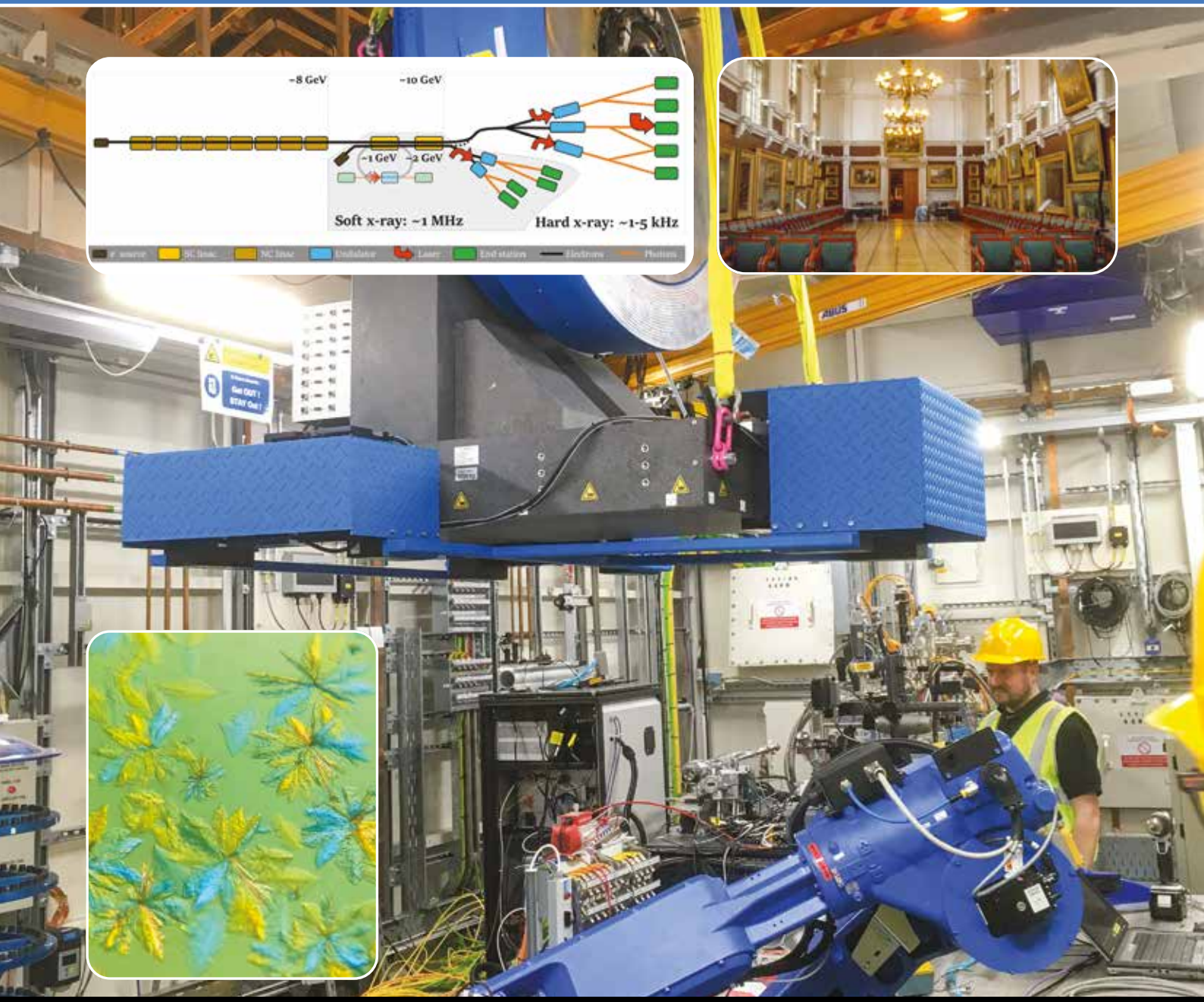


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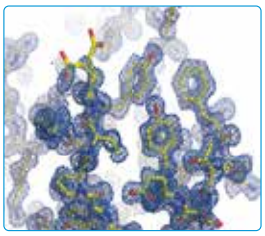
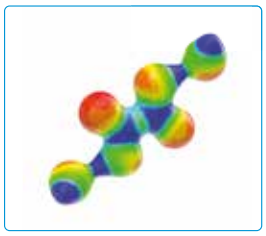
Density maps from a ten minute thaumatin dataset solved by S-SAD phasing





Electron density from a 0.37 Å quantum crystallography measurement of oxalic acid

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British Crystallographic Association

# Bursaries for conference attendance in 2020/21

Bursaries and awards are available as normal to BCA members through the Arnold Beevers Bursary Fund and the BCA Industrial Group.

BCA members who are students/post-docs/junior or non-permanent staff are eligible to apply for bursaries to attend BCA Spring meetings and other crystallographic meetings. Applications should be made via the website:
https://crystallography.org.uk/prizes/bursaries

Additional Carers grants are available to BCA members at any career stage:
https://industrial.crystallography.org.uk/bursaries-and-awards/

Applications for ABBF and IG bursaries can be made at the ABBF portal on the BCA website, and for the Carers award on the IG website

General Assembly and Congress of the International Union of Crystallography
IUCr XXV
Praha 2021
25

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**CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.**
**Please ensure that items for inclusion in the December 2020 issue are sent to the Editor to arrive before 25 October 2020.**

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

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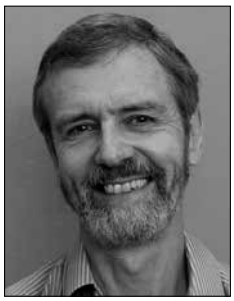
## *This month's cover:*

*DIAMOND I11 diffractometer installation; a conceptual outline UK XFEL; RHUL Picture Gallery; SARS-CoV-2 protease crystals.*

# From the President



**IN my previous column I described the view from my window over an empty village recreation ground where the local children should have been playing football. Now it's July, and the children are back on the field as the lockdown gradually eases, but it's still not life as we know it with social distancing, masks and Perspex screens becoming the norm. We hear a lot about the 'New Normal', and how successful working from home can be, avoiding the commute and communicating via Zoom. Crystallographers already have some experience of this, with remote use of synchrotron data collection, and increased use of automation in the home lab.**

I had an interesting early experience of remote working at a conference in the mid-2000s. I sat next to another crystallographer on a coach, probably one shipping us off to a conference dinner or on a trip, and we got talking. He worked for the Joint Center for Structural Genomics (JCSG), which was based at the Scripps Institute in San Diego and used the Stanford Synchrotron Radiation Lightsource (SSRL), 500 miles away for data collection. He was solving protein structures, starting, in each case, from the gene for the target protein, cloning it, expressing and crystallizing the protein, collecting the data at SSRL, solving and then refining the structure. He dropped the bombshell comment that he actually lived in an apartment in Houston, and did every stage of his projects remotely, only visiting the Scripps lab. occasionally for meetings.

There were people, of course, at JCSG and SSRL supporting the robots, feeding them reagents and supplies, and mounting crystals (a very tricky procedure to automate) etc. The macromolecular crystallographers will remember the excitement in the late 1990s around Structural Genomics, the possibility of using the newly-determined genome sequences to obtain crystal structures for all the proteins in an organism. Projects were set up in Japan, the USA and Europe to address this challenge. High funding levels, and pressure to deliver large numbers of structures, drove efficiency, innovation and automation. Although the holy grail of solving all structures for an organism proved overambitious, huge advances were made in the technology that remain in routine use. Lab. robots and automated remote data collection, for instance, are the norm for macromolecular crystallographers, but no longer their sole preserve.

The experience of my Texan friend was not unlike that of people working from home in the current pandemic, and it clearly worked, but it was riding on the back of impressive innovation and facilities that had been developed previously. I suspect such ground-breaking ideas would be unlikely to emerge from ten people sitting in their individual apartments using Zoom, but more likely if they were brainstorming in a face-to-face meeting in the lab. I think we would all value getting back into the lab., socialising with colleagues and batting ideas around, as well as actually doing experiments. I also worry about the psychological effects of social isolation.

In fact, such a 'New Normal' had actually been foreseen by **E.M. Forster**. Many readers will be familiar with his classic novels, such as 'A Room with a View' or 'A Passage to India'. Remarkably, Forster wrote a short story in 1909 entitled 'The Machine Stops', which is well worth reading. He describes a world where everyone lives individually in underground cells and rarely visits the surface or travels. All their needs, food, water, heating, air etc. are catered for by the Machine, but no-one knows how it works. People communicate using a device uncannily like a modern tablet, complete with video, connected to a system like the internet. They amuse themselves by giving each other lectures on various topics, recipes etc., rather like Facebook, YouTube and Zoom today. It all goes wrong when the Machine starts to run down and no-one can fix it. The idea was picked up by the prolific science fiction writer **Isaac Asimov**, who describes a similar world in 'The Naked Sun' (1957), with more advanced communication using holographic images. Unsurprisingly, things do not go well there either. Asimov was a chemist who taught biochemistry at Boston University, and a friend of **Linus Pauling**. He had many interests including crystals and imaging, once describing a spoof four-dimensional compound, thiotimolene, that was so soluble that its crystals began to dissolve even before water was added, reminding us of those pesky crystals that fall apart before you can get them mounted.

Back in the real world, the crystallographic community is continuing its attack on the structure of the SARS-CoV-2 virus. At the time of writing there are 260 total protein structures, mostly from crystallography, and 75 EM density maps in the databanks. This corresponds to structures for about half the proteins in the virus, and the total will have increased by the time this issue is published. Structures of the spike protein, and its complexes, underpin efforts on possible antibody therapies, drug design and vaccines, while the internal replicase and protease are key targets for novel drug leads.

The BCA Council has continued to meet via Zoom and business is moving forward on its usual schedule. The planning committee for the 2021 Spring Meeting in Leeds met, via Zoom, in July and discussed the prospect of running it as a 'normal' meeting. The conclusion was that it was unlikely to be practical, and the decision was taken to convert it to a virtual meeting. Details appear elsewhere in this issue. The University of Leeds was helpful, and the 2022 Spring Meeting will now be held there, at no additional cost to the BCA.

The BCA Annual General Meeting was held via a Zoom webinar on 18th June. The technology worked well, thanks to our expert Secretary, Alex Stanley, and to the over 40 participants who joined. The full set of presentations is available in the Members' Area of the BCA website, and the minutes will be published later this year. Important resolutions passed included the acceptance of the Examining Accountant's report, and three proposals for updates to the Statutes and By-Laws. The updates were additions to allow formally for the AGM to be held electronically, on keeping the minutes, and some corrections to remove some sections that were not gender-neutral.

I would like to send my best wishes to you, and your families, as we gradually emerge from this crisis.

**Simon Phillips**

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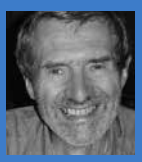

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*(The dates in parentheses indicate the end of the term of office).*
Full committee details on the BCA website **www.crystallography.org.uk**

# From the Editor

**SINCE the early Spring, I expect many of us will have been 'attending' (or giving!) online lectures and/or 'participating' in online conferences or workshops.**

We'll have seen many of the advantages over being there in person. Not having to travel saves us time, allows us to participate while looking after the kids, and reduces our carbon footprint. For international meetings, visa restrictions become irrelevant, so encouraging scientific collaborations across politically restrictive borders. Ease of access to online meetings has encouraged me to 'attend' some that aren't central to my main research interests, widening my view of what is going on and even suggesting I might contribute something in other areas. And we don't have to pay for the travel and accommodation – particularly useful if, like me, you no longer have a research budget. Sadly, however, some conferences still charge a significant registration fee. Can a fee of $250 to 'attend' the American Conference on Neutron Scattering be justified to cover what will surely be a relatively low overhead?

On the other hand, we will have recognised many disadvantages from not being there in person. Forgetting technical issues arising through failure of software or inadequate bandwidth, what has frustrated me most has been the clunkiness of discussions after talks. When you are in the room, you can stick your hand up and wave it around to alert the chair that you are there. But if you are one of a couple of hundred somewhere in the ether, getting recognised is more difficult. If your version of Zoom or Teams supports the 'hand raising' option, then you can try using that. But my experience is that the chair often fails to see such raised hands. Some events use either a 'chat' or 'Q & A' function, in which you type in your question and hope that the moderator picks it up on his or her screen. In one webinar I 'attended', 130 questions were typed in *during the speaker's 30 minute talk itself*. This did seem to me to mean the speaker wasn't getting the attention he should have done as many people were too busy typing in their questions. And a further problem is the difficulty of coming back on a speaker's answer to a question.

Apart from these 'mechanistic' issues, what these virtual meetings cannot reproduce are the personal interactions between scientists – as is also emphasised in Simon Phillips' column two pages back. If I'm using Zoom, I might be able to use the chat function to discuss privately by text issues with certain others 'present'; but this can't replace the discussions 'in the margins' – whether those margins be on a conference outing, over coffee or dinner, or in the bar. Looking back at the scientific collaborations I have had, two of the most fruitful arose quite by accident at conferences abroad. At one of these, neither my future collaborator (a biochemist) nor I (a physicist) could work out why we were invited to this particular conference as it wasn't central to the interests of either of us. We suspected the conference organiser had seen the possible common interests so had slyly got us together over dinner, where our common vinous interests helped to lubricate the beginnings of a very fruitful – and mutually enjoyable – long interdisciplinary collaboration. That people are more likely to develop new ideas and approaches when they meet has certainly been borne out in my experience.

And there is the important matter of trust between scientists. The trust and mutual understanding built up through the initial personal contact makes it easier to have effective subsequent online interaction.

While perhaps most of these positive and negative aspects are fairly obvious, my eye was caught by an article on page 19 of the July 2020 Physics World. Entitled 'The danger of going online only', it was written by a science sociologist (Harry Collins from Cardiff) and two physicists (Bill Barnes from Exeter and Riccardo Sapienza from Imperial College London). While recognising the real advantages of virtual workshops and conferences, they flagged up an issue that at first sight may seem subtle, but is critical to the success of science.

These authors argue that face-to-face communication *plays a fundamental role in the social aspects of science*. The common 'language' that scientists develop at in-person conferences is not only learned there by students but also developed and improved upon by researchers. "It is this process of 'socialization' that teaches values central to science" they assert. Furthermore, they argue that the aspects of science that make it special are developed face-to-face and are unlikely to happen through the web. And what is particularly worrying, "...if the boundary between information and misinformation comes to be fought out over the Internet rather than the seminar or workshop, science will lose the battle" (think climate change and MMR vaccination for example).

They say further: "This means that new generations need to be inducted into the fundamental norm of integrity, which defines the social institution of science and the foundations of the scientific discipline. It starts with education, where at meetings the relationship of authority and truth in science is revealed because a Ph.D. student can, and sometimes does, criticize a Nobel laureate. That truth must be seen to trump authority is another crucial value of science".

Obviously we must capitalise on the advantages of online meetings and improve their effectiveness, but they shouldn't be seen as the most effective way of working. As these authors conclude: "For areas that are well established there is perhaps less danger for a shift to an online world, but for those that involve much disagreement and passion, face-to-face will be the only way to propel the science forward".

Enough of my ramblings. I hope you enjoy the articles – and the puzzle (thanks Bob!) – we have put together for your Autumn delectation. In addition to a preview of the 2021 Spring Meeting programme, these include the exciting possibilities of a UK X-ray free-electron laser, insight into the crystallographic work going on at Diamond, and what is likely to come from Covid-19 work using neutrons at the ILL. For those of you tearing your hair out with the kids at home, there are some new scientific home learning activities for children arising from the ISYP Crystals project. Down Memory Lane is Moreton Moore at previous BCA Spring Meetings, and something for the oldies who remember Algol. And sadly, we say goodbye and thank you to Mark Ladd.

**John Finney**

# Nominations for BCA Council

There will be Council elections this year for the following posts:

- BCA President
- One Ordinary Member
- Education and Outreach Co-ordinator

Any two Members may make nominations. These should be accompanied by the written consent of the candidate to serve if elected.

Nominations must be received by the Secretary (secretary@crystallography.org.uk) by the 30th September 2020.

The successful candidates will take office from the end of the 2021 AGM and serve until the AGM in 2024. Council normally meets twice each year, with one of those meetings during the annual Spring Meeting.

## 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.
- Free insert in the annual Spring Meeting delegate pack.
- Two free non-residential registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly Crystallography News.
- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

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

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### Benefits of Individual BCA Membership:

- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

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

# BCA-BACG 2021 Joint Spring Meeting

## 29th March-1st April 2021 · Online

**READERS of Crystallography News will know that the BCA Spring Meeting planned for Leeds in 2020 had to be cancelled at short notice due to the Covid-19 pandemic. We had hoped that the situation would be improved by Spring 2021, and the Organising Committee planned to keep much of the programme for delivery in 2021 in Leeds, but with the exciting news that the Spring Meeting would be held as a joint event with the British Association for Crystal Growth (BACG). To reflect the interests of both organisations, the intention was to have a series of joint sessions on themes of interest to both BCA and BACG members.**

However, given the current uncertainty with regards to what large gatherings may be possible in the near future, the committees of both BCA and BACG have very recently decided that the 2021 Spring Meeting should be held as a virtual conference, using a virtual conference platform where all the sessions will be available to watch. Details of the sessions will be made available to all those who register to 'attend' the conference. Planning is well under way to provide an exciting scientific programme that should provide excellent synergy between the BCA and BACG as well as Association-specific elements. Brief descriptions of sessions that are provisionally planned are given below.

The joint Programme Team will develop a series of joint sessions on themes of common interest to BCA and BACG members focussed on the areas of crystal engineering, crystal structure prediction and bio-mineralisation. The BACG organisation team will develop sessions on topics unique to the crystallisation community around the themes of nucleation, growth and industrial crystallisation. The BCA team will offer sessions themed around the sub-groups as usual.

The intended format and approach are still being finalised. However, at this stage a vibrant and dynamic programme is envisaged that will also include opportunities for lively poster sessions, sponsor and exhibitor events, and sessions that will allow active networking and discussion. The programme will reflect common interests, passion, enthusiasm for crystals, and crystallography within both organisations and the meeting will provide an opportunity to rekindle and reflect on the historical overlap between crystallisation and crystallography.

Provisional dates are Monday March 29th to Thursday April 1st 2021. The BACG Organising Committee for 2021 is Dr Linda Seton, Dr Grahame Woollam and Prof Nick Blagden, and the BCA Programme Chair is Dr Tom Edwards.

**Tom Edwards**
(University of Leeds)
**Nick Blagden**
(University of Lincoln)

# *Puzzle Corner*

Crystallographers need to know a lot about probability, and a good exercise is calculating the probability of a particular poker hand.

The easiest to calculate, and the least probable to obtain, is the Royal Flush: 10, Jack, Queen, King, Ace, all of the same suit.

What is the chance, if you are dealt 5 cards at random from a full 52 card pack (no jokers), that you will have a Royal Flush in your hand?

# SESSION DETAILS

## YCG/BACG Early Career Satellite Meeting

The YCG/BACG meeting is an opportunity for all early career researchers in the field of Crystallography, from Master's students to postdocs, to present their work in a supportive and friendly environment. Previous YCG meetings have covered a wide range of interests, spanning all the disciplines of the interest groups that make up the BCA community. This year with the incorporation of the early career British Association of Crystal Growth (BACG) community it is hoped that the diversity of research represented will be expanded even further. To reflect the incorporation of the BACG in this event we encourage YCG members to consider highlighting some of the crystallisation approaches that they have employed that often might not be the focal point of their research.

## YCG/IG: A Career In Crystallography: Exploring the Interface of Academia and Industry

Crystallography can lead to a wide range of exciting and varied careers. The start of this session will feature research talks exploring research interests in academia, industry and at national facilities. The session will also offer a question and answer forum to discuss careers in crystallography and crystal growing with a selected panel of crystallographers and crystal growers who have taken different career paths. This session has been designed to provide greater information about the variety of careers available for early career researchers, with attendees able to ask questions they have about the careers of the panellists.

# BSG SESSION DETAILS

## BSG Plenary: Rosalind Franklin Centenary Lecture

**Chair:** **Prof. Elspeth Garman (Oxford)**

**Speaker:** **Prof. Gabriel Waksman (UCL/Birkbeck)**
Mechanism of effector targeting by the Legionella type IV secretion system

## Structure-based drug design

**Chair:** **Prof. Jane Endicott (Newcastle)**

**Keynote:** **Dr Pamela Williams (Astex)**
Structure-based drug discovery: how did we get here and where are we going?

Protein structures can assist drug development at all stages of the discovery pipeline, from choosing targets, through identifying hit matter, to supporting iterative medicinal chemistry to enhance potency, pharmacokinetics and pharmacodynamics. Historically, structure-based drug design has addressed well characterised active sites by identifying potential molecular interactions to inform subsequent chemical synthesis. Application of this approach has already contributed to the development of many potent and selective drugs. However, molecular targets with clear disease linkage can be extremely difficult to find, and for this reason more is being asked of structures in drug discovery campaigns. Examples of these new contributions include characterising and capturing biologically relevant protein conformations to help in the targeting of allosteric sites, and identifying novel classes of target that depend on protein-protein and protein-DNA/RNA/lipid interactions. The keynote lecture will review key advances in the field over the last decade and future possible directions while reflecting on what a drug discovery campaign looks like from the structural biologist's point of view.

## Time-resolved crystallography

**Chair:** **Dr Briony Yorke (Bradford)**

**Keynote:** **Prof. Jasper van Thor (Imperial)**
Optical control of protein structural dynamics by ultrafast X-ray crystallography

Time-resolved crystallography allows the observation of molecular mechanism in real time, providing unique insight into the dynamics that link structure and function. The use of X-ray free-electron lasers has pushed the boundaries of time-resolved crystallography, allowing structural changes to be determined with femtosecond time-resolution. The development of serial crystallographic techniques has also initiated a resurgence in synchrotron time-resolved experiments. This session will focus on the exciting developments being made at free-electron laser and synchrotron sources and the science that has been made possible due to these developments. Contributions describing these and other structural time-resolved methods are welcomed.

## Enzymes

**Chair:** **Dr Wyatt Yue (Oxford)**

**Keynote:** **Prof. Peter Moody (Leicester)**
Using neutron crystallography to watch hydrogens in heme enzymes

Metabolic enzymes catalyse the biochemical reactions associated with survival and homeostasis in living organisms while the processes governing the behaviour of cells are mediated by tightly regulated cascades and complexes of cell signalling enzymes. Enzymes that perform various types of chemistry are therefore studied intensively in the fields of biochemistry and molecular cell biology. The essentiality of metabolic enzymes is underscored by various genetic and common disorders associated with their deficiency. Enzymes are also central to the field of biotechnology, where they are engineered to manufacture novel products or act upon novel substrates. This session will include examples of work in which structural biology methods are answering important questions relating to the activity and regulation of enzymes, with a view to understanding their functional, biotechnological and therapeutic applications.

## Computational biophysics

**Chair:** **Dr Matteo Degiacomi (Durham)**

**Keynote:** **Prof. Franca Fraternali (King's)**
Protein-protein interactions in health and disease: the importance of 3D structure

To successfully carry out their task in an organism, biomolecules must interact with their designated substrates in a controlled manner. The function of a biomolecule thus emerges from its specific atomic structure and associated dynamics. Many computational techniques, as diverse as molecular dynamics simulations, homology modelling and protein-protein/ligand docking, can leverage crystallographic data to characterize molecular structure, dynamics and interactions. This session will focus on the application and development of such techniques.

## Membrane proteins

**Chair:** **Prof. Bonnie Wallace (Birkbeck)**

**Keynote:** **Dr Amandine Marechal (UCL)**
Respiratory supercomplexes: what can we learn from yeast?

Membrane proteins span a wide range of structural and functional types, ranging from multimeric complexes to monomeric or multimeric channels, receptors, and enzymes. They perform very important functions in cells and many are of interest for pharmaceutical development. However, they have proved to be challenging for structural studies due to their amphipathic nature, with both hydrophobic and hydrophilic domains, and the requirement for detergents, amphipols, nanodiscs, and other amphiphiles to solubilise, purify, and stabilise them. This session will include examples of work demonstrating how recent developments in sample preparation and in the complementary techniques of cryo-Electron Microscopy and X-ray Crystallography are enabling structural studies of key membrane proteins.

## Protein-protein interactions

**Chair:** **Prof. Richard Bayliss (Leeds)**

**Keynote:** **Dr Elton Zeqiraj (Leeds)**
Structure and function of ubiquitin signalling complexes

Cellular processes depend entirely upon interactions between proteins, either for the transient or regulated recognition of one molecule by another in interaction networks or the stable assembly of individual proteins into higher order complexes. Specific molecular recognition in protein-protein interaction networks is crucial in cell signalling while protein complexes function in cells as molecular scaffolds, hubs for cell signalling or as molecular machines carrying out concerted functions. This session will include examples of work in which structural biology methods have been used to determine the molecular basis of interaction between proteins and their assembly into multiprotein complexes.

# IG SESSION DETAILS

**IG plenary:** **Marcus Neumann (Avant Garde Materials Simulation)**

**Chair:** **Helen Blade (AstraZeneca)**

**IG/BACG:** **Crystal growth/pitfalls and challenges**

**Chair:** **Natalie Johnson (CCDC, Cambridge)**

**Keynote:** **Adam Keates (Syngenta)**
Crystallisation in agrochemicals: The good, the bad and the ugly

The control and prediction of crystallisation processes is a challenge but vital in many areas of industry. This session will cover practical and computational methods that aim to link understanding with the development of control strategies and predictive approaches. Talks from the perspectives of crystallisation, solid form and characterisation will be welcome.

## IG/CCG: Control & prediction of crystals

**Chair:** **Angeles Pulido (CCDC, Cambridge)**

**Keynote:** **Dr Sten Nilsson-Lill (Computational Scientist, AstraZeneca)**
A Smörgåsbord of Predictive and Analysis Tools for Crystal Structures. Usage in pharmaceutical industry

This session aims to cover a wide range of research used to control and predict crystal structures including both experimental and computational tools. Talks will be welcome for the control and prediction of solid forms, particle and mechanical properties, and will be open to researchers from a wide range of fields: computational chemistry, informatics, solid state/crystallisation and materials science.

# PCG SESSION DETAILS

## Biominerals & Biomaterials

**Chair:** **Julia Parker (Diamond)**

**Keynote:** **Melinda Duer (Cambridge)**
The Bare Bones of Biomineralization: new insights into bone mineral composition, structure and formation

From the exquisite morphologies of coccoliths and the incredible hierarchical architecture of bone, to the engineering of implants and joint replacements, the structure of biominerals and biomaterials plays an integral role in determining their properties and function. This session will examine the importance of structure in both natural systems and biomedical devices, explore how their composition and assembly controls physical properties and look at how this can be exploited in the development of novel bio-inspired materials.

## Entropy & Structure

**Chair:** **Anthony Phillips (QMUL)**

**Keynote:** **Xavier Moya (Cambridge)**
Giant caloric effects near structural phase transitions

In recent years, entropy has become an explicit target of materials design and synthesis: configurational and magnetic entropy can stabilise materials' structures or form the basis of their functionality. Understanding such disorder requires a variety of experimental and computational techniques drawn both from the conventional crystallographic arsenal and beyond. In this session we welcome talks on all aspects of order and disorder: quantifying, designing, and exploiting entropy for materials ranging from high-entropy alloys to calorics.

## Structure and Properties of Low-Dimensional Materials

**Chair:** **Lucy Clark (Liverpool)**

**Keynote:** **Maria Grazia Francesconi (Hull)**
One-dimensional oxide and non-oxide materials

There are many examples of crystalline solids whose structures feature quasi-one-dimensional chains or two-dimensional planes of atoms giving rise to low-dimensional interactions. This results in a diverse array of intriguing physical phenomena, from high-temperature superconductivity in, for example, layered iron arsenides

to pronounced magnetocaloric effects in one-dimensional framework solids. Furthermore, since the isolation of graphene, there has been an explosion of activity in the discovery and characterisation of different classes of two-dimensional crystals with remarkable properties that may underpin future advanced technologies. As such, this session is dedicated to showcasing recent developments of crystallography and complementary characterisation methods in the determination of the fascinating structure-property relationships in a variety of low-dimensional solids.

## Structure and Properties of Higher-Dimensional Materials

**Chair:** **Phil Lightfoot (St Andrews)**

**Keynote:** **Fabio Orlandi (ISIS)**
Superspace formalism and materials properties

This session targets crystals and materials that go beyond a conventional description using three dimensional axes and indices. This includes aperiodic crystals, quasicrystals and incommensurately modulated crystals, structures, magnetic structures etc. Examples may include compounds exhibiting compositional, structural or spin disorder at the 3D level, but which is amenable to better description and rationalisation using 4D or higher dimensionality. We are interested in examples where the dimensionality may significantly affect materials' properties, as well as in the fundamental description and understanding of the higher-dimensional crystallography.

## PCG/CCG Structure Solutions from Powders

**PCG Chair:** **Karen Johnston (Durham),**
**CCG Chair:** **Jeremy Cockroft (UCL)**

**Keynote:** **Kenneth Shankland (Reading)**
Accelerating and enhancing the effectiveness of crystal structure determination from powder diffraction data

This joint session between the CCG and PCG explores structure solution from powders in a variety of organic, inorganic and mixed organic/inorganic systems. Despite considerable advances in the field, structure solution from powder diffraction is by no means routine and, increasingly, complementary methods are being used to aid structure determination. We are interested in recent examples where structure solution has been aided by complementary methods, including *in situ* and *in operando* techniques as well as total scattering methods. Examples where the combination of experimental and computational methods has resulted in successful structure solution are also of significant interest.

## Phase Transitions

**Chair:** **Lewis Owen (Cambridge)**

**Keynote:** **Joe Hriljac (Diamond Light Source)**
Phase transitions in zeolites driven by pressure and ion exchange

Phase transitions are of critical importance to our understanding of a material's structure and its physical and chemical properties. This session will aim to explore a broad range of structural phase transitions; from crystalline solid state transformations to crystalline-amorphous transitions. Particular interest will be placed on novel characterisation including novel experimental set-ups and techniques (e.g. Bragg diffraction, PDF, NMR etc.), data-processing methodologies, and structural parametrisation.

# CCG SESSION DETAILS

**CCG Plenary:** **Franziksa Emmerling (BAM, Berlin)**
Shaken not stirred: enhancing the flavour of mechanochemistry

**Chair:** **Hamish Yeung**

## Hot Structures

**Chair:** **Charlie McMonagle (ESRF)**

**Keynote:** **Sven Lidin (Lund)**
The simple, the challenging and the confusing: Making sense of complexities in reciprocal space.

In this session we look at the latest hot structures coming from the chemical crystallography community. These could be those found at very high temperatures (hot, hot, hot) or that feature an exciting design element or neat properties.

## Chemistry in Extreme Conditions

**Chair:** **Hamish Yeung**

**Keynote:** **Colin Pulham (Edinburgh)**
Putting the Squeeze on Molecular Materials

Crystallography has traditionally been a major technique with which to understand the structures and reactivity of molecules. This session focuses on how crystallography and other methods can reveal insight into phenomena that occur away from ambient conditions, such as at very high or low temperatures, high pressure or in electric fields. Think bonding, mechanics, distortions, phase transformations, changes in physical properties etc. – *in* and *ex situ* studies allowed!

## Advances in Software for Crystallography

**Chair:** **Lucy Saunders (Diamond Light Source)**

**Keynote:** **Florian Kleemis (moving locations)**
NoSpherA2: Non-spherical atom refinements for general application

This session aims to reveal the latest and exciting developments happening in crystallographic software. We encourage abstracts from those in the community working on software for chemical crystallography research. We want to know about the latest tools on offer. This could be in the areas of data processing, structure refinement, property calculation or structure investigation to name a few… and we want to hear about them!

## Electron Crystallography

**Chair:** **Simon Parsons (Edinburgh)**

**Keynote:** **Lukas Palatinus**
**(The Czech Academy of Sciences)**
Structure refinement from 3D electron diffraction: where are the limits?

Electron diffraction is one of the mostly rapidly developing and exciting areas of crystallography. The publication of a number of recent papers describing its application in chemical crystallography has led to a great deal of comment and anticipation in the chemical community. The technique enables crystal structures to be obtained from samples with dimensions of the order of a few microns, or even hundreds of nanometres. The strength of the interaction between electrons and matter that enables such small crystals to be studied carries with it the problem of multiple scattering, meaning that the kinematical model which has

been so successful for X-ray and neutron diffraction no longer applies, and dynamical effects need to be taken into account. This session will give an overview of the most recent advances in the field and progress towards making electron diffraction a more widely used technique in the chemical crystallography community.

# BACG SESSION DETAILS

## Annual Lecture and Medal Talk

Each year the BACG invites an individual who has made a significant contribution to crystal science to present The BACG Annual Lecture on a topic of interest to the community.

## BACG Young Scientists Award

This annual award recognises achievement by a young scientist publishing work in the field of crystal growth. The award is made annually to the candidate achieving the most significant advancement in the understanding of the theory, practice or characterisation of crystal growth processes, published in scientific literature in the previous three calendar years. The winner will receive a cheque for £250 and an engraved medal and will present the work at the annual conference following which the formal presentation of the award will be made by the President of the BACG. Details of criteria and how to enter are available on the BACG website https://www.bacg.co.uk/bacg-young-scientists-award/ Closing date for entry is 30th January 2021

## Nucleation – theory to practice

Integration of approaches is critical to achieve insight into the influence this step in the crystal growth journey imparts on the crystallisation process. This session will cover all aspects of nucleation, exploring the synergy between theory, simulation and experimental studies, along with novel techniques to probe nucleation.

## Crystal Growth – theory to practice

The session offers a platform to present our current understanding of crystal growth theory, including the contribution of simulation in understanding the mechanism and control of growth processes. The scope embraces the nature of the crystal growth front, evolution and intervention of morphology and analytical techniques to probe processes, leading to our observed experimental outcomes imparted, through the fundamentals of which we aim to understand this important process.

## Industrial Crystallisation – scale up / scale out

An industrial perspective of control and theory will underpin this session on all aspects of industrial crystallisation. The scope of the session will include simulation, scale up approaches and new platforms to undertake crystallisation. Contributions on the theme of batch processing case studies alongside continuous processing opportunities are particularly welcomed.

## *In situ* monitoring of crystallisation

This is an area of growing importance and the session has a broad scope. Historically *in situ* monitoring was largely limited to thermal microscopy. However, with advances in analytics, opportunities at light source facilities, and the development of new techniques, probing the detail of crystallisation is possible. This session is a platform to present studies of this type and demonstrate the new insights that can be glimmered. The scope includes contributions outside the area of diffraction or scattering.

## Crystallisation of Pharmaceuticals

All aspects of dosage from selection, pre-formulation considerations and pharmaceutical materials processing are within the remit of this session. The impact of screening, processing and stability on pharmaceutical products along with system specific examples of hydrates, solvates, salts and polymorphs relevant to dosage forms will be included. Contributions in the area of *in silico* tools for aiding screening and selection are of particular interest.

## Carbonaceous Materials

Since the emergence of $C_{60}$, the area of carbonaceous materials and their impact on all aspects of science has come to the fore. We seek to provide an opportunity to reflect this and provide a session where the nucleation, crystallisation and nano applications of these materials can be presented to a wider crystal science audience.

# JOINT BACG/ BCA SESSIONS

## Biominerals & Biomaterials

Joint with PCG. See details in BCA programme above.

## Crystal Engineering 1: Small molecule systems

Within this session the molecular, non-framework aspects of crystal engineering will be explored. The main focus will be the influence the supramolecular process imparts to the crystal science of these materials, and contributions are invited from areas including solid form, particle properties and gel to crystal transformations.

## Crystal Engineering 2: MOFS and open network systems

Within this session the framework aspects of crystal engineering will be covered. The focus is on MOFs and allied extended networks in clays, zeolites and minerals along with energy capture and green processing applications.

## Crystal Structure prediction

From theory to application within crystal structure prediction. This is an opportunity to highlight new approaches, search space and energy ranking optimisation, together with the wider impacts of theory insight into this area. A key feature is to be able to present the ongoing challenges and experiences to date.

# The Science Case for a UK XFEL

**WE offer here a short survey of the Science Case for a UK X-Ray Free-Electron Laser (XFEL) published on the 2nd July 2020. We will briefly highlight potential benefits of this proposed infrastructure to the crystallography community, as well as to the wider science and technology community in the UK. The case was prepared by a team of 25 UK based scientific experts from across a broad spread of disciplines (life scientists, materials scientists, nanotechnologists, physicists, chemists and biochemists) and were aided by over 80 additional expert advisors from both the UK and overseas. The STFC Project Champion John Collier, Director of the Central Laser Facility, has supported the process and enabled the Scientific Lead, Jon Marangos, Imperial College London and the science team to undertake the required discussions with the UK science and technology community and to develop the Science Case document.**

Many of the ideas that were input into the process came from contributions at a series of seven workshops run through the second half of 2019. These workshops were attended cumulatively by over 475 participants, many of whom contributed additional ideas and discussion. The full Science Case, released as a draft in anticipation of further input and augmentation, can be downloaded from the STFC website[1]. We are now extending the consultation until mid-September 2020, when we will update the case with any appropriate additions, after which the case will be reviewed by a panel commissioned by STFC.

The primary science driver for X-Ray Free-Electron Lasers is based around the opportunity they provide for real-time access to the characteristic processes and fluctuations in matter at the quantum scale. This is summarised in Figure 1 where examples in physical, chemical and life sciences are highlighted.

X-ray FELs enable atomic scale structure and electronic state resolution to be determined in a time resolved way, through measurements using a wide array of X-ray scattering and X-ray spectroscopy techniques. This provides information on structural and electronic dynamics on the crucial Ångström spatial and femtosecond temporal scales[2]. In contrast, conventional synchrotron sources, whilst highly suited to static measurements or for targeting longer timescales (microsecond timescale and slower phenomena), cannot access dynamics faster than ~ 100 picoseconds. The capability provided by XFELs is very timely as we are now in an era with many emerging technologies requiring a full understanding of matter at the quantum scale. For example, many sustainable technologies are energised by the light from the Sun, and a full understanding and optimisation of these requires tools to track the dynamics starting from the initial ultrafast photochemical/photophysical event. The high brightness of the X-ray pulses from XFELs also opens new opportunities in X-ray crystallography through enabling femtosecond serial nano-crystallography, that has generated multiple breakthroughs in protein structure determination in recent years[2,3,4,5,6,7], and of course time resolution of biochemical processes has been shown to be in reach through these methods[8,9].

The first XFEL (LCLS, Stanford, USA) began operating just 11 years ago, and in the subsequent decade we have seen, as well as the demonstration of high scientific impact from XFELs, that there have been major technology advances in XFEL sources. These go beyond conventional self-amplified spontaneous emission (SASE) operation and include, for example, improved spectral purity (through seeding schemes) and ultra-short pulse operation (through enhanced SASE operation) into the attosecond domain. High repetition rate operation is now developed using superconducting electron accelerators. For the Science Case we have taken a long view so we looked at what kind of science we will do with an advanced XFEL operating from 2030, extrapolating current

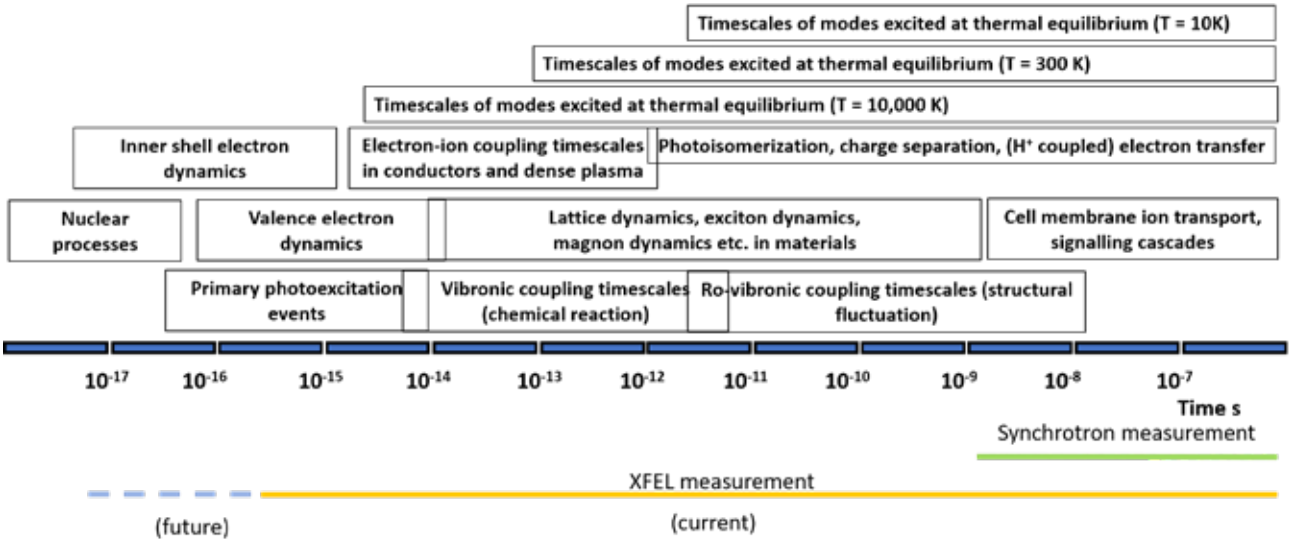



*Figure 1: Ultrafast timescales, from attosecond to nanosecond, which are vital for understanding the fundamental processes in chemical, material and living systems that can be captured with atomic spatial scale resolution using XFELs.*

technology advances to frame what will be possible then if an advanced XFEL is constructed. Whilst there are currently 5 X-ray FELs operating in the world with additional capacity planned in Shanghai (SHINE), along with additionally a handful of XUV/soft X-ray machines, they are already highly oversubscribed and with a continuing growth in user demand are unlikely to be sufficient for international and UK needs beyond a decade or so timescale. Moreover, all the operating machines were designed more than a decade ago, before the many exciting developments mentioned above had fully emerged. These machines were not built to fully benefit from all of that new technology and the exciting auxiliary developments in lasers, terahertz (THz) and electron beam sources that have been made in the meantime. As well as the additional capacity that a UK XFEL can provide, there are significant opportunities for important new capabilities that take full account of the technology developments of the last 10 years and those that are ongoing.

Here we will overview the (275 page) Science Case by looking at some science opportunities enabled by new capabilities that we anticipate will be within the planned specification of a UK XFEL. *Ultrafast X-rays* with ~ 250 attosecond duration across the soft X-ray (SXR) to the hard X-ray (HXR) range will enable probing of attosecond electron dynamics in complex molecules and condensed phase systems, uncover the mechanisms of radiation damage in technological materials and biomolecules and will give us unique access to the elementary processes in chemical reactions involving electron-nuclear coupling at conical intersections. *High X-ray intensity and high data rate* enabled by a high pulse repetition rate exceeding 100 kHz over the SXR range and at least 5 kHz in the HXR range, will allow exploration of the fundamentals of X-ray–matter interaction and the development of new concepts in time resolved imaging at the nanoscopic scale based around coherent diffraction imaging and data driven analysis methods[10]. *High energy/power optical lasers* and *bright X-rays* will provide access to the conditions inside planets, stars and shocked materials of high importance in engineering, defence and fusion energy. *High spectral purity X-rays* and *high data rates* will permit the probing and optimisation of quantum materials, ultrafast magnetisation and functional materials. *X-rays synchronized to ultrafast lasers, THz and electrons* will provide a powerful combination to uncover the fundamentals of chemical dynamics in the environment, space and energy materials. *High rep-rate multi-colour ultrafast X-rays* provide powerful approaches to systematic advances in catalysis by providing simultaneous access to multiple atomic absorption edges in the catalyst and reactant.

For crystallography the opportunities are equally rich. *Controlled X-rays and samples* enabled by a new generation of high brightness stable XFEL modes and advanced sample delivery concepts will extend the power of serial femtosecond nanocrystallography for advancing knowledge and drug discovery. *High data rate* through the high repetition rate XFEL and, equally importantly, high frame rate large dynamic range large area X-ray detectors, will advance the understanding of structural biology and biochemistry under the conditions of life. *Multi time-scale X-ray approaches* from femtoseconds to nanoseconds made possible by an X-ray FEL will unravel the complex dynamics of biochemistry: photosynthesis, vision and enzymology by combining time-resolved diffraction and time-resolved X-ray spectroscopy data. The importance of accessing biomolecular structure under biological conditions of temperature, pressure and aqueous environments are an important aspect of the Life Sciences use case for an XFEL[11].

The full range of science covered in the Science Case is both extensive and diverse. Some of the opportunities may be realised on a shorter time scale through work at existing XFELs, but we have identified a significant number of longer range and ambitious scientific areas that will require a machine with specifications well beyond the current range. In common with the existing machines, we identify that a photon energy range from 200 eV to greater than 20 keV in XFEL fundamental (up to 100 keV in harmonics) will be needed. For really cutting edge science a high repetition rate allowing high data rate acquisition is essential with 100 kHz to MHz repetition rate in soft X-ray, at least 2-3 kHz and potentially > 50 kHz in hard X-rays (HXR). Of the international machines, only LCLS II HE is likely to have specifications that fully match the requirement of reaching 1 MHz repetition rate within 10 years (although European XFEL can partially match this and the planned SHINE machine in Shanghai may also eventually reach this specification).

One aspect that has emerged that has very important implications for applications like X-ray spectroscopy and inelastic scattering is a very high spectral purity (narrow bandwidth). This may be achieved using external seeding to ~1 keV with unprecedently high repetition rates, and self-seeding and high brightness SASE modes across the entire SXR to HXR range. Attosecond and X-ray pump-probe femtosecond modes using enhanced SASE and fresh slice operation with enhanced power using tapered undulators looks to be very promising across the full photon energy range.

As important to the ambitious scientific mission as the raw X-ray capabilities will be the enhanced auxiliary light sources and other capabilities that can be delivered synchronised to the X-rays. A full range of femtosecond laser sources covering the range from 10,000 nm to < 10 nm will need to be provided through the laser fundamental, tunable optical parametric amplifiers (OPAs), harmonic generation, difference frequency generation (DFG) and high harmonic generation (HHG). These will be required with a timing synchronization to < 10 fs with the X-rays, and online time-tools to permit shot-wise time-stamping to sub-femtosecond precision. A high energy (kJ class)/high power (multi-PW class) laser system is required for studying matter under extreme conditions, and here the UK has unique capability in scaleable diode pumped laser systems with the prospects to work at elevated repetition rates > 10 Hz. For studying the dynamical modes in a large range of chemical, biological and materials science systems we will require picosecond THz sources of high brightness; these may be provided by radiators using the primary and auxiliary electron beams. There are some really exciting new scientific possibilities in basic physics, chemistry, materials and radiation chemistry if a relativistic e-beam interacts at the sample synchronously with the X-rays (both co- and counter- propagating). A gamma source from Inverse Compton Scattering of a laser from primary e-beam is used; if this can be done for a 1 GeV electron beam in an energy recovery linac pre-accelerator, it would provide the world's brightest source with application in nuclear science, technology and security.

A number of conceptual outline designs are sketched in the appendix of the Science Case. For example, we have looked at a normal conducting/superconducting accelerator in a hybrid machine (see figure 2). This could be a cost-effective way to access most of the science identified in the Science Case, but full coverage can only be realised using a fully superconducting system.

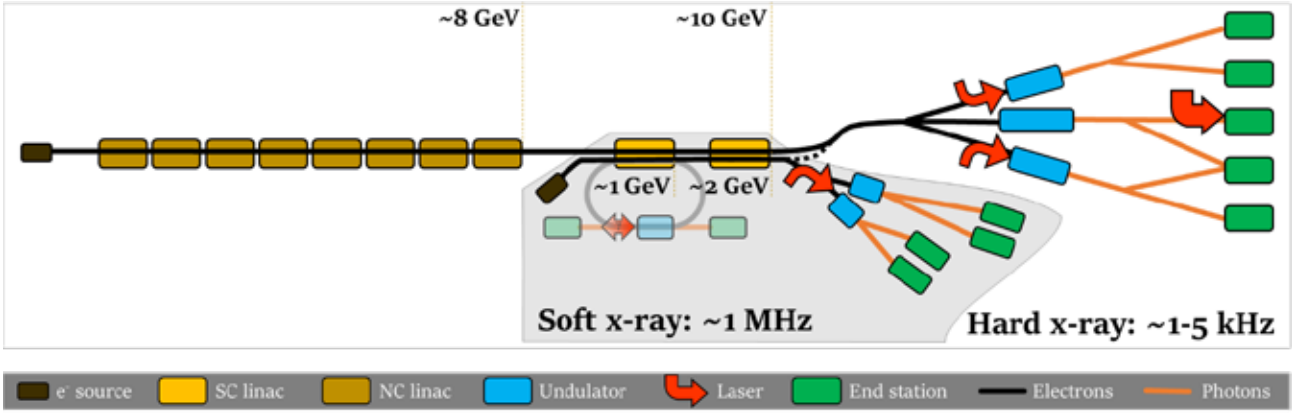
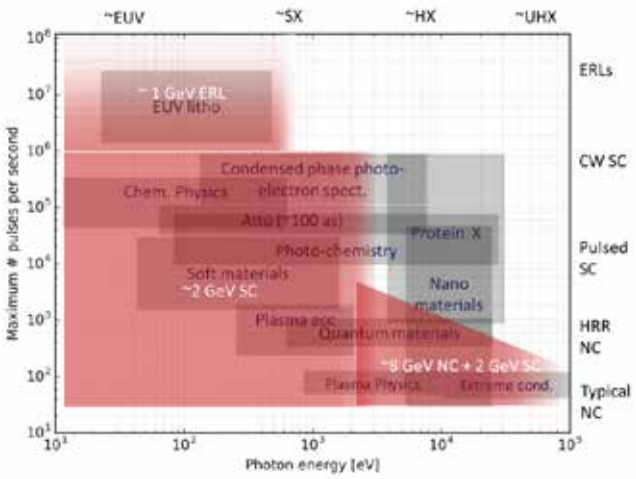



*Figure 2. An example of the conceptual outline machines considered at this preliminary stage. Here a hybrid normal+ superconducting accelerator combination is considered. This could be an excellent match to the greater portion of science opportunities identified in the Science Case (see image below).*




We have identified compelling reasons to proceed with a UK XFEL. Unique emerging X-ray capabilities can be optimised for new science with such a facility. It creates also opportunities in e-beam science, THz sources, high-power lasers and γ sources. A multidisciplinary capability will be established that puts the UK at the centre of some of the most advanced science and innovation. The facility would be a stimulus for the UK forming exciting new global scientific partnerships. Moreover, by building a national machine of international class we retain full control over the science and technology programme whilst bringing direct benefits to UK economy from construction, procurement and operation. In the longer term such a national facility will safeguard future capabilities for industry and defence. It also will provide a golden opportunity for a national "levelling up" agenda – the machine could be built anywhere in the UK with some suitable flat land and reasonable access to transport infrastructure and proximity to regional universities. The presence of such a facility will build, and help retain, a wide range of skills in the UK workforce, as well as attracting the best scientists from around the world to the UK. It will also be a national flagship for attracting young people to STEM subjects and for increasing public appreciation of science.

**Jon Marangos**
Blackett Laboratory Extreme Light Consortium,
Imperial College London

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# The possible contribution of neutrons at the ILL to the fight against SARS-CoV-2

**MAINTAINING good health is one of the most important aspects in our quality of life. Neutron-based research can play an important role in uncovering the subtleties of living processes as well in contributing to research on treatments that enable us to live long healthy lives.**

The current pandemic of Coronavirus Disease 2019 (COVID-19), a newly emerging infectious disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), has demonstrated that viral diseases represent an ever growing threat to our society. The full genome sequence of SARS-CoV-2 is known and the sequencing has allowed the expression of many proteins present in the virus. Their three-dimensional structures have been determined and those have proven useful in the search of inhibitors for virus replication. Nevertheless more information is needed and modern analytical tools such as synchrotron X-ray radiation, cryo-electron microscopy and neutron scattering are indispensable for important insights into the morphology and functionality of viruses.

Indeed, a full understanding of a virus's life cycle requires the study of the mechanism the virus uses to penetrate the host cell. SARS-CoV-2 is one of those viruses, like HIV, possessing a viral envelope composed of lipids, proteins and sugars. Viruses are not capable of independent replication. In order to replicate and spread, they must hijack living cells. When SARS-CoV-2 finds a suitable cell, the virus binds to and penetrates it.

Although all the three critical structural proteins (Spike, Membrane and Envelope, see Figure 1) of SARS-CoV-2 encounter cellular membranes both at the time of entry and exit of the host cell, the virus crucially relies on the spike (S) protein to gain entry, and thus initiating infection. The spike acts as a natural ligand by binding to the cell surface receptor *Angiotensin-converting enzyme-2* (ACE-2), triggering conformational changes, leading to membrane fusion between the viral and host cellular membranes and delivery of the virus genome in the cytoplasm. The spike glycoprotein is therefore a key drug target due to its indispensable function for viral infection and fusion with the ACE-2 receptor.

## Neutron scattering

At micrometre scales, various techniques can be used to probe the structure and elastic properties of biological matter such as optical microscopy or light scattering. At the much smaller molecular level scale, nuclear magnetic resonance, or numerical simulations are used to elucidate in detail the relationships between the chemical structure and the physical properties of lipids, proteins and nucleic acids. Between the molecular and micrometre scales, neutron scattering techniques play a privileged role.

Neutrons, the uncharged subatomic particles found in atomic nuclei, have a mass of $1.67\times10^{-27}$ kg. Their speed, v = 2.2 km/s at room temperature and energy ~ 0.025 eV correspond to a wavelength $\lambda$ = 0.18 nm. Neutron scattering is thus a (non-destructive) tool for characterizing the structure and dynamics of biomimetic systems at scales ranging from tenths to tens of nanometers and from nanoseconds to microseconds. A further strength of neutrons is their power of sample penetration: because their electric charge is zero, they can penetrate materials without being retarded by a Coulomb barrier. They thus can probe the interiors of samples, access buried parts of them and allow the use of complex sample environments.

Sensitive to light elements (H, C, O, N, P…), a further advantage of neutrons comes from the possibility of performing isotopic substitution in order to highlight the parts of interest in the studied systems. Of particular importance here is that protium and its isotope deuterium have similar chemical properties, but they have different interaction potentials with neutrons.

This feature is heavily exploited for example in *small-angle neutron scattering* studies of macromolecular structures that provide low-resolution 3D information on molecular shape without the need for crystallization. While crystallography, NMR and cryo-electron microscopy provide the detailed atomic-resolution structures of small biological assemblies, neutron scattering allows us to see full molecular complexes at lower resolution. The technique's ability to distinguish specific regions (RNA, proteins and lipids) of the virus enables us to map out the arrangement of the various components. It can thus give invaluable information in structural studies of SARS-CoV-2 and should allow to map out the structure of the complex formed by the spike protein and its human receptor. Neutron scattering is also well suited to determining the structures of functional membrane proteins in physiological conditions.

Viruses in their physiological environment are highly dynamic systems. The understanding of how they move, deform and cluster is essential for the optimisation of diagnostic and therapeutic processes. Neutron spectroscopy is ideally suited to provide information on the motion of matter, from the small chemical group to large macromolecular assemblies.

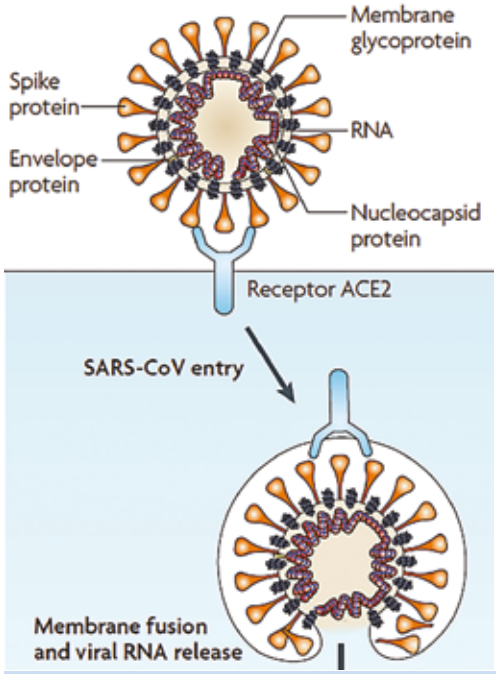


***Figure 1. Internalization of the virus into the human cell.***

*Reprinted by permission from Springer Nature, Nature Reviews Microbiology, "The spike protein of SARS-CoV — a target for vaccine and therapeutic development", L. Du* et al.*, Nature Revs Microbiol. **7**, 226-236 (2009). https://www.nature.com/nrmicro/*

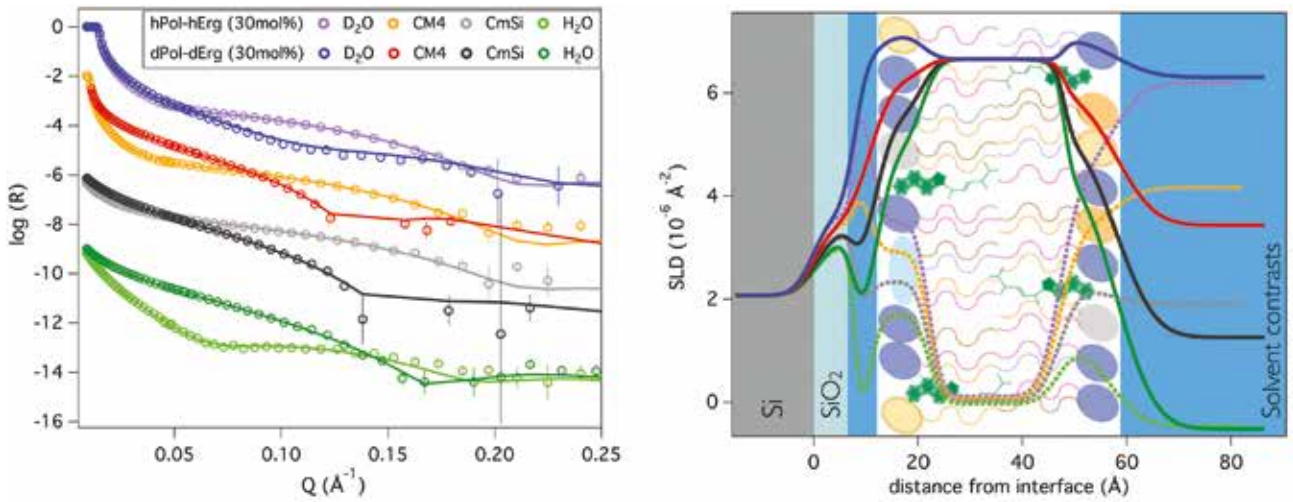


***Figure 2. Neutron reflectivity profiles (left) and scattering length (SLD) profiles (right) corresponding to the best fits to the data of lipid membranes composed of the phospholipids extracted from* Pichia pastoris *with 30mol% ergosterol both in the fully deuterated (dark colours) and fully hydrogenous form (light colour). CMSi and CM4 correspond to 38 mol% and 66 mol% content of $D_2O$, respectively. A schematic illustration of the bilayer is given together with the SLD profiles.***

*Reprinted from Current Opinion in Colloid & Interface Science,* ***38****, G, Fragneto* et al.*, "Neutrons and model membranes: Moving towards complexity", Pages 108-121. Copyright (2018), with permission from Elsevier.*

Neutron diffraction (for structural characterisation down to the Å scale), small angle scattering (for characterisation in bulk solution and physiological conditions of complex assemblies), reflectometry (for thin planar films studies), inelastic scattering and spin-echo (to look at the dynamics of drugs and membranes), are the techniques that will be used at neutron large scale facilities including the Institut Laue-Langevin (ILL) in Grenoble to contribute a better understanding of virus replication and interaction with cells.

Assembling the data from all of these neutron-based analyses of the coronavirus will be essential to control its spread and limit its societal impact over the long term. Below we will describe in more details the areas where ILL studies will be primarily involved.

## Cell membranes and thin films studies

The cell is the structural and functional unit of most living organisms. Each of them is surrounded by a membrane. A rough estimate indicates that the total area of cell membranes in our body is equivalent to about three hectares. The membrane surrounding the cell is a vital structural and functional element in every living being.

The currently accepted description of cell membranes, the *Fluid Mosaic Model*, implies that they consist of a two-dimensional liquid, into which proteins are incorporated. Lipids are then considered an inert medium in which proteins perform all membrane associated functions.

Different types of amphipathic molecules are found in the lipid constituents of membranes like phospholipids, as well as glycolipids, sphingolipids and sterols. Phospholipids represent the majority of cell lipids. These are molecules that have a hydrophilic headgroup and hydrophobic carbon chain tails. In the presence of water, these lipids are able to self-assemble as a continuous bilayer barrier: they present their heads to the aqueous media inside and outside the cell, with the hydrocarbon tails sandwiched in between. Membrane proteins can integrate between the lipid tails and participate in the exchange of material from one side to the other of the membrane.

At the ILL we have been running an ambitious programme to mimic as closely as possible cell membranes by producing lipid bilayers from natural extracts of deuterated yeast cells. This allows a fine characterisation of the interaction of different biological molecules as well as drugs with membranes by using for example the reflectometry technique. Examples of measurements from deuterated and hydrogenous lipid bilayers on a planar substrate are shown in Figure 2.

Neutron reflectometry will be used to assess the binding mechanisms of the CoV2-S protein with membrane bilayers of varying compositions (each one biomimicking a specific cellular organelle) in the presence and absence of the mammalian ACE-2. This will require building *in vitro* model systems that essentially replicate the viral protein-host cell membrane interaction. Such an approach will allow us to understand the kind of interaction strategy coronaviruses exert with their

***Figure 3. The reflectometers D17 (left) and FIGARO (right, layout of components) at the ILL (http://www.ill.eu).***

cognate receptor to achieve the affinity that is required for effective cell entry. Besides exploring the structural features of the binding mechanism, the technique will give access to the stability, interaction strength, and dynamics of the interaction between the viral spike and the human hACE-2 receptor as well as with cellular membranes.

Furthermore, neutron reflectometry (see Figure 3 for a picture and the layout of two ILL reflectometers) can provide information on the molecular structure and composition of the outer surface of the virus, enabling the interaction process to be better understood, as research carried out in 2017 at the ILL achieved for the hepatitis C virus[i].

## Useful insight for drug development

Neutrons can help in the development of antiviral drugs. For these to be efficient, the drug should be strongly bound to the protease, the enzyme responsible for the cleavage. In this way the treatment can be effective in the long-term despite mutations of the protein. *Neutron crystallography* can provide high-resolution structures of proteins, including the locations of individual hydrogen atoms that have been exchanged for deuterium to make them particularly visible. Indeed, the technique can provide unique information at physiological temperatures on the chemistry of enzymatic reactions that often involve proton transfer. Unlike X-rays, neutrons can "see" protons – an invaluable feature in many areas involving biological processes. In the particular case of viruses, proteases capable of cleaving polypeptide chains at precise locations can be inhibited by appropriate anti-retroviral drugs, blocking in this way virus replication. Key details become accessible about the hydrogen atoms that play an essential role in the binding of drugs to their target protein through hydrogen bonding. Finding how the inhibitors position themselves, and what exactly the bonds are that they have made with the protein is how neutron crystallography can help improve the development of antiviral drugs – indeed this is what has already been done with the HIV-1 protease[ii] on the instrument LADI-III at the ILL. A new instrument optimised for these studies, DALI, will be commissioned in summer.

High-resolution X-ray data on the protease of SARS-CoV-2 are already available and at the moment efforts are being deployed to obtain crystals for neutron crystallography studies (see Figure 4).

***Figure 4. Microscopic view of the SARS-CoV-2 protease crystals grown in Oak Ridge National Laboratory's Protein Crystallization and Characterization laboratory (US). Once crystals reach a certain size and shape, they will be used in neutron scattering experiments.***

*Reprinted with permission of Daniel Kneller and Andrey Kovalevsky, ORNL. From: https://neutrons.ornl.gov/content/history-insightful-hiv-research-inspires-neutron-scattering-approach-studying-covid-19.*

Besides proteases, neutron crystallography can provide essential information on the virus spike proteins responsible for mediating the attachment and entry into human cells, of great relevance for developing therapeutic defense strategies against the virus. In fact, unique information about the precise coupling mechanism of the virus and the receptor proteins of the cell membrane can be obtained.

**Giovanna Fragneto**
Large Scale Structures Group Leader & Head of Soft Matter Science & Support Group
Institut Laue-Langevin

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i T. Soranzo *et al*., "Coupling neutron reflectivity with cell-free protein synthesis to probe membrane protein structure in supported bilayers", Scientific Reports **7**, 3399 (2017)

ii O. Gerlits *et al*., "Room temperature neutron crystallography of drug resistant HIV-1 protease uncovers limitations of X-ray structural analysis at 100K", J. Med. Chem. **60**, 2018-2025 (2017)

# Crystallography at DIAMOND

**THE Crystallography Science Group at the Diamond Light Source currently comprises 32 people: 20 beamline scientists or postdocs, five dedicated technicians and seven joint Diamond-University Ph.D. students. There are four instruments in the group: the High-Resolution Powder Diffraction beamline (I11) with a team led by Chiu Tang, the Extreme Conditions beamline (I15) whose team is led by Christine Beavers, the X-ray Pair Distribution Function (XPDF) beamline (I15-1) led by Phil Chater, and the Small-Molecule Single-Crystal Diffraction beamline (I19) led by Dave Allan. I15 was one of the first seven beamlines built at Diamond, a so-called Phase 1 beamline, and became operational in 2007. I11 and I19 followed in Phase 2 and I15-1 in Phase 3.**

Internal organisation of the science program at Diamond evolved into the present structure in 2018 and that is when the Crystallography Science Group was formed, first under Heribert Wilhelm and then from March 2019 under Joe Hriljac when Heribert moved to become the Managing Director of the Helmholtz Institute in Ulm. Bringing these beamlines and teams together into one science group means we can fully exploit the technical and scientific expertise to provide the basis for future development and pioneering experiments. There is much sharing of ideas between the teams on science, beamline and software development. Recently Dean Keeble moved from a position on I15-1 to become part of the Scientific Software Group as a Data Analysis Scientist for Diffraction; he and Ben Williams (who supports I19) take the lead in software development to underpin the Group's activities. An overview of each beamline is given below. More details and contacts can be found at https://www.diamond.ac.uk/Instruments/Crystallography.html.

One of the most exciting developments at the moment across Diamond is the planning for the proposed upgrade to Diamond-II. Part of the design would include an increase of the electron beam energy from 3.0 to 3.5 GeV. For the two crystallography instruments on undulator sources, I11 and I19, this would significantly improve the X-ray flux at high energies. For the two instruments on the I15 superconducting wiggler source, I15 and I15-1, the flux increase would be less substantial but still benefit the crystallography community. More details about Diamond-II can be found at https://www.diamond.ac.uk/Home/About/Vision/Diamond-II.html

## I11 – the High-Resolution Powder Diffraction beamline

This high brightness beamline uses monochromatic X-rays in the range of 6 – 25 keV for high-resolution and time-resolved powder diffraction experiments in the first Experimental Hutch (EH1) or for Long Duration Experiments in EH2. It facilitates experiments to the busy user programme throughout the year, in particular for non-ambient applications and experiments requiring unusual hardware setups such as toxic/corrosive gas absorption studies at cryogenic temperatures, resonant diffraction at high temperature and time-resolved *in operando* lithium-ion (Li-ion) battery work.

After running for ten years, many components such as the monochromator, diffractometer and multi-analyser crystal (MAC) detector began to show signs of wear. An upgrade plan, endorsed by the Scientific Advisory Committee (SAC) and the Diamond Industrial Science Committee (DISCo) at the end of 2017, to replace these components started in 2019. The construction and installation of a new high stability monochromator were completed during the June 2019 shutdown. A new Newport diffractometer was delivered in late 2019 and its installation began in March. The image shows the diffractometer being craned into EH1. Installation was suspended during the site shutdown due to COVID-19, but at the time of writing work has resumed and installation of the MAC and position sensitive (PSD) detectors is expected to be completed in September so that user operations can resume. A superconducting undulator to replace the original in-vacuum system and provide better flux at high energy has undergone extensive specification and early prototype testing, and this should be complete and ready for installation in early 2021. Finally, an upgrade to the linear PSD in EH1 is planned, and it is anticipated that a next-generation detector should be available in 2021/22.

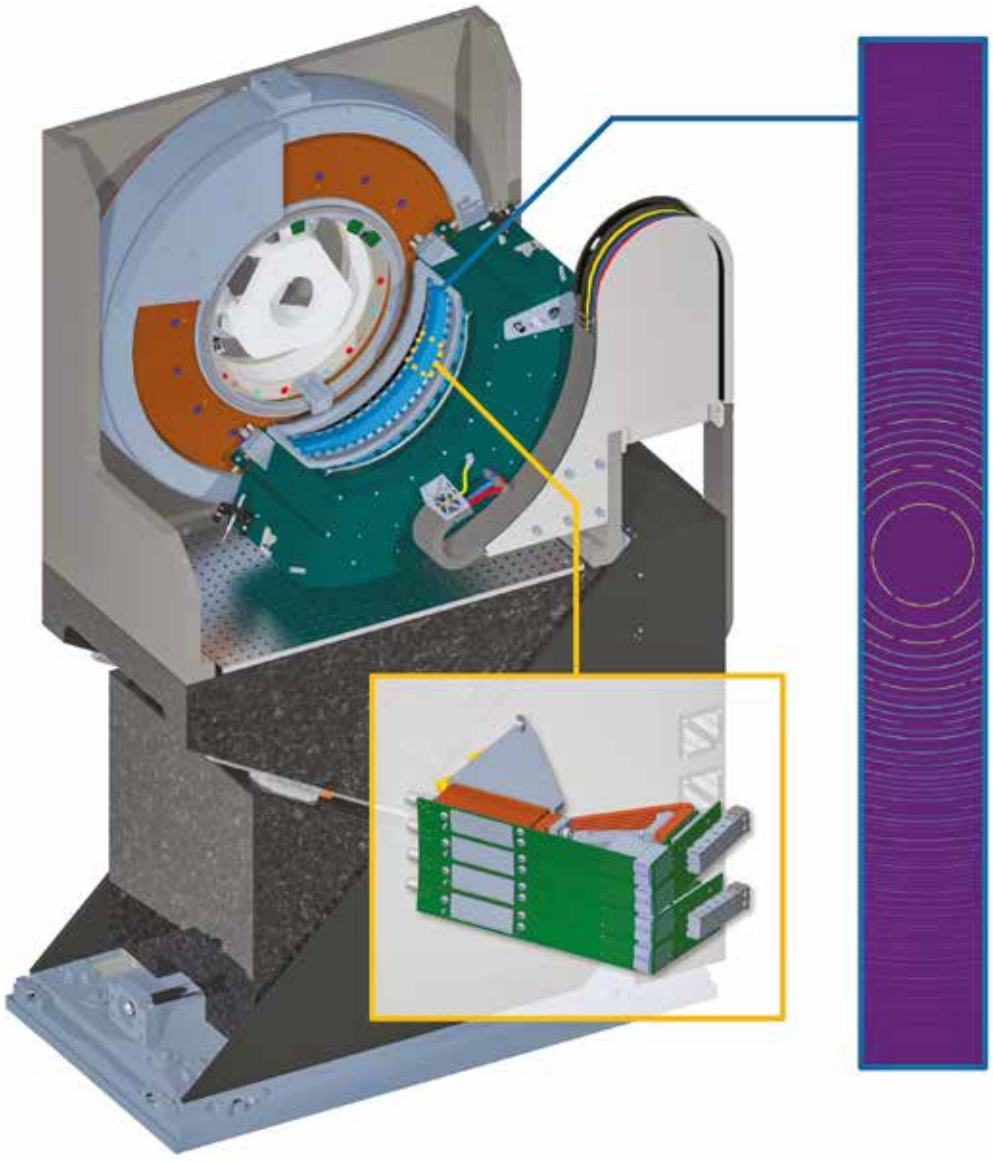
## I15 – the Extreme Conditions beamline

I15 employs high energy X-rays to explore the structure of materials at high pressures, high and low temperatures, as well as under other *in situ* and *in operando* conditions. The beamline receives an X-ray continuum from the superconducting wiggler; this allows for experiments that require monochromatic X-rays between 20 and 80 keV, as well as polychromatic beam. I15 was originally designed to serve the mineral physics community, which it has, whilst also assisting material scientists, chemists and solid-state physicists with their structural investigations, at pressure or otherwise.

I15 continues to offer capabilities and support that few extreme conditions beamlines do. Its users have pre-experiment access to bespoke assistance and training from our highly skilled staff in diamond anvil cell (DAC) preparation and loading, as well as the loaning of DACs for I15 experiments. The high-pressure gas loader available at I15 offers users the choice of many possible gases to use as their pressure transmitting media (PTM), allowing them to optimise for hydrostaticity with helium or neon, or choosing a PTM based on desired interactions with the sample at pressure. Work is underway to add hydrogen to the gas loading capabilities in 2020. The recent addition of the laser heating system adds a further unique capability – the I15 system is capable of quickly ramping the laser power to perturb a sample without delivering too much heat to the bulk. Several small upgrades started in 2019; these include improved network infrastructure and a better design of the laser system. In 2020 a low-temperature cryostat for DAC work will be commissioned and, significantly, the beamline is procuring a vastly improved detector – a DECTRIS PILATUS3 X CdTe 2M that will provide much greater sensitivity to high-energy X-rays and the capability for much faster data collections. Software and hardware improvements to take advantage of the speed and sensitivity offered by the new detector are being explored. Diffraction mapping with automated processing has been successfully tested with the existing Perkin Elmer detector – this functionality will be improved with the CdTe PILATUS3. Further upgrades to I15 to take full advantage of fast hardware-based scanning and mapping are planned.

## I15-1 – the X-ray Pair Distribution Function (XPDF) beamline

I15-1 is dedicated to producing high-quality X-ray total scattering data for Pair Distribution Function (PDF) analysis. Operational since 2017, I15-1 has illuminated samples from diverse fields, from Earth sciences to pharmaceuticals, as well as materials science and chemistry. I15-1 receives X-rays from the inside edge of the wiggler fan, and this light is monochromated and directed to the end station in one of three energies: 40, 65 or 76 keV. PDF data are collected at high energies to produce the low sample absorption and high Q-range required for successful interpretation. Gaining structural information on amorphous samples is a primary goal of many XPDF experiments, but crystalline samples can also display local structure variations such as defects and disorder, which can be studied via PDF analysis. PDF data collections are rarely available at home institutions, so in order to allow more people to exploit this powerful technique, I15-1 complements the standard proposal route with popular Rapid and Easy Access routes, where PDF data can be collected via a mail-in procedure.



Consisting of a sample position, with an optional sample-changing magazine, and two large area detectors, the end station is highly flexible and has been adapted to many *in situ* and *in operando* experiments, including variable temperature, gas flow, hydrothermal synthesis and electrochemical cycling. For more routine measurements, the 15-position sample changer has been a popular choice, allowing automatic data collection. Further upgrades including a new end station and a sample-changing robot are in progress, and both should be commissioned

during 2020. The final aspect of the current upgrade is a new detector based on CdTe sensors that will be much more sensitive at high energy and with faster electronics for data readout. A schematic diagram of the new end station and detector are shown here. These upgrades will be a synergistic addition to the existing auto-processing infrastructure and will allow users to collect better data with less manual intervention.

## I19 – The Small-Molecule Single-Crystal Diffraction beamline

I19 uses X-rays in the 5 – 25 keV energy range to determine the structures of small-molecule and extended three-dimensional systems, e.g. metal-organic frameworks, with single-crystal diffraction techniques. These methods can be applied to the characterisation of novel materials or for investigating the variation in the structure of a crystalline material under an external physical influence such as a change in temperature, the exposure to a gas, photo-excitation or through the application of high-pressure.

The use of the robotic sample changer, and remote access, is now well established in Experimental Hutch 1 (EH1) of the beamline, where pre-mounted samples are sent to Diamond under cryogenic storage, and users then run their beamtime from their home institutions. This mode of operation makes it possible to carry out chemical crystallography studies in a more responsive manner as beamtime can be scheduled in more regular, and shorter, periods. We now schedule individual shifts, rather than whole one-day (three shifts) blocks of beamtime, for those wishing to run their beamtime via the remote access route. For Experimental Hutch 2 (EH2), we have recently developed a cell which allows a high static electric field to be applied to the sample crystal. The application of electric fields to materials can result in a variety of responses that may have important technological applications, spanning electronic and ionic conductivity to piezo- and ferro-electricity.

In 2019, the original monochromator was replaced with an upgraded one of a new design, and this now affords greater beam stability and ease of wavelength change. The data collection software has also seen substantial work with greater integration of the SynchWeb interface to the ISPyB database (making remote operation much easier and more like a macromolecular crystallography (MX) beamline) and the in-house dials/xia2 data processing software. There has also been local development particularly relevant to chemical crystallography in terms of optimising sample screening and choice of attenuation to minimise exposure times and subsequent beam damage. Overall, these have led to data collections at 2-4 times faster rates than before with equally good quality.

**Joe Hriljac**
(Diamond)

# The 2020 Winter Crystallography Meeting

## November 2nd-3rd 2020
## Milton Hill House Hotel
## Steventon, Abingdon, Oxfordshire

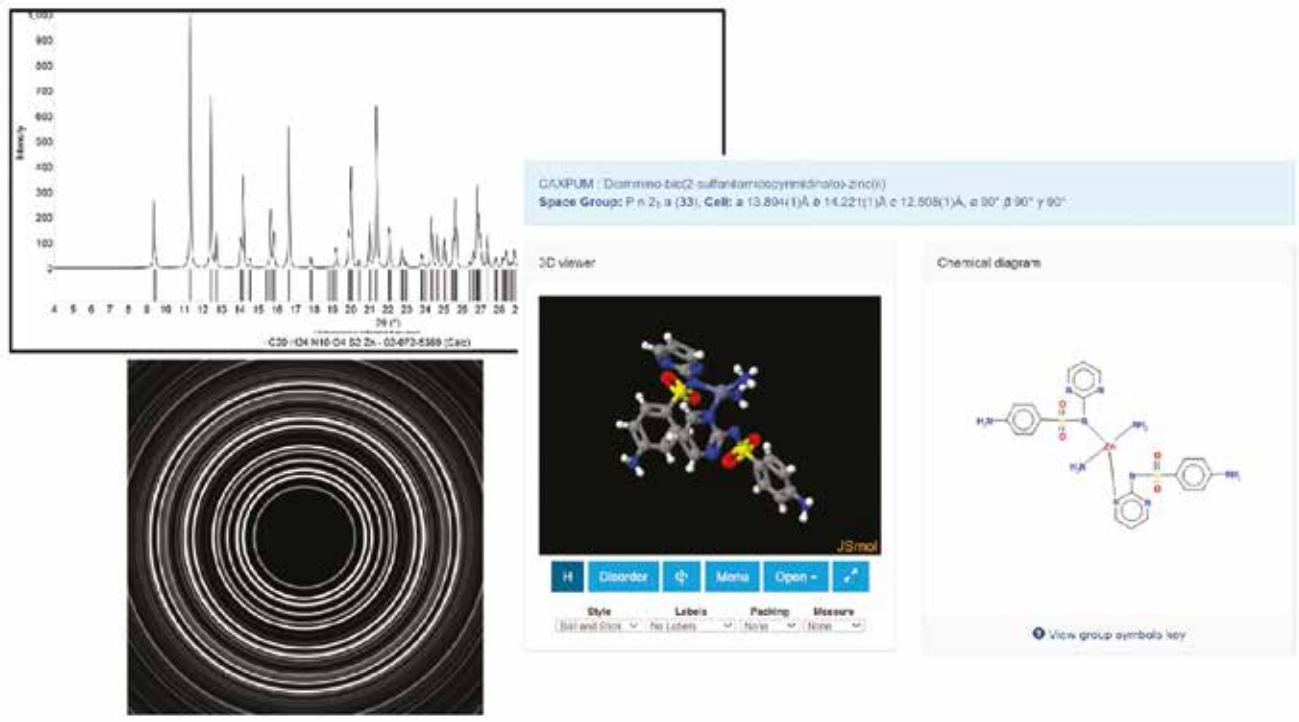
The Winter Crystallography Meeting brings together ISIS & Diamond users with members of the BCA Physical Crystallography Group in a two day celebration of structural science.

As always we hope to put together a diverse and exciting programme. Ph.D. students and early career researchers are particularly encouraged to apply to give talks and present posters!

More information will be posted on www.pcg-scmp.org in due course. Registration will open in September.

# New Data Partnership between ICDD and CCDC

***Leaders in chemistry data management combine to deliver unified data resource for materials characterisation.***




*The ICDD CCDC partnership will see the power of powder and single crystal data combined.*

**TWO of the largest chemical data repositories – The International Centre for Diffraction Data, ICDD and The Cambridge Crystallographic Data Centre, CCDC have announced a new partnership which will allow greater utility and insights in the development of new drugs and materials, and drive greater opportunities in pharma and materials development.**

ICDD, publishes the PDF® (Powder Diffraction File) and has managed the curation, publication and distribution of X-ray powder diffraction data for 75 years, while CCDC curates and maintains the CSD (Cambridge Structural Database) – the world's repository for small-molecule organic and metal-organic crystal structures. Both non-profit organisations have a strong focus on data quality, with entries edited and verified manually to ensure accuracy and standardized format.

The partnership will see the ICDD calculate and publish diffraction patterns, including atomic co-ordinates, from structures found in the CSD. By combining powder and single crystal data in this manner, the ability to match samples to known structures will be enhanced – enabling, for example, rapid analysis in the pharmaceutical industry from the discovery of active pharmaceutical ingredients through drug delivery formulation.

*"This collaboration between our two organizations is a win for the scientific community. Materials characterization is enhanced by this symbiotic relationship, particularly in the areas of phase identification and quantitative analysis. The goal is straightforward, to get more data into the hands of more analysts to help them get the right answer."*
Tom Blanton, Executive Director ICDD.

*"CCDC and ICDD have a common aim of collating, enhancing and making high-quality structural chemistry data available to scientists across the world. I am delighted that this collaboration helps extend our commitment to the FAIR data principles increasing the findability, accessibility, interoperability and reusability of this important dataset."*
Juergen Harter, CEO CCDC.

As discoveries and developments made using or even exclusively by informatics-based approaches continue to rise, this partnership could open further opportunities for innovative research in the ever-changing pharmaceutical and organic materials landscape.

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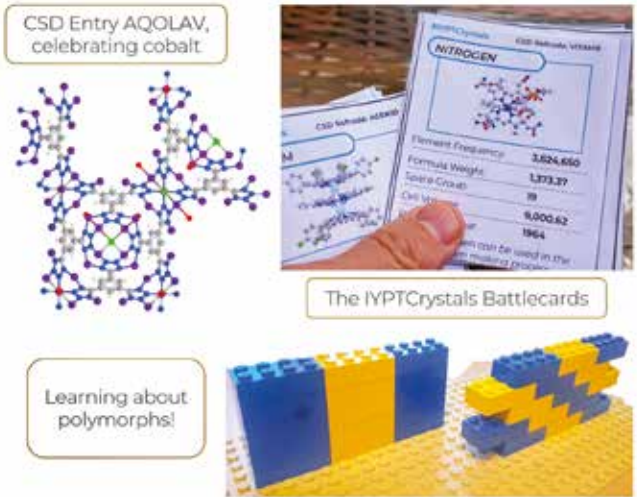
# New Scientific Home Learning Activities for Children

**SINCE the start of lock-down, many of us have had to adapt to new ways of working and this has been particularly true for school children. With schools closed, children and parents faced the difficult task of home schooling. This cannot have been easy, and so at the Cambridge Crystallographic Data Centre (CCDC)[i] we have been busy creating fun scientific activities that can be enjoyed by the whole family. And what a better place to start than by building on the resources we had already created through the IYPT[ii] through Crystals project[iii], working with the BCA[iv] and NCS[v] (National Crystallography Service)?**

The beginning of summer brought many updates from this project: the periodic table of crystals is nearly complete thanks to the contributions of the crystallographic community; the champion element was crowned; and the first educational game was released, becoming immediately the most popular educational resource on the CCDC website and leading the way in our new CCDC Home Learning Collection.

The #IYPTCrystals competition opened on the 4th of May, and everyone could vote for their favourite element among the six shortlisted: carbon[vi], chromium[vii], cobalt[viii], europium[ix], germanium[x], and tellurium[xi]. From all the elements, these six were selected by a panel of judges based on their engaging and informative content and on the interaction received on social media and on their webpages. After one month and over 2,000 votes, cobalt was the winner! Congratulations to Alexis Graybeal and Chiara Lagioia, authors of this elements page. Chiara and Alexis are students at Illinois State University, and they told us that they chose to curate the page of cobalt not only because of its beautiful colour, but also as they had recently studied transition metal complexes. They celebrated cobalt with CSD Entry AQOLAV[xii] (see image).




To further promote engagement and learning with this interactive periodic table of crystals, the next step was the development of educational resources that could be used in schools, science festivals, and by families at home. The first resource is the IYPT Crystals Battlecards (find them here[xiii]), a fun and educational game, developed with the NCS. Elements from hydrogen to xenon have each a dedicated battlecard in the deck, with their celebrative crystal structure and their properties, which are the grounds for the game. These battlecards represent a window for children and players of any age and background on the crystallographic world and offer a fun way of learning.

Since launching this game, the CCDC have been busy expanding the CCDC Home Learning Collection. Children can learn about polymorphs through the wonders of LEGO® and chocolate as well as participate in a fun detective activity based on common substances you can find at home. To see this growing collection of activities for kids and families you can visit the CCDC Home Learning webpage[xiv]. For the latest news from the IYPT through Crystal project and CCDC Home Learning you can follow CCDC on their social media (Twitter: @ccdc_cambridge, Facebook: @ccdc.cambridge, Instagram: @ccdc_cambridge, and Linkedin). If you would like to collaborate with CCDC on new educational material, you can email hello@ccdc.cam.ac.uk.

**Ilaria Gimondi**
On behalf of the IYPT through Crystals and CCDC Home Learning Project Teams

## References

i https://www.ccdc.cam.ac.uk/
ii The International Year of the Periodic Table
iii https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/
iv https://crystallography.org.uk/
v http://www.ncs.ac.uk/
vi https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Carbon/
vii https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Chromium/
viii https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Cobalt/
ix https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Europium/
x https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/Germanium/
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xii https://www.ccdc.cam.ac.uk/structures/search?id=doi:10.5517/ccdc.csd.cc1m5tqb&sid=DataCite
xiii https://www.ccdc.cam.ac.uk/Community/educationalresources/PeriodicTable/activities/
xiv https://www.ccdc.cam.ac.uk/Community/educationalresources/activities-for-kids/lego-chocolate-polymorphs/

# BCA Spring Conferences remembered

**THE British Crystallographic Association (BCA) is more than just the sum of its individual groups. In the late 1970s there were many discussions regarding a possible coalescence of the Chemical Crystallography Group of the Royal Society of Chemistry (RSC) and the Physical Crystallography Group of the Institute of Physics (IoP). In particular, joint meetings and a combined newsletter were proposed. For a number of years, I had been the Editor of the Newsletter for the IoP Crystallography Group; and I became the Editor of the RSC/IoP Crystallography Newsletter, and thereafter the BCA *Crystallography News*. At a jointly-arranged meeting in Durham in 1982, these chemical and physical crystallography groups were formally united together, and the BCA was officially launched with the financial support of 42 distinguished Founder Members. Their signatures are shown on page 26 of the March 2020 issue of *Crystallography News* (underneath my calligraphy!).**

The meeting of the BCA for the following year (1983), was arranged by myself at Royal Holloway College, University of London. The poster sessions were exhibited in the College's ornate, Victorian, Picture Gallery (see image), which greatly impressed Jerry Karle (1985 Nobel Laureate), who had attended the meeting on behalf of the American Crystallographic Association, and who wrote an appreciative piece at the time for *Crystallography News*. It was at this conference in Egham that Sir Aaron Klug (1982 Nobel Laureate) addressed the meeting; and the Biological Structures Group and the Industrial Crystallography Group were inaugurated. Thus the BCA became more than just chemistry + physics, and cross-fertilization of ideas among the groups was abundant. The Young Crystallographers' Group was added later, covering all aspects of crystallography and giving a forum for wide discussion of hot topics. An important component of each BCA Spring Conference has been the staging of a vibrant commercial exhibition, and companies have also bought space for advertisements in *Crystallography News*, which we gratefully appreciate.

The new BCA required a logo and a competition was organized. I'm pleased to say that my design found favour and I won a bottle of Lagavulin single-malt whisky!

Initially it was thought that the BCA Spring Conferences should be held alternately at universities in the North and South of the UK. You can see from the table that we have indeed visited most areas, some more than once. I have attended every one (except for Sheffield 1991, when I had been teaching at the BCA graduate school and unfortunately I couldn't spare any more days away from home). I still have the 1985 Bristol T-shirt and numerous useful canvas shopping bags! I'm sure that the years and venues listed in the table will bring back many happy memories of conferences gone by. I hear you say: "Gosh! Was that Spring Meeting as long ago as that?"

| | | |
|---|---|---|
| 1. | 1982 | Durham |
| 2. | 1983 | Royal Holloway College University of London, Egham |
| 3. | 1984 | Nottingham |
| 4. | 1985 | Bristol |
| 5. | 1986 | York |
| 6. | 1987 | Warwick |
| 7. | 1988 | Heriot-Watt University, Edinburgh |
| 8. | 1989 | Oxford |
| 9. | 1990 | Exeter |
| 10. | 1991 | Sheffield |
| 11. | 1992 | Liverpool |
| 12. | 1993 | Manchester |
| 13. | 1994 | Newcastle |
| 14. | 1995 | Cardiff |
| 15. | 1996 | Cambridge |
| 16. | 1997 | Leeds |
| 17. | 1998 | St Andrews |
| IUCr | 1999 | International Union of Crystallography Congress, Glasgow |
| 18. | 2000 | Heriot-Watt University, Edinburgh |
| 19. | 2001 | Reading |
| 20. | 2002 | Nottingham |
| 21. | 2003 | York |
| 22. | 2004 | Manchester |
| 23. | 2005 | Loughborough |
| 24. | 2006 | Lancaster |
| 25. | 2007 | Canterbury |
| 26. | 2008 | York |
| 27. | 2009 | Loughborough |
| 28. | 2010 | Warwick |
| 29. | 2011 | Keele |
| 30. | 2012 | Warwick |
| ECM | 2013 | European Crystallographic Meeting, Warwick |
| 31. | 2014 | Loughborough |
| 32. | 2015 | York |
| 33. | 2016 | Nottingham |
| 34. | 2017 | Lancaster |
| 35. | 2018 | Warwick |
| 36. | 2019 | Nottingham |

*Royal Holloway University of London Picture Gallery, where the Poster Sessions of the 1983 Spring Meeting were held.*

Long before the formation of the BCA, the Bragg Lecture Fund (BLF) had been organizing pairs of lectures on crystallographic topics which were delivered to the public at the places where Sir William Henry Bragg and Sir Lawrence Bragg had worked: Adelaide, Cambridge, Leeds, London and Manchester. The same lecture was given in two different places in order to raise public awareness of the great achievements of crystallography. I was the Secretary of the BLF in the 1980s and I organized four such pairs of Bragg Lectures. I understand that the fund is still administered by the Royal Institution; and it is sufficient to cover lecture expenses and to ensure that Bragg Lectures are given free of charge to those attending. In recent years, Bragg Lectures have been given at the BCA Spring Meetings and to gatherings of crystallographers elsewhere.

I'd like to end by paying my own personal tribute to Carl Schwalbe, who was such an excellent Editor of *Crystallography News:* quietly efficient, highly knowledgeable and a great companion at conference dinners. We will all greatly miss him.

**Moreton Moore**
Royal Holloway University of London
m.moore@rhul.ac.uk

# Correction to June reminscences on Cyrus Chothia

**I was wrong to attribute to César Milstein the preparation and crystallization of the Fab fragment of the monoclonal antibody D1.3.**

Roy Mariuzza, Simon Phillips and Roberto Poljak (who also died last year) at the Institut Pasteur first created and solved the 2.8 Å crystal structure of the Fab fragment of the D1.3 monoclonal antibody in a complex with its antigen hen egg white lysozyme. They gave César Milstein, (now Sir) Greg Winter, and colleagues at the LMB early access to the structure and sequence, initiating a collaboration that later allowed Greg to express the smaller Fv fragment of D1.3 in *E. coli*. The LMB was of course well supplied with expert protein crystallographers, and César tramped up and down the corridor hoping to persuade one of them to solve the Fv complex structure. He hoped to keep this project in the building. But for some reason they all turned him down. Roberto and his group took on the D1.3 Fv-lysozyme problem, a natural continuation of their earlier work, and were able to collect higher-resolution data. César and Roberto had close personal as well as professional relations, as they had been students together in Argentina – and of course they shared a very keen interest in these structures.

**Arthur Lesk** (Penn State)

# Algol revisited

**IN my working days I used to write crystallographic computer programs in Fortran, the programming language widely used for that purpose at the time. As a student I had experimented with Algol 60, and recently thought it might be fun to write something in Algol 68.**

Here is a program for doing calculations on an ideal air-source heat pump (quite topical I think), with an example applied to a home installation when the outside temperature is -10 degrees.

| | |
|---|---|
| Source | -10.00 deg C |
| Final | +77.73 deg C |
| Coefficient of Performance = | +3.00 |
| Temperature difference = | +87.73 deg C |

Required output taking specific heat of air at constant pressure to be 1.0 kJ/kg/K

or 1/1.225 kJ/m^3/K is +107.473 kJ/m^3

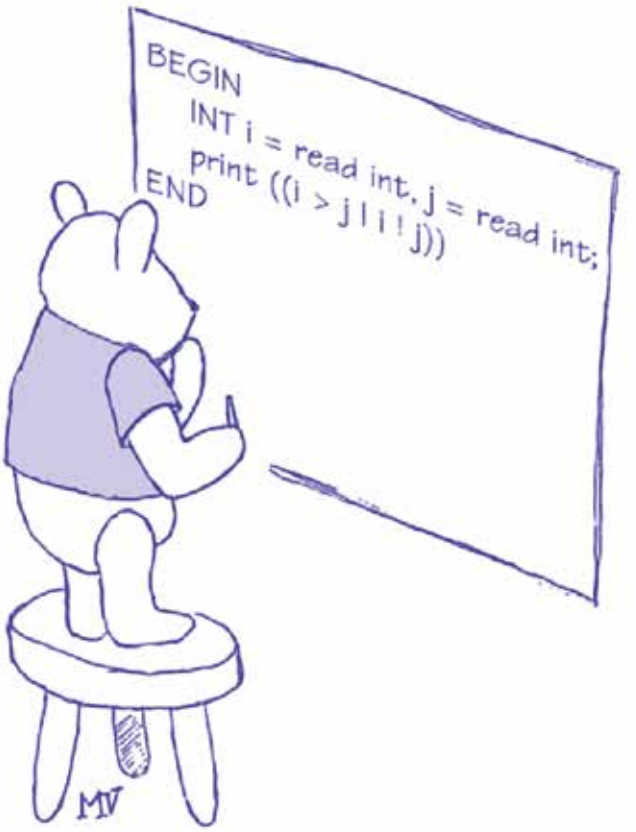
Input to heat pump required for warming a room size 50 m^3 by +87.73 deg C in 1 hour is +0.498 kW

Corresponds to flow rate 14 l/s with output +1.493 kW

For anyone who would like to try this, I found the a68g compiler on my Ubuntu system and the manual "Programming Algol 68 Made Easy" on the internet (see http://www.nunan.myzen.co.uk/algol68/pame.pdf ). Actually I didn't find it easy!

– – – – – – – – – – – –

```
BEGIN

COMMENT

Heat pump calculation ref. Physical Chemistry P.W. Atkins Chapter 4

Illustrates use of Algol 68 procedures and routines

END COMMENT

FILE outfile;
establish (outfile,
        "results", stand out channel);

REAL tc, th, coef;

PROC final = (REAL tcold, thot, coeff) REAL:
            COMMENT Equivalent Fortran would be
            REAL FUNCTION final(tcold, thot, coeff) ...
            final = thot – tcold
            END
            END COMMENT
```




*Reproduced by permission of Marcel van der Veer.*

```
BEGIN

put (outfile, (newline, "Source", fixed(tcold, 10, 2), "deg C",
newline, "Final", fixed(thot, 10, 2), "deg C",
newline, "Coefficient of Performance =",fixed(coeff, 10, 2),
newline, newline, "Temperature difference = "));
thot – tcold
END;

PROC roomtemp = VOID:

BEGIN

        COMMENT

        VOID here signifies procedure is a subroutine (in
        Fortran terminology) rather than

        a function, i.e. the name itself doesn't have a value.
        Equivalent Fortran would be

        SUBROUTINE roomtemp

        COMMON tc, th, coef

        ... END

        END COMMENT
```

```
put (outfile, (fixed(final(KTOC tc, KTOC th, coef), 10, 2), " deg
    C", newline));
put (outfile, (newline, "Required output taking specific heat of
    air at constant pressure to be 1.0 kJ/kg/K",
newline, "or 1/1.225 kJ/m^3/K is", fixed((th – tc) * 1.225, 10, 3),
    " kJ/m^3", newline));
put (outfile, (newline, "Input to heat pump required for warming
    a room size 50 m^3 by ", fixed(th – tc, 10, 2)));
put (outfile, (" deg C in 1 hour is", fixed((th – tc) * 1.225 *50/
    (3600*coef), 10, 3), " kW", newline));
put (outfile, (newline, "Corresponds to flow rate 14 l/s with
    output", fixed((th – tc) * 1.225 * 50/3600, 10, 3), " kW"))
END;

OP KTOC = (REAL ktemp)REAL:

    COMMENT example of a routine to convert K to
    C END COMMENT
    ktemp – 273.2;

COMMENT **** main program **** END COMMENT

print ((" enter source and final temperatures (deg C),"));
print ((" coefficient of performance ")); print(newline);
print ((" (value -1 means calculate from the other two, source
can be down to -100C)"));
print(newline);

tc := read real; th := read real; coef := read real;
tc := tc + 273.2; th := th + 273.2;

IF tc < 173.2 COMMENT allow tc down to -100C
END COMMENT
THEN

    tc := coef*th/(1 + coef); print(newline);
    print ((" Tc = "));
    print (fixed(tc – 273.2, 10, 3)); print ((" deg C", newline));
    roomtemp

ELSE

    IF th < 273.2

    THEN

    th := (tc + coef*tc)/coef; print(newline);
    print ((" Th = "));
    print (fixed(th – 273.2, 10, 3)); print ((" deg C", newline));
    roomtemp

    ELSE

    coef := tc/(th – tc); print(newline);
    print ((" Coefficient = "));
    print (fixed(coef, 10, 3)); print(newline);
    roomtemp

    FI

FI

END
```

**Paul Mallinson**
Glasgow University

# The 18th BCA/CCG Intensive Teaching School


The School will be run for the first time as an online school from the 10th – 18th April, 2021. We are intending to have the usual mixture of lectures, tutorials and social activities which will give you the opportunity to get to know your fellow participants whilst covering the usual crystallographic content. For those of you that have heard the rumours about the intense nature of the school from previous participants, fear not for we are adjusting the timetable and content delivery to include regular breaks and to avoid 'online fatigue'. Registration for the course will open in Autumn 2020 and close in early January 2021 to allow for place assignment and the complete course notes to be sent out to those who have registered. We are very much looking forward to welcoming people virtually! Any queries please get in touch using the email on the school webpages (https://community.dur.ac.uk/durham.x-ray-school/).

**Hazel Sparkes**
(University of Bristol)

*See advert on page 29*

# Obituary – Dr Marcus Frederick Charles Ladd 1926 - 2020

**MARK Ladd's long association with the University of Surrey goes back to the 1950s. As a young graduate, he was employed by GEC in their Hirst Research Centre in Wembley, travelling there daily from Tottenham on his trusty moped. One part of GEC was investigating the structural aspects of a range of materials considered to be of commercial interest to the company and Mark joined the X-ray crystallography group. Their remit was wide ranging and covered both the development of a range of techniques to study the properties of a large range of polycrystalline and single-crystal materials, and this is where his interest in the solid state and its characterisation began to evolve.**

He may well have stayed at GEC had it not been for developments which were taking place in Higher Education. In 1956 the then Battersea Polytechnic, following a government White Paper, became one of the Colleges of Advanced Technology (CATs). In keeping with this advanced technology remit a new department was created, 'Chemical Physics and Spectroscopy', under the headship of Prof. Victor Griffiths. 'Griff' as he was always known was keen to recruit academic staff who had good experience of industry. It is not clear how 'Griff' and Mark Ladd first met although 'Griff' was well known for having a wide net of industrial contacts, but Mark always remembered his first meeting over a cup of tea in a café in Battersea Park Road. Soon after, he was on the teaching staff of the new CAT as a junior lecturer. The new department was situated in an annexe some distance away from the main college in an old school building in Falcon Road, Battersea which resembled a rabbit warren. New staff were not given offices and the whole arrangement was very open plan.

'Griff' was always keen that his staff had the opportunity for postgraduate study and in 1958 Mark registered for a Ph.D. at Birkbeck College on a part-time basis working on the crystal structure of Euphenyl Iodoacetate with Dr C.H. Carlisle as his supervisor. There was little X-ray diffraction equipment available at Falcon Road so most of the experimental work was carried out at Birkbeck College. In his spare time away from teaching duties, Mark would travel to Birkbeck to carry out the experimental work, setting up multiple film packs on a Weissenberg camera. "This was hard work going back and forth to Birkbeck but fortunately the exposures often took a few days so I could leave them running with the technical staff at Birkbeck looking after them". Later in his career he loved to explain to students the real labour of love to get a set of X-ray intensity data measured by eye with a calibrated film strip coupled with the necessary scaling from successive films.

In the early 1960s the college had purchased a new computer, an Elliot 503, and this to Mark's delight was sited at Falcon Road. He taught himself ALGOL which was the only programming language available and was able to carry out some of the calculations required for his research. Unfortunately, the relatively small capacity of the machine and its lack of availability during the day meant that some of the long calculations had to be performed overnight. Three-dimensional electron density maps required intermediate summations to be output on punched paper tape which then had to be subsequently re-input, and Mark had a camp bed installed so that he could keep track of all the calculations. His Ph.D. was awarded in 1965.

Apart from his teaching duties in his own department, Mark was keen to interact with other departments at Battersea so when the head of chemistry asked if he would like to "do something on crystallography" for a final year physical chemistry course he jumped at the opportunity. "When I asked how many lectures I could have, back came the reply, "just one"". But he did it. It was done at a fast pace with a lot of detailed handouts but it also gave him the opportunity to advertise the new M.Sc. course in crystallography which he was in the process of organising.

In 1968, the college was granted its royal charter and it moved to Guildford as the University of Surrey. The departmental name was changed to Chemical Physics and Mark was charged with organising the layout of the department. "If it was going to be done, it had to be done properly. I remember going to see 'Griff' with my requests for equipment. He would disappear to see someone he knew from industry and use his very persuasive powers to find either money or second-hand equipment". The results of his efforts were fully equipped teaching and research laboratories with a complement of single-crystal cameras, powder diffractometers and a 4-circle Siemens single-crystal diffractometer. In addition, there was a crystal optics laboratory and a well-resourced model room. The geographical position of Chemical Physics within the campus allowed the setting up of interactions with the departments of Metallurgy, Physics and Chemistry and the proximity of organisations such as the Royal Aircraft Establishment allowed the M.Sc. course to be run on a part-time as well as full-time basis.

As Head of Department and Reader in Chemical Crystallography Mark was always committed to chemical physics as a separate discipline and to this end, he made sure that all the undergraduate and taught postgraduate students had the opportunity to study mathematics, "proper maths" as he called it.

At this time, there was little or no opportunity to use computers to enhance lectures so all visual aid material was constructed by hand and he produced a large number of expertly drawn transparencies to explain the many aspects of crystal geometry and symmetry, as well as producing a collection of some 300 35mm photographic slides. Fancy automatic slide projectors did not exist or were too expensive, so he acquired an ancient slide projector which was brought along to his lectures.

The 1970s were a time of change. Personal computers were evolving, and Mark saw this as a real opportunity to enhance the chemical physics degree. Within this framework, he developed the concept of two distinct themes, the science of measurement and the science of structure. The former was based around the use of microcomputers as a means of monitoring and controlling a range of scientific processes. The latter expanded the solid-state themes into studies of surface structure, electron diffraction and crystal growth in collaboration with the metallurgy department.

In 1981 the Higher Education sector in the UK suffered severe financial cutbacks. Several departments at Surrey were closed and Chemical Physics was subsumed into Chemistry as a sub-department, although still retaining its independence and academic head. However this gave Mark the opportunity to form stronger links with the various synthetic chemistry groups which were further strengthened when he persuaded the university to purchase a new Enraf Nonius Cad4 diffractometer, and he got great pleasure in persuading many Ph.D. students in these groups to think about including structure determination of some of the molecules that they were synthesising.

However, as time progressed numbers of students on both the undergraduate chemical physics and taught masters courses started to decline and eventually the university decided to close both of them. It was with great sadness that Mark agreed to this, although he did persuade the chemistry department that some of the chemical physics modules would make ideal final-year options and he continued to contribute to these.

Over his long career Mark authored or co-authored many textbooks. The first of these, Practical Radiochemistry, was co-authored with W.H. Lee, a physical chemist working in the chemistry department at Battersea. This was the start over several years of a whole series of books covering Physical Chemistry, Structure and Bonding, Symmetry in Molecules and Crystals, and Structure Determination by X-Ray Crystallography (with R. A. Palmer). Even after retirement he was insistent that the textbooks should be kept up to date. Many underwent subsequent revisions with new sets of problems and computer-based material which was made available on an accompanying website.

Outside of the university Mark was passionate about music. He played the double bass as a member of the Croydon Symphony Orchestra and also played the viola. Students undertaking some of the practical modelling classes which he supervised would find a classical melody playing quietly in the background as 'relaxation' for them. None of the students dared ask whether they could have something a bit more modern!

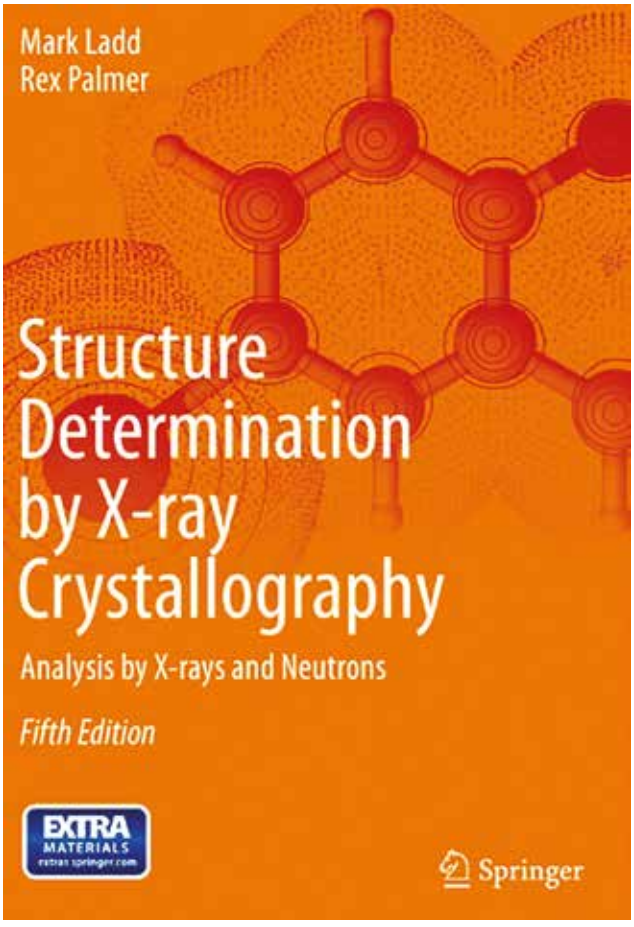
He became interested in Doberman dogs after a friend gave them their first Doberman. This developed into showing the animal at Crufts where it won best in breed and was the start of more than a hobby. Mark moved into breeding Dobermans, importing animals from the USA and eventually producing a book on Doberman genetics. He was also president of the Surrey Doberman Society for several years. The first that anyone new about the developing interest in dogs was when one was proudly brought into the department, much to the anxiety of the departmental secretary – not a dog lover! Feeling that she had to say something she asked Mark what the name of the animal was. Mark with his usual attention to detail came out with the long Kennel Club registered name. "I shall never remember that" said the secretary. "The dog is brown in colour. I shall call him Mr Brown". From that day on, everybody in the department, staff and students, knew Mr Brown who used to sit quite happily in the corner of Mark's office.

At the age of eighty, and indicative of his adventurous spirit, he and his wife decided to swap the comfort of suburban Farnham to a more remote existence in Bramshott where he continued with his writing, and he was often to be found in the chemistry department talking about some ideas about a new book he was planning.

Sadly, declining health curtailed many of his activities although he was still active in writing and his final book "The Essence of Crystallography" was published at the end of 2019.

He lost his beloved wife of 69 years, Val, only five weeks before he died, and he leaves two sons, Tony, a Professor in the Chemical Engineering Department at the University of Florida, and Nick, a Church of England Minister.

**David Povey**
(University of Surrey)



# Meetings of interest

In the current pandemic situation, many meetings are being cancelled or postponed. At the time of writing, all the meetings listed here were scheduled to go ahead either in-person or online, but there are likely to have been further changes since going to press. Further information may be obtained from the websites given. Assistance from the IUCr website is gratefully acknowledged.

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

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

**2nd Sep 2020 - 6th Sep 2020**
Euroscience Open Forum (ESOF2020)
Trieste, Italy.
**https://www.esof.eu/en/**

**14th Sep 2020 - 17th Sep 2020**
60th Anniversary Meeting of The British Biophysical Society
Via Zoom.
**https://bit.ly/31p61xC**

**14th Sep 2020 - 16th Sep 2020**
Science@FELs 2020
Online meeting.
**https://indico.desy.de/indico/event/24279/**

**23rd Sep 2020 - 25th Sep 2020**
ILL and ESS European Users Meeting
Lund, Sweden.
**http://neutrons4europe.com/**

**28th Sep 2020 - 2nd Oct 2020**
ICDD Clinic - Rietveld Refinement & Indexing
Newtown Square, PA, United States.
**http://www.icdd.com/rietveld/**

**4th Oct 2020 - 6th Oct 2020**
2nd Joint Meeting of the "Young Crystallographers" (DGK) and the "Young Crystal Growers" (DGKK)
Freiberg, Germany.
**https://dgk-home.de/aks/jkyc/freiberg-2020/**

**12th Oct 2020 - 16th Oct 2020**
Cristallographie et Grands Equipements 2020
Gif-sur-Yvette, France.
**https://www.synchrotron-soleil.fr/fr/evenements/ecole-cristallographie-et-grands-equipements-2020**

**1st Nov 2020 - 5th Nov 2020**
Crystallography for Space Sciences
Addis Ababa, Ethiopia.
**letaeyasu@yahoo.com**

**8th Dec 2020 - 10th Dec 2020**
MLZ User Meeting and Deutsche Neutronenstreutagung
Munich, Germany.
**https://indico.frm2.tum.de/event/225/**

**28th Jan 2021 - 29th Jan 2021**
DESY Photon Science Users' Meeting
Hamburg, Germany.
**https://photon-science.desy.de/users_area/users'_meeting/index_eng.html**

**29th Mar 2021 - 1st Apr 2021**
British Crystallographic Association Spring Meeting
Online conference.
**https://crystallography.org.uk/spring-meetings/#next-meeting**

**18th Apr 2021 - 23rd Apr 2021**
Imaging Materials with X-Rays – Recent Advances with Synchrotron and Laboratory Sources
Seattle, WA, United States.
**https://www.mrs.org/meetings-events/spring-meetings-exhibits/2021-mrs-spring-meeting/call-for-papers/detail/s21/ct03/Symposium_CT03**

**23rd Apr 2021 - 27th Apr 2021**
Crete 2021 - 1st International CryoEM Symposium/Workshop
Heraklion, Crete, Greece.
**https://cryoemcrete.com/**

**14th May 2021 - 16th May 2021**
10th International Conference of the Hellenic Crystallographic Association
Athens, Greece.
**https://sites.google.com/view/hecra2020/home**

**14th Jun 2021 - 18th Jun 2021**
16th International Conference on Surface X-ray and Neutron Scattering (SXNS16)
Lund, Sweden.
**https://www.sxns16.org**

**29th Jun 2021 - 2nd Jul 2021**
AFC 2020: Congress of the French Association of Crystallography
Grenoble, France.
**https://afc2020.afc.asso.fr**

**4th Jul 2021 - 10th Jul 2021**
6th European Crystallographic School (ECS6)
Budapest, Hungary.
**https://www.ecs6.chemcryst.hu/**

**18th Jul 2021 - 23rd Jul 2021**
11th Liquid Matter Conference
Prague, Czech Republic.
**http://www.lmc2020.cz/**

**30th Jul 2021 – 4th Aug 2021**
71st ACA Annual Meeting
Baltimore, MD, United States.
**https://www.amercrystalassn.org/future-meetings**

**9th Aug 2021 - 14th Aug 2021**
IUCr2020 Computing School
Nove Hrady, Czech Republic.
**https://www.xray.cz/iucr/workshops/nh/default.htm**

**11th Aug 2021 - 13th Aug 2021**
School on SAXS/SANS and BioSAXS/BioSANS data analysis
Kutná Hora, Czech Republic.
**https://www.xray.cz/iucr/workshops/kh/default.htm**

**11th Aug 2021 - 14th Aug 2021**
Electron Crystallography School
Tabor, Czech Republic.
**https://www.xray.cz/iucr/workshops/tabor/default.htm**

**12th Aug 2021 - 14th Aug 2021**
TOPAS Intensive Course
Prague, Czech Republic.
**https://www.xray.cz/iucr/workshops/topas/**

**14th Aug 2021 - 22nd Aug 2021**
Twenty-Fifth Congress and General Assembly of the International Union of Crystallography
Prague, Czech Republic.
**http://www.iucr2020.org/**

**6th Sep 2021 - 8th Sep 2021**
Understanding Crystallisation: Faraday Discussion
Leeds, UK.
**https://www.rsc.org/events/detail/41849/understanding-crystallisation-faraday-discussion**

**12th Sep 2021 - 17th Sep 2021**
15th Biennial Conference on High Resolution X-Ray Diffraction and Imaging (XTOP 2020)
Minsk, Belarus.
**https://www.xtop2020.atomicus.by/**

**16th Sep 2021 - 18th Sep 2021**
23rd Heart of Europe Bio-Crystallography Meeting (HEC23)
Vierzehnheiligen, Franconia, Germany.
**https://www.hec23.uni-bayreuth.de/en/index.html**

**19th Sep 2021 - 23rd Sep 2021**
23rd European Symposium on Quantitative Structure-Activity Relationship
Barcelona, Spain.
**https://www.euroqsar2020.org/**

# #RSCPoster @britcryst ??

I was on a coach to Glasgow for a live music gig (remember those?) and I was scrolling my Twitter feed when I found out about the Royal Society of Chemistry 2020 #RSCPoster Twitter Conference due to be held on that same day. Back in March, before the Covid-19 pandemic forced this new lockdown reality upon us, online conferences were not really "a thing" and I never attended one. However, since I had a three hours journey ahead with nothing to do, I made the impromptu decision to join in. Luckily, I already had prepared a poster for another conference. Participating was simple: the only thing I had to do was to register online and tweet a picture of my poster with a title and one or more relevant subject categories. I was a bit sceptical at first, as I am not very confident with handles and hashtags, but as soon as my tweet went online, likes and interactions came in. With about 800 registered poster presenters spanning across the chemical sciences, over 4700 attendees from all corners of the globe and more than 9900 tweets, the potential audience was huge. In 24 hours, my poster only was seen more than 19000 times, certainly way more than all the presentations I have ever given combined together! Overall, the event turned out to be incredibly fun and engaging.

Now, online conferences and webinars are slowly becoming the new norm. These virtual events have no environmental impact and the benefit of attracting a broader participation, although some are saying that it will never be possible to replicate the networking opportunities offered by raising a few (sometimes too many) glasses together (*Nature* **582**, 136, 2020; *Science*, doi:10.1126/science.caredit.abc5170, 2020). In my opinion, the unique online format of #RSCPoster provided an exciting way of presenting and networking on the move: I retweeted my poster and answered questions even while waiting for the band to get on stage! It was possible to browse amazing posters and interact with scientists from all disciplines in a friendly environment, a great thing especially for young scientists who sometimes may feel intimidated to engage with more senior peers in the usual conference setting.

Virtual meetings surely have several downsides, and online poster presentations risk to be dull and with no real exchange of opinions (*Nature* **582**, 166, (2020)). However, with its immediacy, the familiar Twitter style undoubtedly encourages discussion and allows participants to freely use their creativity in promoting their science. Twitter could provide an excellent stage for informal and accessible scientific presentations, characteristics which are particularly attractive to the younger generations of scientists. Not only do I highly recommend readers to take part to the next edition of #RSCPoster, but I also strongly advocate a similar initiative to be held by the BCA (especially its Young Crystallographers Group) in order to create an event entirely dedicated to connecting members of the crystallographic community in such a dynamic way.

**Sacha Fop**
University of Aberdeen

## Editor's comment

*Sacha is being very modest – his poster on Hexagonal Power was runner up in the Materials section and won him £60! You can see it in all its glory (except we've had to get it to fit on an A4 page) overleaf. Successful science on a long-distance bus!*

*#RSCPoster will be returning in 2021 for another 24 hours of sharing, networking and engaging with fellow chemists across the globe. The event will be held from 12:00 (UTC) 2 March 2021 – 12:00 (UTC) 3 March 2021. Follow @RoySocChem and #RSCPoster for further details to come.*

*It's also perhaps worth mentioning that the Institute of Physics Publishing ran a similar event (#IoPPposter) in July 2020 – see https://ioppublishing.org/news/iop-publishing-launches-social-media-powered-poster-conference-ioppposter/. So it's worth looking out for their 2021 version also.*

# Hexagonal Power

## Hexagonal perovskites for ceramic fuel cells

*Sacha Fop & Abbie C. Mclaughlin*

1495 UNIVERSITY OF ABERDEEN

## $CO_2$ emissions in the UK

**451** million tonnes in 2018


51% of $CO_2$ emissions in the UK from automotive and energy sectors

**0** target set for 2050

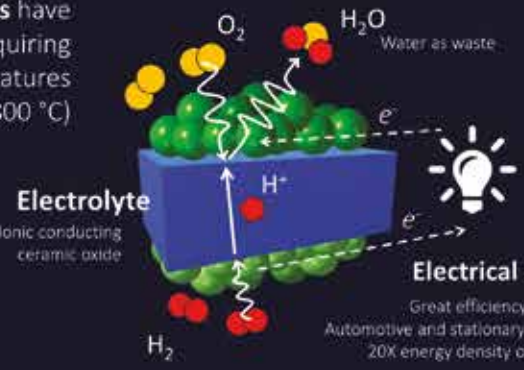
**Climate change is a threat - now.**

$CO_2$ emissions from fossil fuel use must be reduced to limit global warming

## Clean energy production: ceramic fuel cells

**Drawback**

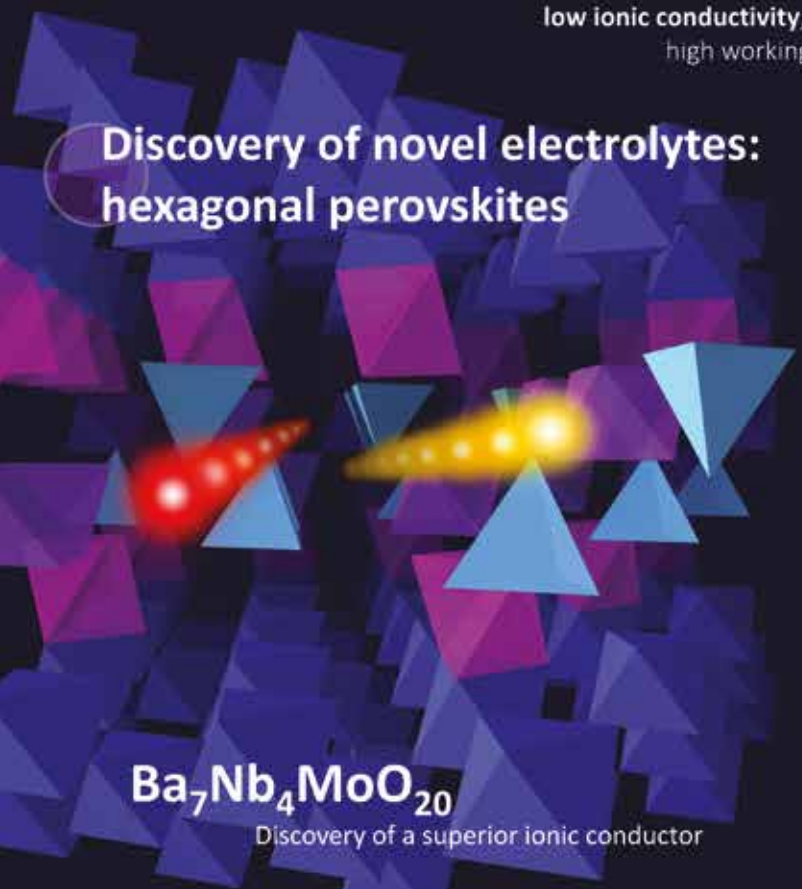
Available **solid state electrolytes** have **low ionic conductivity**, thus requiring high working temperatures (> 800 °C)




**Electrical energy**

Great efficiency (up to 80%)
Automotive and stationary applications
20X energy density of Li-batteries

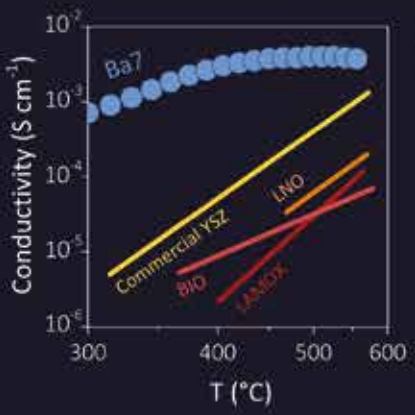
## Discovery of novel electrolytes: hexagonal perovskites



### $Ba_7Nb_4MoO_{20}$

Discovery of a superior ionic conductor

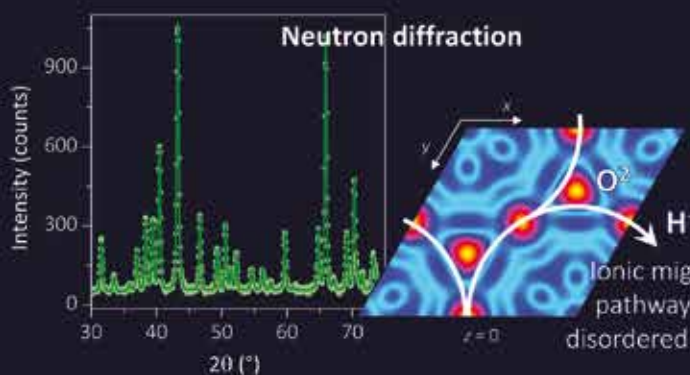
**$Ba_7Nb_4MoO_{20}$: remarkable ionic conductivity**




**10 – 100 times higher** than best commercial electrolyte, YSZ

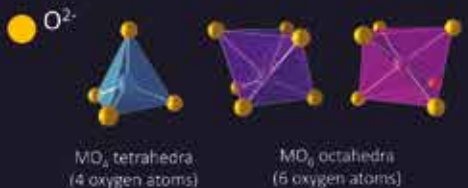
**Game changer** development of fuel cells operating at temperatures ≤ 500 °C

Study of the **crystal structure** (i.e. the arrangement of atoms in a material) is **essential** in order to design top-performance electrolytes




Ionic migration pathway along disordered layers

**Structural disorder enables fast ionic conduction**




Mixture of *corner-sharing* □ and *face-sharing* ○ **polyhedral units**



- Paris Agreement, UNFCC, 2016.
- UK Greenhouse Gas Emissions, National Statistics, BEIS, 2018.
- S. Fop *et al*, *Nature Materials*, accepted (in press), 2020.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@AbSSChem

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