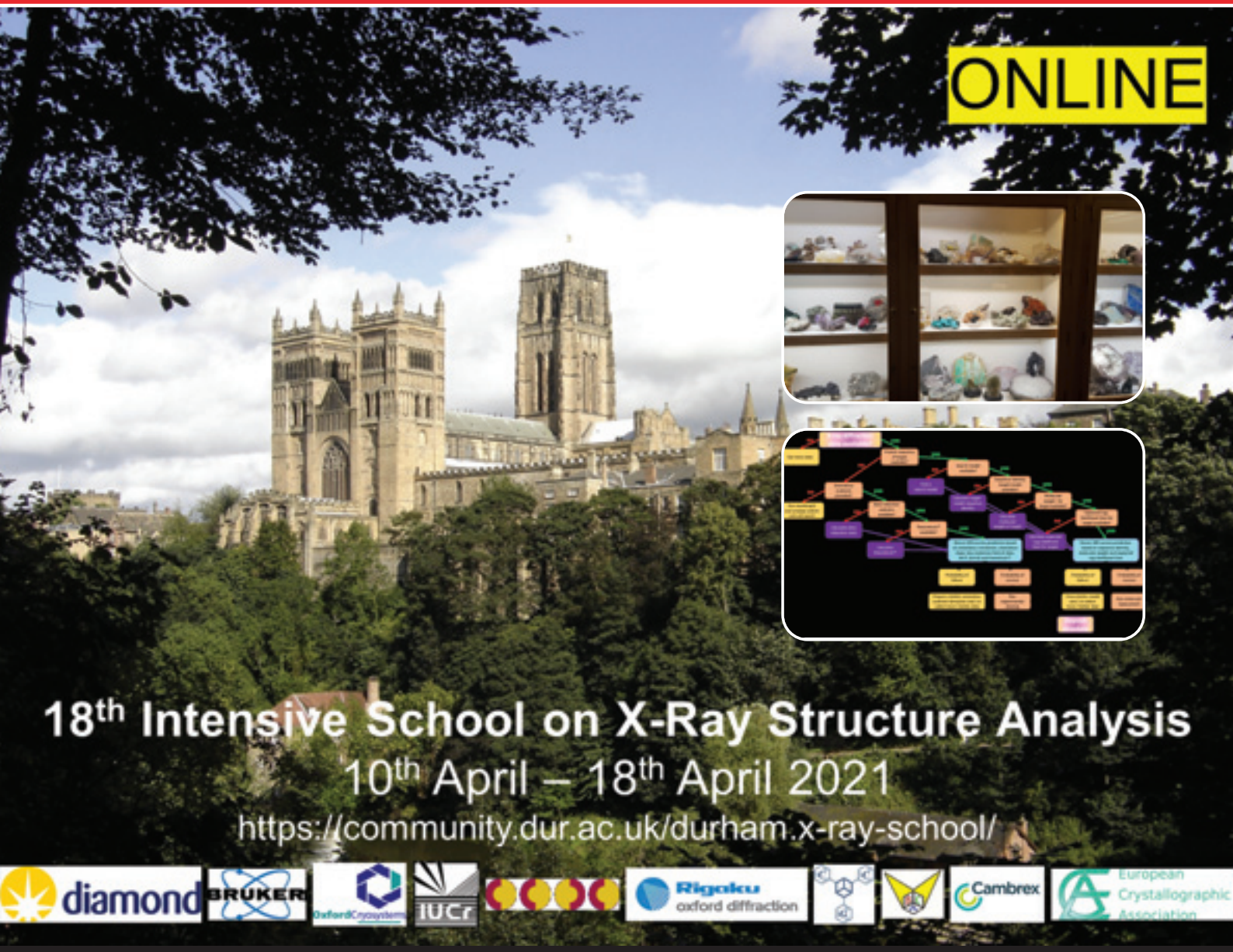
# Crystallography News

## British Crystallographic Association

Issue No. 155 December 2020
ISSI 1467-2790




## AI & Open Science at Large Scale Facilities


# IμS DIAMOND – Simply Brilliant

## ‘Diamonds are a crystallographer’s best friend‘

The extreme hardness of diamonds has allowed crystallographers to study materials at pressures greater than the core of the Earth. Now, the extreme heat conductivity of diamond gives crystallography a new X-ray source without equal: the IμS DIAMOND source. Diamond conducts heat five times more efficiently than any other known material, making it perfect to cool the intense heat loads in a modern microfocus source.

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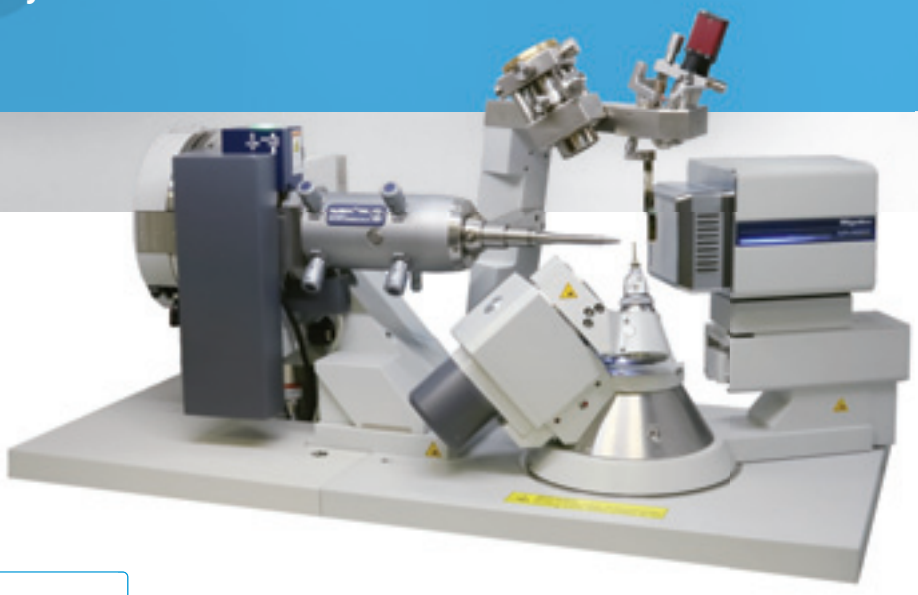
Crystallography

Innovation with Integrity

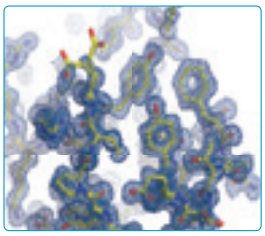
# THE EVOLUTION OF DUAL-WAVELENGTH TECHNOLOGY: XtaLAB Synergy-DW VHF

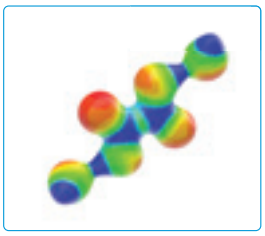
- New VHF optic produces 50 percent more fluence
- One source, two wavelengths, computer switchable
- Hybrid photon counting detector with massive dynamic range
- Perfect instrument to share between SCX and PX research
- Best-in-class data quality



Rigaku oxford diffraction

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

In 2004, a revolution in crystallography was started when the Gemini dual-wavelength diffractometer was introduced. The experimental versatility of having two different wavelengths available to carry out diffraction experiments was quickly recognized as being important for a modern X-ray lab. The XtaLAB Synergy-DW VHF is an evolution of that original concept and greatly extends the range of crystal sizes that can be measured by utilizing a dual-wavelength rotating anode X-ray source and a new VHF optic that increases the fluence at the crystal by 50 percent.

Rigaku



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British Crystallographic Association

# Bursaries for conference attendance in 2021

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 (in person or virtual). Applications should be made via the website:

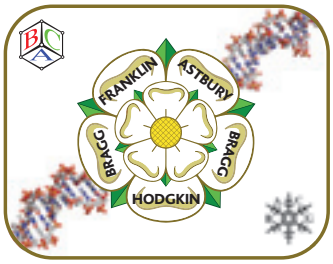
https://crystallography.org.uk/prizes/bursaries

Additional carers grants are available to BCA members at any career stage; these are awarded by the Industrial Group.

https://industrial.crystallography.org.uk/bursaries-and-awards/

Applications can be made at the BCA and IG websites.





# Contents



## *This month's cover:*

*Durham Cathedral; Exhibits in the Smithsonian Museum; Machine Learning Predictor Decision-making Steps*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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 March 2021 issue are sent to the Editor to arrive before 25 January 2021.

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

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

# From the President

**IT'S mid-October. I am, once again, sitting at my PC, looking out of the window over the village recreation ground. The cricket pitch markings have made way for football pitches, and I have a strong sense of déjà-vu. The Covid-19 pandemic is accelerating again and restrictions are tightening, although with regional variations this time. I do not know what the situation will be when you read this article, but it is likely to be worse. The BCA, however, continues to operate as normally as possible via Zoom, although we would all like to see friends and colleagues in the flesh, and preferably in the lab. or a bar.**

Virtual conferences do work, however, and we should be grateful for the relatively recent technology that makes this possible. The ACA, for instance, held its annual meeting in a virtual format in August, attracting large numbers of posters and abstracts. The offer of cheap ACA membership and attendance for BCA members was an innovative move, spawning an ongoing discussion between our two associations on the possibility of future reciprocal membership arrangements. I attended the British Biophysical Society (BBS) 60th Anniversary meeting in September and was pleasantly surprised by how enjoyable such a virtual meeting can be. It attracted a larger number of participants than usual, many from outside the UK. This seems to be a general trend, and an interesting article in *Science* (doi:10.1126/science.caredit.abe9591) explores it in more detail, analysing a number of recent conferences in the USA. The virtual format allows researchers and students from other countries to attend where they could not normally afford to come in person. It also benefits other groups who find it difficult to attend, such as those with disabilities. The record attendance increase reported, 500%, was for the American Association for Cancer Research, with most conferences surveyed showing more modest changes from previous years. The planning committee for the 2021 BCA Spring Meeting foresaw the looming second Covid wave, and decided that the meeting would have to take place virtually. When things are back to normal post Covid, we should be considering how a virtual component might be added to meetings in the future.

The international research assault on the SARS-CoV-2 virus continues apace, with a number of vaccine trials progressing well and crystallography still featuring strongly. Amongst many interesting studies, one that caught my eye was by **Pamela Bjorkman** at Caltech, on the structures of eight different antibodies, identified from patients convalescing from Covid-19, and their complexes with their target antigen, the spike (S) protein from the coronavirus surface. As I write this, her paper is available online in *Nature*, but not yet in print. The antibodies are 'neutralising', i.e. they bind to the S protein and inhibit viral entry to cells. She used the increasingly popular combination of high-resolution crystal structures and cryo-EM to show where and how they bind, and how specific mutations in the S protein would prevent antibody binding. Different antibodies bind to different regions and conformations of S. This knowledge informs the design of antibody 'cocktails', where two or more antibodies can be chosen such that a single mutation of S would inhibit binding of one but not the other(s), so that the virus could not escape neutralisation. This approach is key to emerging treatments with such antibody cocktails, including the one developed by Regeneron and used on the US President.

The Nobel Prizes have just been announced and, once again, winners have connections with crystallography. **Jennifer Doudna** shared the chemistry prize for work on gene editing using the CRISPR system. She was interested in catalytic RNA molecules, or ribozymes, in her Ph.D. research, and realized that knowing the 3D structure is essential to understanding the catalytic mechanism, just as for protein enzymes. She learnt crystallography and solved the first ribozyme structure in 1996, becoming a leading light in the challenging area of RNA crystallography. The CRISPR work retains this dependence on structural studies. **Roger Penrose** shared the physics prize for work on black holes, but his work on tessellation of a surface to generate long range five-fold symmetry, 'Penrose Tiling', solved a problem that crystallographers used to think was impossible. It was extended to three dimensions by **Alan Mackay** at Birkbeck and shown to explain the five-fold symmetry in the diffraction pattern of quasicrystals by **Daniel Shechtman** (Chemistry Nobel Prize, 2011).

I am pleased to report that nominations have been received for the three positions, President, Ordinary Member and Education and Outreach Coordinator, available in the Council membership elections. I would encourage all members to use their votes, having read the candidates' statements in this issue. Electronic voting is easy, and recent political history should teach us all that it is important to register your vote.

Registration is now open for the BCA 2021 Spring Meeting, that was to be held at the University of Leeds but will now be virtual, so please get out your pens/keyboards, start writing your abstracts and sign up at https://registrations.hg3conferences.co.uk/hg3/165/home. This meeting is special in that it will be held jointly with the British Association for Crystal Growth (BACG), and will exploit the synergies between the two organizations and their members. We have secured the use of a sophisticated virtual platform, which will allow parallel sessions, poster sessions and a commercial exhibition, reproducing most of the conference experience, with the exception of the bar and ceilidh. If you cannot do without the last two you will have to arrange for them yourself in the privacy of your own home. Registration fees are lower than usual, and the lack of travel and accommodation costs will make for greatly reduced costs for attendees. The programme appears elsewhere in this issue, and includes joint sessions between the BCA and BACG, and the Bragg lecture from **Richard Henderson**. I would strongly urge members to register and support this meeting and the BCA in these difficult times. I would also extend my thanks to the meeting planning committee, who have worked tirelessly in the face of the challenges posed by the pandemic, and for a period extending over two years instead of the usual one. I look forward to seeing you all there.

I hope you are all well and wish you the best in these challenging times.

**Simon Phillips**

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

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

# From the Editor

**IN the September issue, both Simon Phillips and I talked about the pros and cons of remote as against in-person conferences. One of the generally accepted advantages of on-line meetings is a reduced carbon footprint – after all, the aviation industry is responsible for about 2% of global $CO_2$ emissions, and driving fossil-fuelled cars is a major contributor to our carbon footprint.**

However, the analysis done by one of my colleagues comparing the carbon footprint of a recent three-day on-line UK conference with that of actually going to the same meeting in a conference-centre hotel got me to question some of my assumptions.

For example, the internet requires supercomputers cooled by giant cooling systems: just to keep it running for a year consumes 416.2 TWh of electricity, which is more than the annual UK consumption of electricity. What fraction of this do we eat up in using the web, and in a Zoom call (...other platforms are available...)? What's the carbon footprint of staying in our own home compared to that of the chosen conference centre? And although I have blithely assumed that the carbon footprint of flying to a conference is a *really bad thing* in terms of adding to global warming, how does that stack up against the other $CO_2$ costs involved in attending a conference from home?

## Typical carbon emissions ($kgCO_2$)

| | | |
|---|---|---|
| Use Zoom | 0.282/hour | About 1 hr Netflix; 1.5 miles car journey |
| Load web pages | .006/page | |
| Home energy | 7.8/day | Less for 'eco homes' |
| Home food | 3.9/day | Less for flexi/vege/tarians |
| Driving | 0.20/mile | Much less for electric car. Sharing less than train. |
| Train | 0.16/mile | |
| Air | 0.22/mile | Varies with fuel efficiency and passenger load factors. Includes radiative forcing. |
| Hotel | 31.1/room/night | Accepted hospitality industry standard |

The table gives some 'standard' or 'typical' figures from various 'carbon calculators'. I have used these to estimate the carbon footprint of attending, on-line and in-person, a three-day UK meeting (BCA Spring Meeting?). For the on-line version, I would have generated about 41kg of $CO_2$ – of which 14% would have come from Zooming 20 hours over the three days. For in-person participation, assuming an average return travel distance of 200 miles, 50% travel by (non-electric) car, 20% of attendees sharing a car, and 30% travelling by train, and an average hotel stay of 2.5 days, the average $CO_2$ bill per person would have been 107kg, 28% of which would have been from travel. So the in-person event would have been 2.6 times more $CO_2$ costly than staying at home. Q.E.D.

But wait a moment!

What struck me forcefully was that the whole equation is dominated, not by travel but by the footprint of the conference centre compared to that of staying at home. The figures given in the table for both these 'costs' are highly variable: our own 'home' footprints will depend on our particular diet and how we heat our home, and some hotels are making big efforts to reduce their footprints. One quoted in a 2018 issue of HOTELS Magazine (**https://considerategroup.com/carbon-emissions/**) has reduced it to a fifth of the industry standard. Substituting that figure into the equation brings the per person $CO_2$ bill for an in-person meeting down from 107kg to 44kg – within 'error', the same as staying at home.

Of course, the stay-at-home costs can also be decreased to make that option more climate-friendly, and in your absence your house could still be occupied by the rest of your family. But what this exercise has underlined to me is that it's not the travel to a UK conference that dominates the carbon equation, but the carbon costs of both staying at home and occupying the conference venue. We can affect both these by in the first case reducing our own at-home footprint, and in the latter case by asking questions of potential conference venues. Until these 'residential' costs are reduced, the travel involved would not be the major contribution to an individual's carbon footprint in attending an in-person conference in the UK. Unless you are travelling electric with 'green' energy in your battery (which would make a major change to the travel element), this conclusion becomes progressively less valid as the distance travelled increases. And if you are flying a serious distance, for example to the U.S., then even though the per mile figure is similar to that of driving on petrol or diesel, the flight will indeed totally dominate your $CO_2$ emissions (for example 1.5 *tonnes* for a return flight to Boston to attend a Gordon Conference). So at least one of my earlier assumptions was correct...

Finally, to conclude with a non-controversial matter, it would be very amiss of me not to thank Mark Comer for his excellent design work for the last three issues of *Crystallography News*. He stood in for our regular designer Tony Hopps when Tony had to take time out for medical treatment. We are delighted that Tony is back with us for this issue, and are extremely grateful to Mark for holding the fort so effectively.

**John Finney**

# Puzzle Corner

**SOCIAL** distancing is a topic in which crystallographers can give advice. The Church of Scotland has suggested that the maximum number of people in a hall should allow 8 square metres per person. This is very generous, in terms of space, not people. What is the amount of space per person if people are "packed" in a hall 16 m x 10.5 m, so that no one is less than 2 m from anyone else?

## *Answer to September's puzzle:*

The number of arrangements of cards you may be dealt is 52x51x50x49x48. These will not be all different, as any particular hand may have been dealt in 120 (5!) orders. Finally, there is one Royal Flush in each of the 4 suits. Thus the chance of getting one of these is 1 in (52x51x50x49x48/120)/4 = 649,740.

## BCA Corporate Membership

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

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

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

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### Benefits of Individual BCA Membership:

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

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

# BCA-BACG 2021 Joint Spring Meeting

## 29th March-1st April 2021 · Online

https://registrations.hg3conferences.co.uk/hg3/165/home.

## YCG-BACG Early Career Satellite Meeting

## SESSION DETAILS

### YCG/BACG Early Career Satellite Meeting

**Monday 29 March, 2021**

**09.30 – 17.40**

Chairs: Natalie Tatum (Newcastle) and Tom Roseveare (Sheffield)

The YCG satellite meeting is an opportunity for all early career researchers in the field of Crystallography to present their work in a supportive and friendly environment, and will be run by fellow early career scientists. This year's meeting will be the first joint meeting with BACG early career members and will be held virtually. There will be four sessions of talks on Monday chaired by: session 1: Stephen Dodsworth; session 2: Emma Wolpert; session 3: Natalie Tatum; session 4: Natalie Johnson, along with a short presentations session (chaired by Tom Roseveare and Natalie Pridmore) with presenters given 2-3 mins to present their data (similar to flash presentations).

### 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 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.

**09.30 – 10.00**

### YCG Plenary talk

Speaker: Cheryl Doherty (GSK)

***Exploring digital design for pharmaceutical solid forms***

**13.20 – 13.50**

### Parkin Lecture

Speaker: Elizabeth Driscoll (Birmingham)

***The building blocks of battery technology: Inspiring the next generation of battery researchers***

## BCA-BACG 2021 Main Meeting Programme

**Tuesday 30 March, 2021**

**09.45 – 10.00**

**Opening remarks and welcome to the conference**

## 10.00 – 11.30 Parallel Sessions

### Parallel Session 1
### CCG: Advances in Software for Crystallography

Chair: Lucy Saunders (Diamond Light Source)
Keynote: Florian Kleemis

***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!

### Parallel Session 2
### BSG: 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.

## Parallel Session 3
## BACG: *In situ* monitoring of crystallisation

Chair: Tariq Mahmud (Leeds)
Keynote: To be confirmed

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.

## Parallel Session 4
## BACG: Crystal Growth – theory to practice

Chair: Linda Seton (Liverpool)
Keynote: To be confirmed

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.

# 13.30 – 14.30 Parallel Plenary Talks

## CCG Plenary

Chair: Hamish Yeung
Speaker: Franziksa Emmerling (BAM, Berlin)

***Shaken not stirred: enhancing the flavour of mechanochemistry***

## IG Plenary

Chair: Helen Blade (AstraZeneca)
Speaker: Marcus Neumann (Avant Garde Materials Simulation)

***Title to be confirmed***

## PCG Plenary

Speaker: Vaclav Petricekval

***The role of crystal structure analysis in investigation of crystals with important physical properties***

## BSG 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***

# 15.30 – 17.00 Parallel Sessions

## Parallel Session 1
## PCG: 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.

## Parallel Session 2
## CCG: 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.

## Parallel Session 3
## BSG: 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.

## Parallel Session 4
## BACG: Nucleation – theory to practice

Chair: Joop Horst (Strathclyde)
Keynote: To be confirmed

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.

# Wednesday 31 March, 2021

# 10.00 – 11.30 Parallel Sessions

## Parallel Session 1
## PCG: <3D: 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.

## Parallel Session 2
## BSG: 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

## Parallel Session 3
## IG/BACG: Crystal growth: pitfalls and challenges in industrial crystallisation

Chairs: Natalie Johnson (CCDC, Cambridge) and Helen Blade (AstraZeneca)
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.

## Parallel Session 4
## CCG/BACG: Crystal growth of framework materials (incl. MOFs)

Chairs: Nick Blagden (Lincoln) and Michael Zaworotko (Limerick)
Keynote: Michael Zaworotko (Limerick)

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.

# 12.00 – 13.00 Exhibition Session and live Q and A chat

## 13.30 – 15.00
## Bragg Lecture

Speaker: Richard Henderson (Cambridge)

# 15.30 – 17.00 Parallel Sessions

## Parallel Session 1
## PCG: >3D: Structure and Properties of Higher-Dimensional Methods

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.

## Parallel Session 2
## BSG: 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.

### Parallel Session 3
### BCA/BACG: Control and Predictions of Crystals

Chairs: Angeles Pulido (CCDC, Cambridge) and Helen Blade (AstraZeneca)
Keynote: Dr Sten Nilsson-Lill (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 on 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.

### Parallel Session 4
### BACG: Crystallisation of Pharmaceuticals

Chair: Grahame Woollam (Novartis)
Keynote: Dr Sten Nilsson-Lill (AstraZeneca)

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.

## 17.30 – 18.30 BCA AGM

# Thursday 1 April, 2021

## 10.00 – 11.30 Parallel Sessions

### Parallel Session 1
### CCG: Chemistry at Extreme Conditions

Chair: Hamish Yeung (Birmingham)
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!

### Parallel Session 2
### CCG/PCG: 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.

### Parallel Session 3
### BSG: 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.

### Parallel Session 4
### BCA/BACG: Crystal Engineering

Chairs: Nick Blagden (Lincoln) and Bucar Kreso (UCL)
Keynote: Bucar Kreso (UCL)

***Respiratory supercomplexes: what can we learn from yeast?***

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.

## 12.00 – 13.00 Poster Session and live Q and A

### 12.00 – 13.00
### Lonsdale Lecture

Speaker: Lucy Clark (Liverpool)

### 13.30 – 15.00
## BACG 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.

## 13.30 – 15.00 BCA Early Career Prize Lectures

## 15.30 – 17.00 Parallel Sessions

### Parallel Session 1
### PCG: 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.

### Parallel Session 2
### BSG: 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.

### Parallel Session 3
### CCG: 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.

### Parallel Session 4
### PCG/BACG: Biominerals and Biomaterials / Carbonaceous Materials

Chair: Julia Parker (Diamond)
Keynote: Melinda Duer (Cambridge)

***The bare bones of biomineralization: new insights into bone mineral composition, structure and formation***

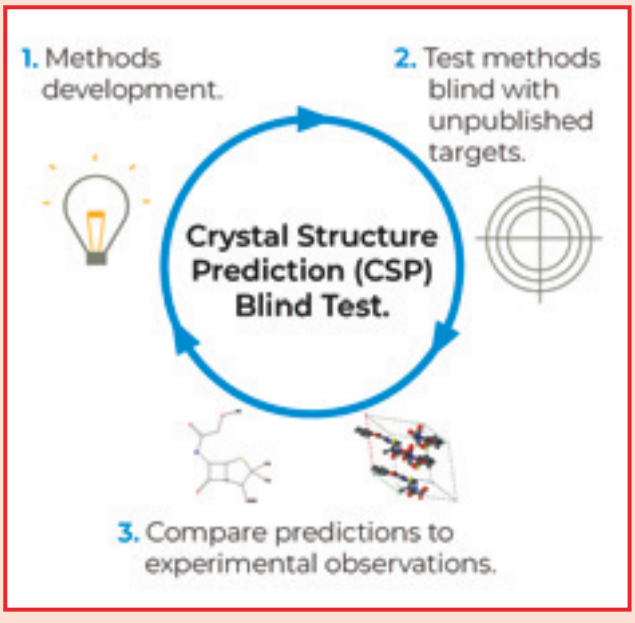
From the exquisite morphologies of coccoliths and the incredible hierarchical architecture of bone, to the engineering of implants and joint replacements, the structure of biominerals and biomaterials plays an integral role in determining their properties and function. This session will examine the importance 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.

# The 7th Crystal Structure Prediction Blind Test has begun!

**This major challenge in computational chemistry will see the world leading methods in Crystal Structure Prediction put to the test on real targets - with a high bar set by previous work. The seven test systems have been sourced from leading experimentalists in industry and academia for prediction.**

The first phase ends in October 2021,

Fancy your chances? New participants can still sign up. Full details on the CCDC website at **https://www.ccdc.cam.ac.uk/**.



# BCA Council Elections 2021

## Candidate Statements

**NOMINATIONS for BCA President, Ordinary Member of Council and Education and Outreach Coordinator have been received. Elections will be held by electronic ballot of the BCA membership. The short CVs and statements produced by the candidates are given below; the order in which they are given for each post is random.**

## President Candidate:

### Richard Cooper

**Current position:**
Head of Chemical Crystallography and Associate Professor, Department of Chemistry, University of Oxford.

**Career:**
M.A. (Oxon) Chemistry; D.Phil. in Inorganic Chemistry, University of Oxford; PDRAs at University of Oxford; Software Specialist, Oxford Diffraction Ltd; R&D Manager, oXray Ltd; Software Developer, InhibOx Ltd.

**Activities:**
Scientific Director of the UK Intensive Crystallography School; Acta C co-editor; Contributor to international crystallographic teaching schools, ECA and IUCr Computing Schools; Chair of Departmental Public Engagement Committee; Fellow of the Royal Society of Chemistry; Python and Fortran hacker; Karateka; Cycling advocate.

**Research Interests:**
I am fascinated by finding patterns and rules in structural data for understanding and controlling material properties. This has led to development of classification models for predicting crystallizability of molecular materials. I dedicate some of my time to developing crystallographic software tools that improve our ability to extract useful information from experiments. Recent applications have included determination of hydrogen ($^{1}$H) positions using neutron Laue diffraction combined with complementary experimental and computational data. Software tools are often incorporated into the crystallographic analysis package, CRYSTALS, for wider use.

**Statement:**
Can you see my slides? This could have been the catchphrase of the year, but it will struggle to beat "Your microphone isn't on". These are trivial effects of a terrible pandemic, but reflect disruptive changes that many of us are experiencing. Yet if you are willing to embrace interesting times, why not offer to serve as BCA President?

I have been a BCA member since my student days and have chaired the CCG, and served on the BCA Council for many years as Vice President, Council member and webmaster. I value being part of a friendly and supportive community which provides regular opportunities to share and discover research across a range of disciplines.

The BCA serves the UK community in many ways: organising meetings, providing bursaries for travel and supporting teaching schools; promoting and supporting scientific and educational projects at a national and international level; and sharing resources to support public engagement about crystallography and our research. These common goals motivated the creation of our Association, and I believe we should continue to enthusiastically pursue them.

There is a timely opportunity to take advantage of online meetings to connect a diverse range of speakers with a wider audience. We have also encouraged collection of outreach material via our learn.crystallography website for several years, and we can utilize these efforts to meet the demands for remote learning activities in the coming months.

It is exciting to see emerging science that builds upon crystallographic knowledge. We should continue to engage with developments that inform our own subject, such as the forthcoming joint meeting with the British Association of Crystal Growth and the inclusion of electron diffraction, computational simulation and time-resolved crystallography in our meeting programmes.

Understanding the structure of matter is the heart of crystallography, and it remains essential for determining and controlling the behaviour of molecules and materials from ionic solids to viruses. I will work to ensure that the BCA continues to broaden its range of activities and opportunities for sharing research, and supporting training and outreach within our subject.

## Ordinary Member Candidates:

### Anthony E. Phillips

**Current position:**
Reader in the Physics and Chemistry of Materials, Queen Mary University of London.

**Education and career:**
B.Sc. (Inorganic Chemistry)/B.A. University of Sydney; Ph.D. (Physics), University of Cambridge; fellow then academic, Queen Mary University of London.

**Previous BCA roles:**
I have recently come to the end of my term on the PCG committee, first as YCG rep (2012-13), then after a short hiatus as Treasurer (2014-17) and Chair (2017-20). In that capacity, I served on the Program Committee of the 2013 ECM in Warwick, and have chaired sessions at many recent Spring and Winter meetings.

**Research Interests:**
Typical of the physical crystallography community, my work sits somewhere between solid-state chemistry and condensed matter physics. I am especially interested in framework materials, their phase transitions and polymorphism, and the anomalous thermodynamic, electric, and magnetic behaviour that so often results. I am a longstanding user of total scattering and pair distribution function methods to determine local structure in disordered materials, and also use X-ray and neutron spectroscopy to provide complementary measurements of structure and dynamics. I am an experienced user of synchrotrons and neutron sources worldwide, and serve on review panels for ISIS (Crystallography) and ANSTO.

**Statement:**
Both the scientific expertise of the British crystallographic community and its friendliness and openness have enriched my professional life immeasurably over the past decade. I am thus pleased and grateful to have been nominated to serve this community as an Ordinary Member of the BCA Council.

As I see it, we face a twofold challenge: to maintain and develop crystallography itself, and to build strong links to our scientific neighbours. Thus, on a local level, we must continue to support the educational programmes and meetings that nurture our own community, while engaging with the closely related communities with whom we often share members (spectroscopists, computational chemists, electron microscopists, …). And, in the context of the wider scientific landscape, we must continue to demonstrate that crystallography is an active, relevant, and important science in its own right, working as needed with other scientific societies (RSC, IOP), the Research Councils (EPSRC, STFC), and international organisations (IUCr, ESS).

Of course, none of these are new ideas – our work in all of these directions is thoroughly established already. I believe I have both the technical expertise and the community knowledge to help support this work, and to contribute towards a flourishing BCA in the years ahead.

## Cheryl Doherty

**Current position:**
Scientific Leader at GSK in Chemical Development.

**Education:**
M.Chem. in Chemistry at the University of Bath (2001); Ph.D. in Chemistry, University of Bath (2005).

**Professional Activities:**
Member of the British Crystallographic Association and Ordinary Member of BCA Council 2019-2021 (Bursary Officer). BCA Industrial Group committee member 2009-2018, chair (2013-2016), vice-chair (2016-2019). Meeting and session organiser of numerous Industrial Group meetings during this time. Diamond Industrial Science Committee DISCo (2013-present day). Royal Society of Chemistry member, Fellow and Chartered Chemist.

**Research/Professional Interests:**
Small molecule crystallographer and pharmaceutical materials scientist working in the pharmaceutical industry. Primary focus on developing robust dosage forms for drug candidates. Guiding the solid form selection including experimental screening, characterisation and analysis of the candidate molecules. This involves using models and structural information to digitally design a program of action for these projects. Candidates range from early research (before first in human studies) all the way through to those in Phase III clinical trials. Focus areas include using laboratory and synchrotron diffraction methods, crystal polymorphism, structure-property relationships and the digital design of drug products.

**Personal Statement:**
I have enjoyed and valued my membership in the BCA since I joined as a student member. I moved to the Industrial Group as I started my career in the pharmaceutical industry and served on committee there as an ordinary member, vice chair and chair over 10 years. I was pleased in 2019 to stand as ordinary member on BCA Council and have served in that time as Bursary Officer, supporting student attendance at our Spring Meeting. I am also delighted to have been nominated to stand again for an Ordinary Member position on BCA Council. I work primarily with formulators, medicinal chemists and process chemists with little background in the structural sciences. The impact crystallographic information can have on all these other areas is profound and I have supported outreach efforts in this area, such as by contributing to the RSC Medicinal Chemistry Residential School last few years. Membership of the BCA has provided a vital contact with structural scientists in academia and industry for me, and I am looking forward to many more rewarding collaborations in the future.

# Education and Outreach Coordinator Candidates

## Ilaria Gimondi

**Current Position:**
Education and Outreach Officer at the Cambridge Crystallographic Data Centre (CCDC).

**Education and Career:**
Bachelor and Master in Chemical Engineering, both awarded with honours (2013 and 2015) at Politecnico di Milano (Milan, Italy). Ph.D. in Chemical Engineering (awarded in 2020) at University College London (London, UK).

During my Ph.D. years, I volunteered at the Science Museum (London, UK). I also did some Post-Graduate Teaching Assistant work in the Dept of Chemical Engineering at University College London (London, UK).

**Research Interests:**
I have recently completed a Ph.D. on the study of polymorphism using molecular modelling techniques. We used molecular dynamics and metadynamics to study transitions between polymorphs of carbon dioxide and to investigate conformational polymorphism in succinic acid. Part of this work is published in four papers.

**Statement:**
I am very pleased to be nominated for the Education and Outreach Coordinator role for the BCA. This is a very thrilling and welcome opportunity for me, just at the beginning of my career after Ph.D.

I believe that education and outreach are fundamentals to create and support the next generation of scientists and crystallographers. I, personally, was tremendously inspired by my teachers and the volunteers and educators that I met throughout my journey, who taught me to love learning and encouraged me to pursue a career in science. It is now our turn, and responsibility as a community, to inspire young learners and support them with their steps into our world.

This belief is what pushed me to start my career outside academia as Education and Outreach Officer at the CCDC. The synergy and collaborations between the CCDC and the BCA are certainly not new, sharing a number of values and belonging to the same community. In the education and outreach department, we have seen this collaborative effort bringing to life the Periodic Table of Crystal Structures, project in which I am currently involved, for example contributing to the creation of the Battlecards, a fun game to learn about elements and crystals.

In the current worldwide scenario, we all had to adapt to a more digital and virtual way to work and live. It is thus important that also our educational resources and efforts move in this direction, as the BCA education and outreach department has been doing. In these regards, over my first months at the CCDC, I have gained experience adapting hands-on activities to home-friendly resources (CCDC Home Learning), curating the webpages for these activities, and drafting social media posts. As part of my role at the CCDC, I will be travelling (restrictions allowing) to a number of conferences.

As Education and Outreach Coordinator for the BCA I would be an active Council member working with the Association to ensure education and outreach activities remain a key focus. I feel that our community should be at the heart of everything we do and so establishing new ways to collaborate with members to create resources to inspire the future generation of structural scientists will be important. In practise this will involve building on the online resources that already exist and establishing new ways to support and engage young scientists.

I am looking forward to joining the BCA community and working with you to inspire young and future scientists.

## Christine Beavers

Hello, I am Christine Beavers, Principal Beamline Scientist of I15 at Diamond, and a candidate for the Education and Outreach Council position. Education and outreach are of paramount importance to me as a crystallographer and beamline scientist. More chemists, physicists and material scientists are using crystallographic tools and methods; it is our responsibility, as crystallographers, to make sure that everyone who depends on crystallography can become well versed in it. I have been actively involved in educational outreach for all of my career: during my graduate studies at UC Davis I entertained and educated during the beloved Chemistry Magic Show; at the ALS I was awarded a Directors Award for my tours and outreach activities; most recently at Diamond I have been active in open days and school visits. I was an invited speaker at the US National Neutron and X-ray School for most of the last decade, and in the most recent edition of the Durham Single Crystal School, I was a tutor. I am proud of what crystallography has accomplished and I am eager to help spread the news of what it does today.

# 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

# The PaNOSC FAIR Data Policy

## Introduction

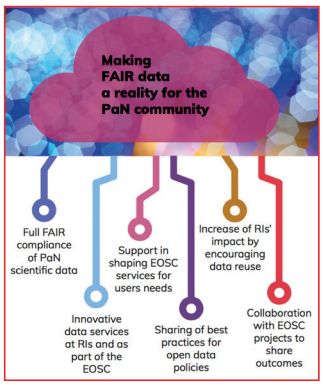
**DATA are the main result produced by experiments carried out at photon and neutron sources. Researchers derive results from data and eventually publish them. The need to share data as open data or as part of a traditional publication in text form is one of the principles of Open Science[i]. Having access to data is essential to understanding, reproducing and extending research. The trend towards constantly increasing volumes of data, and more and more powerful algorithms being developed, is forcing researchers to turn to the data instead of relying only on the text in traditional publications[ii]. Researchers faced with huge volumes of data need help in managing these data in order to publish them and make them reusable. These reasons, as well as the need to manage data, means data producers like photon and neutron sources need to define the policy under which data are produced, curated and made available. A data policy describes which data are covered by the policy and who has access to the data. Without a data policy which describes the rights and obligations of researchers there is little incentive for research institutes to manage huge volumes of data for the long term (decades).**

## The last ten years

The photon and neutron communities were in advance of the 'Findability, Accessibility, Interoperability and Reusability' (FAIR) data movement when in 2010 they released the data policy of the Photon and Neutron Data (PaNdata) infrastructure initiative[iii]. This policy listed best practices for data curation and advocated making data open after an embargo period. The PaNdata data policy was designed to be a framework which could be adapted by any institute or community to their needs prior to being adopted. ISIS and ILL were the first institutes to adopt the PaNdata data policy. They were followed by ESRF and eventually by almost all the photon and neutron sources in Europe. Sites that have not adopted a PaNdata-like data policy are becoming increasingly rare as the FAIR principles[iv] become widely accepted by communities and publishers. The publication of the FAIR guiding principles in 2016 generated a lot of interest in the scientific community and became the guiding principles for data for the European Commission's Open Science Cloud (EOSC)[v]. With the wide adoption of the FAIR principles by the scientific community, including the protein crystallography community[vi vii], it has become urgent to update the PaNdata data policy to include the recommendations and research on FAIR data management[viii].

## The PaNOSC data policy

The Photon and Neutron Open Science Cloud (PaNOSC) project (**https://panosc.eu**) is one of five cluster projects financed by the European Commission's H2020 INFRAEOSC-04 call. It groups the six photon and neutron sources on the European Strategy Forum on Research Infrastructures (ESFRI) roadmap. The PaNOSC partners are ESRF (synchrotron), ILL (neutron source), EuXFEL (free electron laser), ELI-DC (optical laser sources), ESS (neutron source), together with the ERIC CERIC-ERIC (a distributed research facility that includes three photon and neutron sources), e-infrastructures EGI (partner) and GÉANT (contributor). PaNOSC works closely with the national photon and neutron sources via the H2020 project ExPaNDS (**https://expands.eu**). The PaNOSC data policy framework[ix], published in May 2020, is one of the deliverables of the PaNOSC project. The data policy was developed together with ExPaNDS partners over a period of 12 months. The 10 year old PaNdata data policy was taken as the starting point.




The first step was to gather feedback on the PaNdata data policy from sites that had adopted and implemented it. The next was to integrate this feedback into the new data policy. The final step was a critical analysis of the new data policy for its compliance to FAIR based on the FAIR Data Maturity Model (FDMM) recently published by the working group of the Research Data Alliance (RDA)[x]. The FDMM details 41 criteria for evaluating if a data object takes the FAIR principles into account. By applying it to the PaNOSC data policy framework it was possible to ensure that all 41 criteria were covered either by the data policy or by the local implementation. The PaNOSC data policy introduced a series of Implementation Notes for criteria to be addressed by the local implementation.

## The main points of the PaNOSC data policy are:

1. Scientific research data are managed in accordance with the FAIR principles.
2. The raw data produced at the source should be managed by the institute operating the source as custodian of the data.
3. Raw data will be available to the team who produced the data for exclusive use during a period referred to as the embargo period.
4. The definition of raw data does not necessarily mean the output directly from the detector but depends on the technique and what data can be useful to reconstruct the derived results.
5. The length of the embargo period will be decided by the institute operating the source (the guideline of three years is based on the average length of a Ph.D.).
6. The embargo period starts after the last data have been collected.
7. All curated data are made available as open data after the embargo period.
8. The investigation team can make data open before the end of the embargo period for publication or other purposes e.g. if the data are of critical importance to society.
9. The data policy identifies and provides guidelines for different types of data and metadata which can be curated i.e. data can be raw, processed, auxiliary or results data.

10. Scientists are required to provide metadata for their samples and their own equipment.
11. Open data are made available via a machine readable open protocol.
12. Data are available internally for machine learning training for improving user services at the source.
13. Scientists are encouraged to follow best practices of linking software used to analyse data.
14. Data are curated for ten years within reasonable financial constraints.
15. Users must cite data persistent identifiers (DOIs).
16. User persistent identifiers (e.g. ORCID) are linked to the data.
17. Data are made available under Creative Commons licence (e.g. CC-BY, CC-BY-NC or CC0).
18. Data are curated in well known formats e.g. Nexus/HDF5 for photon and neutron data.
19. Users are encouraged to prepare Data Management Plans.
20. Proprietary research data do not fall under the data policy unless a special request is made to make data available with a persistent identifier.
21. Principal Investigators have special rights e.g. they can add or remove members from the investigation team, distribute copies of the data, create DOIs for individual datasets etc.
22. Data are curated as read-only; modifications to the metadata create a new version of the metadata.

All details can be found in the data policy document[ix].

The PaNOSC data policy framework has the same purpose as the PaNdata data policy framework i.e. a framework for sites that need to implement a data policy. It requires some modifications before being adopted. The minimum modification is to add the legal information of the site to the framework. In most cases, the framework will need some modifications to take into account local site specific issues e.g. the length and mechanism for extending the embargo period, local legal obligations, the definition of raw data etc.

## Implications for researchers

The main implications for researchers are that the data generated during their beamtime at the source will be managed and curated correctly. This is a significant step forward for users of photon sources who are increasingly being challenged by the huge data volumes generated by faster, larger detectors and new techniques like fine slicing and serial crystallography. Sites adopting the PaNOSC data policy framework will be able to offer FAIR data management to protein crystallography scientists as recommended by the IUCr[vi].

## Future activities

The PaNOSC and ExPaNDS projects are working on additional services like linking Protein Data Bank (PDB) entries to raw data to further enhance the FAIRness of data in the PDB. A common solution for Data Management Plans will be developed to assist users in creating and maintaining those plans. Both projects are collaborating on adopting existing standards for the metadata vocabularies part of the Nexus standard (**https://nexusformat.org**) e.g. the "Gold standard"[xi] for macromolecular crystallography, while defining vocabularies for new techniques for which Nexus standards do not yet exist e.g. for XFELs and laser facilities.

## Conclusion

The recently published PaNOSC data policy updates the ten year old PaNdata data policy framework to be Findable, Accessible, Interoperable and Reusable – i.e. FAIR. The new framework addresses the FAIR principles in detail and includes guidelines on best practices and implementation notes for sites adopting the framework. The six photon and neutron source institutes of the PaNOSC project will update their data policies to adopt the PaNOSC one and make open data available to the EOSC. All photon and neutron sources are encouraged to adopt or be inspired by the PaNOSC data policy to update their data policies to be compliant with the FAIR principles. The updated data policies will help users to manage the huge quantities of data being produced and help make results compliant with FAIR.


### Acknowledgements:

The author would like to thank all co-authors (J. Taylor, R. Dimper, J-F. Perrin, F. Gliksohn, D. Roccella, K. Wrona) and contributors (A. Ashton, H. Fangohr, A. Gonzalez-Beltran, A. McBirnie, A. Markvardsen, B. Matthews, R. Pugliese, D. Salvat) of the PaNOSC data policy. Special thanks to J.R. Helliwell who suggested writing this article.

PaNOSC has received funding from the European Union's Horizon 2020 Research and Innovation programme under Grant Agreement No 823852.



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On behalf of the PaNOSC project


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# AI for Science at Large-Scale Experimental Facilities

## Introduction

**THE Deep Learning revolution in Artificial Intelligence (AI) that we are now witnessing dates back to the ImageNet project that was led by Professor Fei-Fei Li from Stanford University based on over 14 million high-resolution images collected from the Web[1, 2]. Objects in the images were labelled by human labellers recruited using Amazon's Mechanical Turk. This was followed by a landmark breakthrough in image classification in 2012, by Geoffrey Hinton and two of his PhD students, Alex Krizhevsky and Ilya Sutskever. Their neural network implementation, now called AlexNet, used a 'Deep Neural Network' consisting of five convolutional layers and three fully connected layers and was implemented on two graphics processing units (GPUs). Their paper won the 2012 ImageNet competition and reduced the error rate by an astonishing 10.8% compared to the previous winner[3]. There were further developments to this, but the most notable one was the effort by a team from Microsoft Research who won the competition in 2015 using a very deep neural network of over 100 layers that achieved an error rate for object recognition comparable to human error rates[4].**

In this article, we shall use 'AI for Science' as a shorthand to mean the application of Deep Learning (DL) and other Machine Learning (ML) technologies to large scientific datasets. The Harwell Campus near Oxford hosts several large-scale experimental facilities that now generate large volumes of increasingly complex scientific datasets. These are the UK national synchrotron and the Electron Bio-Imaging Centre (eBIC) both operated by Diamond Light Source, the ISIS Neutron and Muon Facility, and the UK's Central Laser Facility. The Scientific Machine Learning (SciML) group at the Rutherford Appleton Laboratory is working with researchers and beamline scientists at these facilities to apply state-of-the-art ML technologies both to their data and to their experiments. The SciML group also partners with the Alan Turing Institute, the UK's national institute for data science and artificial intelligence, in their 'AI for Science' research theme. In addition, the group supports the PEARL 'AI' computing service for researchers at Turing and at the Science and Technologies Facilities Council (STFC) working on AI for Science on two NVIDIA DGX-2 GPU systems.

After some introduction to the vision and scope of scientific applications of AI and ML technologies at the Harwell campus, we give details of two important examples - X-ray macromolecular crystallography (MX) and cryogenic electron microscopy (cryoEM) before a few words in conclusion.

## Scientific Machine Learning

Our vision for the 'AI for Science' activities at Harwell goes well beyond just applying machine learning techniques for the final data analysis. The SciML research group at the campus has been focussing on this problem from two different viewpoints. One of them is in the development of robust AI/ML techniques that can facilitate the end-to-end processing of scientific datasets from these beamlines. Our key emphasis is on the need for these AI/ML techniques to coexist with conventional methods and software. If the overall end-to-end processing is to be treated as a pipeline of stages, we aim to ensure that AI/ML technologies can be integrated within the pipeline, along with other techniques, to enable the best outcomes. We show one such example pipeline used in cryo-EM processing in Figure 1.


*Figure 1: End-to-End Processing in Structure Identification in Cryo-EM Data.*

Although AI and ML technologies may ultimately overtake conventional techniques, this approach enables a progressive transformation that is particularly needed within operational settings where practical constraints take precedence over pure research-driven concerns. These AI and ML technologies can play a role in a number of stages here, such as minimising or removing unwanted information from experimental datasets (noise removal), identifying structural objects (segmentation), understanding experimental outliers (anomaly detection), and enhancing the quality of datasets, such as those of images and signals. Developing AI/ML frameworks that can coexist with existing processing chains and that can progressively transform the science is a key challenge for the community.

While applying AI and ML techniques to analyse the final datasets remain a key route for advancing science, we believe that the use of AI/ML technologies to optimize the actual experimental runs is equally important. Although this may sound a very operational issue, the use of AI and ML technologies could be truly transformative here. For example, using AI and ML techniques to obtain the best experimental settings (such as those of beamline parameters) based on initial scans can not only improve the results but also improve the efficiency and throughput of the facilities. Although this work is still at the exploration phase, we believe this will ultimately be found to be essential for the optimal running of the facilities and beamlines.

## Crystallography at the Diamond Light Source

At the Diamond Light Source, recent technological developments (e.g. photon-counting detectors) have fundamentally changed the way data are collected at X-ray macromolecular crystallography (MX) beamlines, particularly when combined with a fully automated, unattended, collection set-up. At beamline I04-1 for example, this means that a full 360° rotation data set, including sample exchange, can now be collected in just under a minute which results in 1380 datasets in 23 hours of beam-time. Such vast amounts of data can no longer be assessed manually by individual users but instead offer the opportunity to develop machine learning applications for data triaging, assessment and interpretation. There has also been an ever-increasing need to support structural biologist users as many now work in multi-disciplinary environments and are no longer highly trained experts in MX.

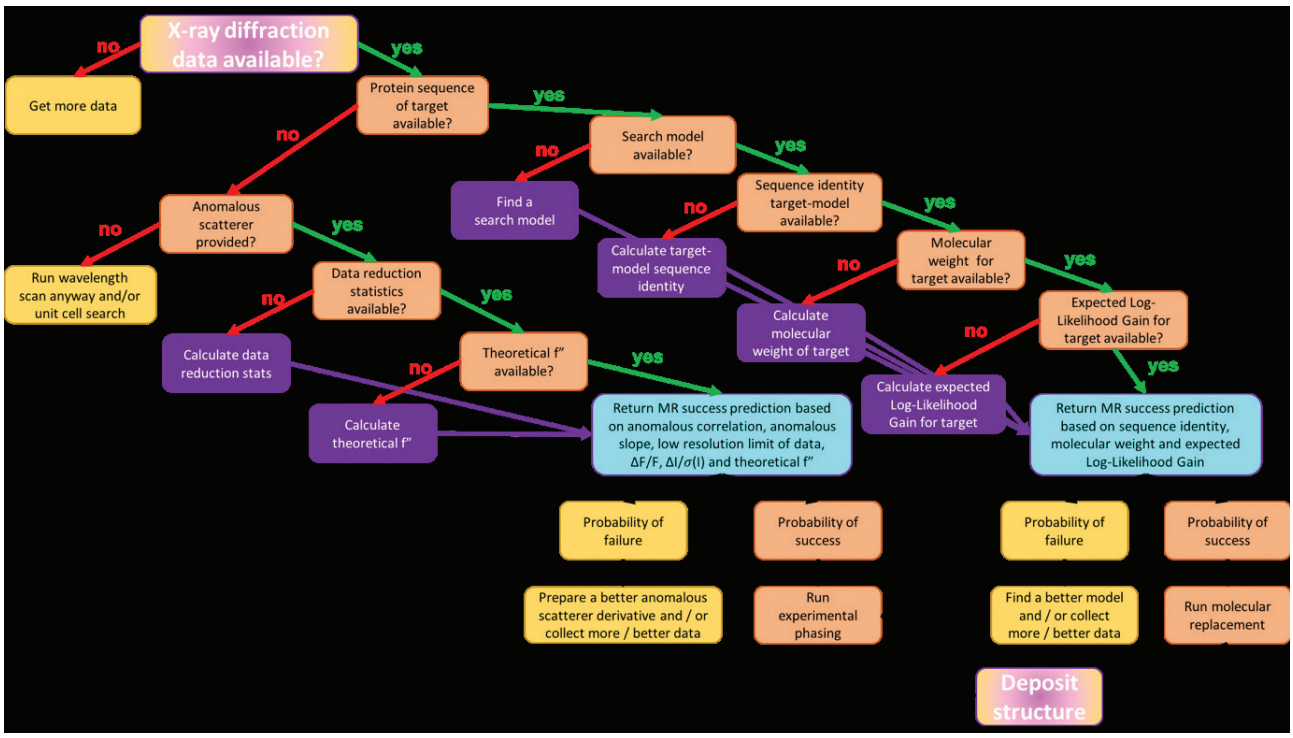


*Figure 2: Schematic Overview of Decision-making Steps during Data Reduction and Integration of ML Predictor.*

As the result of a collaboration between Diamond and the CCP4 MX software consortium[5], users now benefit from two machine learning predictors within the automated data analysis pipelines, run routinely after each data collection. These predictors assess the chances of each data set leading to a successful phase determination either by experimental phasing[6] or by molecular replacement. Both predictors are based on decision tree algorithms with AdaBoost implementation and were trained using metrics calculated during a data reduction step. The information output by either system allows the user or the automated pipeline to decide on which data sets to focus and progress for further analysis, and which ones to discard. The results of these predictors are evaluated, and the associated data are then used to re-train the system with the aim of improving the accuracy and reliability for the users.

In addition, a system is currently being developed in which, after deciding to take certain data forward for phasing, the achieved initial phases are evaluated as to whether they are going to be of sufficient quality to allow for model building. This assessment uses convolutional neural networks and works directly with the 3D electron density maps from phase determination to identify features that are specific to a protein and will lead to successful model building. Ultimately, it is expected that such an AI-based system will be able to place atoms and complete the map interpretation. This will leave the user only having to fix errors made by the algorithm in places where human intuition and experience is still superior. A prototype for identifying electron density maps that will allow for model building is already in place. Present work is now focused on improving performance and being able to use maps calculated in situations where the map quality is reduced because data may be incomplete, resolution may be low, or a molecular replacement model is a distant homologue.

The bottleneck for successful structure solution is no longer the availability of protein crystals, beamtime and diffraction data but the computational resources available. The aim of the developments described here is to give guidance to users and assist them in decision making and therefore reduce the time spent on given data and instead focus on the most promising results and make more efficient use of computational resources.

## Cryogenic Electron Microscopy

The field of cryoEM has matured quickly in recent years, and many structural biologists now use a combination of MX and cryoEM techniques. CryoEM shares many characteristics with crystallography that make it attractive for machine learning and AI, notably large amounts of experimental data that benefit from fast assessment and triaging, through to molecular volume data that requires interpretation.

High-end Titan Krios microscopes are deployed at several centres throughout the UK, each capable of generating one to ten terabytes of data in a day, depending on detector and mode of operation. In particular, the national centre at eBIC operated by Diamond on the Harwell Campus currently has five Krios microscopes together with additional support or specialised instruments. Efficient use of these expensive machines would benefit from fast feedback on the data collection strategy, for example, enabling scientists to answer questions like “Is the ice thickness and/or the particle distribution good enough to generate a high-resolution reconstruction?”. At eBIC, a pipeline for single particle analysis based around the early steps in the Relion software has been implemented to give rough-and-ready two- and three-dimensional class averages, without human intervention, for assessment during a user session. The most problematic step in this pipeline is the automated picking of particles from low signal-to-noise micrographs, a task which has traditionally relied on the tuned eyesight of human scientists.

Two-dimensional image analysis, including object detection, has been one of the big successes of Deep Learning and it is not surprising that these techniques have been applied to cryoEM particle picking. Popular software includes the Topaz, crYOLO and Warp systems. All these are based around convolutional neural networks but differ in implementation

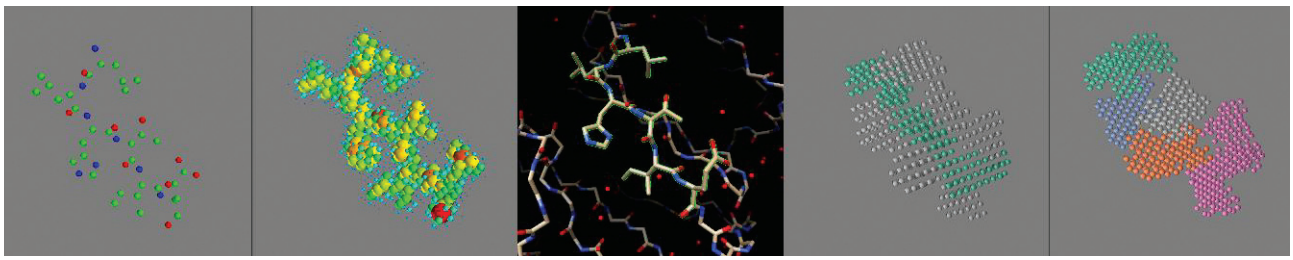

*Figure 3: Automated Segmentation and Annotation of Three-dimensional Volumes from CryoEM Reconstructions.*

details and in the underlying training data. At eBIC, crYOLO has been incorporated into the automated data processing pipeline to allow an initial selection of particles and hence downstream two- and three- dimensional analysis. Currently, the main purpose of the automated data processing at eBIC is ensuring optimal setup and performance of the instrument, for which an approximate analysis using heavily coarsened data is sufficient. With improvements in ML algorithms and computational infrastructure, there is clearly scope for more ambitious uses of automation.

The other principal area in which AI has been applied to cryoEM, and which has obvious overlaps with crystallographic structure solution, is the interpretation of three-dimensional volume data arising from single particle reconstruction or potentially from electron tomography. While standard crystallographic model building software can be used for high resolution cryoEM structures, most structures are still at too low a resolution for physics-based approaches to be reliable. As more structures are solved, the expectation is that data-driven approaches can be developed to learn to identify secondary structure elements or particular domains. Currently available software includes Emap2sec and Haruspex which use three-dimensional deep convolutional neural networks to detect secondary structure elements. Again, there are many implementation details which can influence the success of these approaches for a particular structure, and the CCP-EM consortium[7] is working closely with the SciML group on further improvements to this approach (see Figure 3).

Longer term, machine learning and AI technologies are likely to impinge on all aspects of cryoEM data processing. For example, work from the Relion developers is looking to exploit prior knowledge about biological structures through a convolutional neural network to improve the regularisation step of reconstruction. At a fundamental level, these are data-driven approaches and will improve as more data become available. The SciML and CCP-EM groups are currently benchmarking the cryoEM workflow so as to motivate and direct these anticipated improvements. Where the aim is to learn features of macromolecules, the data may come from various sources, and AI may ultimately help to unify the disciplines of structural biology.

## Concluding Remarks

The ImageNet success of the Deep Learning revolution relied on labelled datasets – a form of 'ground truth' that can be used to train the AI and ML systems. However, for data from the facilities, such curated datasets with labels are very rare, not only for MX and cryoEM, but also for other areas of experimental science. Developing AI/ML techniques to overcome this limitation remains a key challenge for the whole 'AI for Science' community. In fact, understanding which AI/ML techniques work better on which problem and which computer systems and how these 'black boxes' arrive at their conclusions remains largely a mystery.

The SciML group, through a collaboration with a number of major US Department of Energy laboratories, has been attempting to address this problem by assembling an appropriate 'Scientific Machine Learning' benchmark suite. The overarching goal of the benchmark suite is to include examples of a number of scientific problems (including MX and cryoEM) with curated labelled datasets and reference implementations that scientists can easily use. The resulting benchmark suite can then not only help scientists understand the basics of AI/ML techniques but also encourage them to evaluate or benchmark their preferred techniques against the reference implementation. It is worth stressing that the intention is that the benchmark suite will be openly available, including the curated datasets.

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# South West Structural Biology Consortium (SWSBC) Meeting, 20-21 July, 2020

**THIS year the meeting was organised by Ivo Tews (Southampton), Leo Brady (Bristol) and Kim Watson (Reading), who must be thanked for assembling a fascinating programme. Meeting virtually for the first time, participants were made aware of the advantages of this conference format, such as audio-posters and the ability to type questions for presenters or make comments online, as well as screen-grabbing slides and downloading posters, to name just a few.**


*Fig 1: A Microsoft Teams eye-view of organisers and session chairs of SWSBC 2020: **Jenny Littlechild** (Exeter), **Ivo Tews** (Southampton), **Kim Watson** (Reading) and **John McGeehan** (Portsmouth), shown clockwise from top-left.*

The meeting began with a session entitled: *CryoEM of molecular machines and assemblies* which was chaired by **Bertram Daum** and **Vicki Gold** (Exeter). The session started with a lecture by **Patricia Gil Diez** (Exeter) who described microsporidia – subcellular fungal parasites which infect animals and humans. Germination of the parasite spores involves the ejection of their contents into the target host cell through structures known as the polar tubes. Single-particle cryoEM has been used to show that the ribosomes of the *Spraguea lophii* parasite dimerise at this stage which, at least in prokaryotes, is associated with silencing of the translation apparatus. The speaker concluded by presenting a model for the injection of ribosomes into the host cell. The next presentation was by **Alexander Neuhaus** (Exeter) who described cryoEM and mass-spectrometric studies of the type-IV pili of *Thermus thermophilus*. These structures are involved in bacterial motility, biofilm formation and uptake of DNA. The speaker presented 3D reconstructions of the two forms of type-IV pili (wide and narrow) which are found to be extensively glycosylated. Next up, **Lavinia Gambelli** (Exeter) gave an interesting presentation on the monolayer of glycoprotein surrounding cells of the hyperthermophilic and acidophilic bacterium *Sulfolobus acidocaldarius*, known as the S-layer. This layer, which lies outside the periplasmic membrane, is 5-20 nm thick and 70 % of it is formed by pores. The speaker mentioned the possibility of coating magnetic beads with S-layer components and using them in magnetic swimmer therapy for delivering drugs or antibodies in cancer treatment. Extraction of the proteins from the S-layer by use of detergents has allowed the structure of one of them, slaA, to be determined by cryoEM. This protein determines the lattice spacing of the S-layer while the other, slaB, acts as a membrane anchor.

This talk was followed by a presentation from **Kapil Gupta** (Bristol) who described studies of an unexpected free fatty acid binding pocket in the SARS-CoV-2 spike protein. The structure of the spike was analysed by cryoEM at 2.85 Å resolution and established that linoleic acid binds to the receptor binding domains of this trimeric protein. Since these domains are necessary for viral infection, the discovery of this site has implications for drug design. Next, **Kaïn van den Elsen** (Exeter) gave a lecture on the structural basis of flavivirus replication. Flaviviruses such as Denge and Zika are single-stranded positive-sense RNA viruses which form localised replication centres that are associated with the endoplasmic reticulum (ER) of the infected cell. The speaker described cryoEM studies of the complexes in purified ER as well as reconstituted complexes made from proteins expressed in *E. coli*. **Nick Harmer** (Exeter) presented the idea of establishing a South West facility for micro electron diffraction. This technique allows structural studies of nanocrystals which are placed on an EM grid for data collection by rotation of the sample stage. Radiation damage is low by this technique and ion-beam milling is available if the crystals to be analysed are larger than optimal. The final presentation of this session was given by **Ufuk Borucu** (Bristol) who described the GW4 cryoEM facility which was opened in a joint effort between the Universities of Bath, Bristol, Cardiff, and Exeter, and houses an FEI Talos Arctica. The speaker outlined studies of f-actin in the microtubule lumen, the SARS-CoV-2 spike protein and a system of epitope display for use in vaccine development (the ADDomer platform).

The next session was entitled *Enzymes 1* and was chaired by **Jim Spencer** (Bristol) who introduced the first speaker **Greg Pollard** (Bristol), whose lecture focussed on biocatalysts for industrial crosslinking of polymers, specifically the enzyme lysyl oxidase. This enzyme is involved in remodelling the extracellular matrix by oxidising the side chain of lysine to an aldehyde such that adjacent residues can crosslink by condensation. The difficulty of working with the human enzyme meant that it was necessary to use the enzyme from an archaeal species which allowed studies with the diamine substrate cadavarine to be undertaken. Next, **Rachel Bolton** (Southampton/Diamond Light Source DLS) described data collection strategies for the radiation-sensitive, ferric iron-binding protein, FutA, which is associated with an ABC transporter mediating iron uptake by cyanobacteria. The system has been studied by serial femtosecond crystallography at the SACLA XFEL facility in Japan and at DLS, demonstrating damage to the iron centre at high doses. **Charlie Collingham** (Reading) spoke next on neurodegenerative diseases which are the second leading cause of death worldwide, and on how bile-acids have a beneficial effect. Structural studies of a yeast protein and its complex with a putative drug molecule were outlined. This was followed by a lecture from **Simone De Rose** (Exeter) who described a class of molecules known as extremolytes which are produced by extremophilic bacteria as molecular stabilisers and have applications in the food and drug industries. The talk focussed on two enzymes involved in biosynthesis of the extremolyte cyclic diphosphoglycerate which have been expressed in *Thermus thermophilus* using codon-optimised genes; the structure of one enzyme has already been solved. The final talk

of this session was presented by **Geoffrey Masuyer** (Bath) who described the ADP-ribosyltransferase known as endotoxin A which is produced by the pathogen *Aeromonas hydrophila*. The toxin is activated by the protease furin following endocytosis, and engineered forms of it have applications in a number of biological therapeutics. The structure of the toxin was determined at 2.3 Å revealing three domains, of which the third is catalytic, i.e. most likely is involved in the attachment of ADP-ribose to the host cell elongation factor EF2 at a diphthamide-modified histidine residue.

Lunch was followed by a plenary lecture given by **Alan Cheung** (Bristol) which was chaired by **Vicky Gold** (Exeter). The speaker gave an introduction to the workings of RNA polymerase II and the role of transcription factors (TFs) such as TBP, which binds to the TATA box first and other TFs then follow. The nucleosomes making up chromatin have extensive post-translational modifications on their tails which are exposed on the surface. The talk focussed on the SAGA and NuA4 N-acetyl transferases which are huge complexes of co-activator proteins that are involved in remodelling of chromatin to form the pre-initiation complex in order for a gene to be transcribed. The speaker described fantastic cryoEM studies of yeast Tra1 protein kinase which is a half megadalton component of both SAGA and NuA4 that forms a diamond ring structure made by α-solenoids. The speaker then described cryoEM studies of the whole SAGA complex revealing that the transcription factors form a large assembly, adjacent to and of comparable size to Tra1, that has structural similarities with the nucleosome core.

The afternoon session entitled *Protein interactions and disease* was chaired by **Dafydd Jones** (Cardiff) and began with a talk by **Hayden Fisher** (Southampton) about the effects of disulphide shuffling in the hinge region of antibody molecules. The speaker described a range of Cys-to-Ser mutants which had been generated and studied by molecular dynamics and SAXS. The more active form of the antibody was found to be more compact and less flexible than the inactive form. The next presentation was by **Rhys Dunphy** (Bath) who began with an introduction to the complement system. The project concerned the complement protein C3d which has been solved in a dimeric state. The speaker explained how the bacterium *S. aureus* can evade the complement system by producing the immune evasion protein Sbi which interacts with C3d. X-ray studies have shown that Sbi causes the N-terminal helices of the C3d dimer to swap over and a range of Sbi mutants have been analysed by CD and structural studies. Next, **Rory Munro** (Southampton) described how the calcium-binding protein S100A9 is involved in deposition of amyloid fibres in neurodegenerative disorders. Solid state NMR is being used to analyse the interactions between this protein and other amyloidogenic proteins such as Aβ and α-synuclein. This was followed by a lecture from **Alessandro Agnarelli** (Sussex) who described the transcription factor IRF4 which is involved in interferon signalling by binding to response elements in DNA as a dimer. Knockdown studies have implicated the protein in multiple myeloma, and ligands which prevent its dimerisation have potential therapeutic applications. The speaker explained how the structures of the DNA-binding domain bound to a variety of response element sequences have been determined but the structural basis of IRF4 dimerisation remains elusive. The session concluded with a lecture by **Daren Fearon** (DLS) who described an astonishingly fast fragment screening project for the SARS-CoV-2 main protease which was undertaken at the XChem facility and completed within a month of receiving the gene for expression and crystallisation. A total of 23 non-covalent active site hits were obtained spanning the S3 to S1' subsites of the protease and an additional 48 covalent hits were found in a mass-spectrometric screen. Coupling of selected non-covalently bound fragments had resulted in inhibitors with nanomolar (nM) affinity. The speaker outlined an international crowd-sourced drug-design and synthesis project targeting the enzyme, known as the Covid Moonshot. Work on an aminopyridine family of inhibitors and a quinoline series had led to the discovery of compounds with nM affinity.

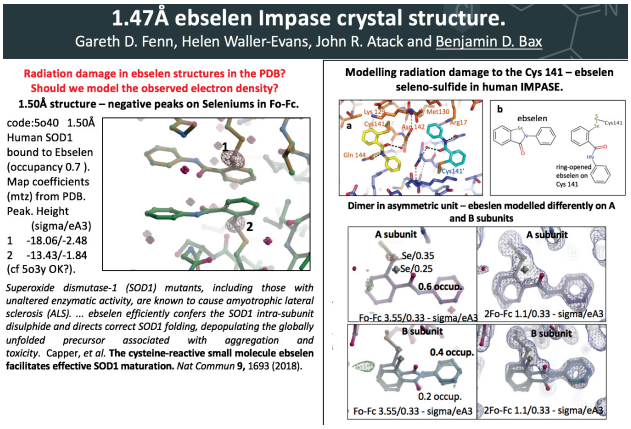



*Fig 2: A sample of one of the excellent virtual posters.*

This session was followed by poster presentations which were expertly hosted by **Ivo Tews** and **Phil Williamson** (Southampton) and an amusing quiz which was organised by **Charlie Collingham** and **Kim Watson** (Reading). It was very useful to be able to leave comments and questions on posters for the presenter to address later on.

The second day began early with computing workshops organised by **CCP4** and **CCP4N** which were followed by a plenary lecture by **Allen Orville** (DLS) who described methods for dynamic structural biology using XFEL sources that can work with extremely small crystals. The speaker explained that since the average enzyme-catalysed reaction takes around 60 ms, these processes are amenable to study by XFEL sources due to their use of femtosecond pulses, known as serial femtosecond crystallography (SFX). The speaker outlined the establishment of an XFEL hub at DLS to assist users wishing to do SFX and other experiments at the six XFEL facilities which are currently available worldwide. He described the issues of sample delivery which have been tackled successfully by the use of the lipidic cubic phase and more recently by the use of a special tape carrying droplets of crystals into the beam. Substrate can be added to the crystals by acoustic droplet injection which allows precise timing of events. The speaker concluded by describing in detail the fascinating work undertaken in collaboration with Chris Schofield (Oxford) to study the mechanism of isopenicillin N-synthase by the simultaneous use of SFX and X-ray emission spectroscopy.

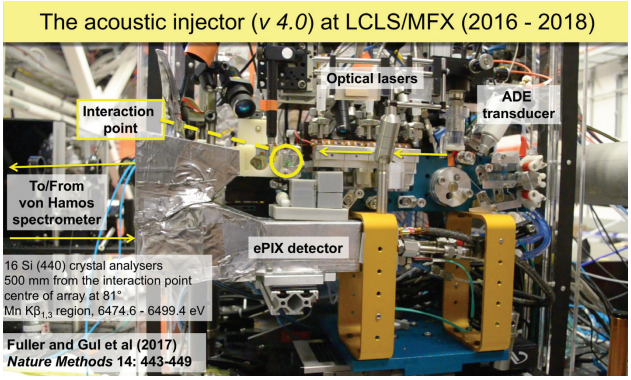



*Fig 3: A slide from the plenary lecture on the UK XFEL hub by **Allen Orville** (DLS).*

The following session on Biotechnology was chaired by **John McGeehan** (Portsmouth) who introduced the first speaker, **Erik Landin** (Bristol). Erik described signalling by G-protein coupled receptors (GPCRs) with a focus on the adenosine 2A receptor which is the target for two FDA approved drugs. The receptor has been studied by molecular dynamics, mutagenesis and $^{19}$F-labelling for NMR spectroscopy which confirmed conformational changes within the receptor caused by an antagonist that binds at a novel allosteric site. Next, **Alex Lander** (Cardiff) described studies of antibacterial peptides, which are produced by bacteria known as bacteriocins. Two such peptides, aureocin A53 and lacticin Q, were both studied by total chemical synthesis of the L- and D-stereoisomers for crystallisation of the racemic mixture. The resulting atomic resolution structure of aureocin suggests how it may target the phospholipid membrane surrounding Gram-positive bacteria. This was followed by another topical and interesting talk on surveillance of the COVID-19 epidemic given by **Sam Robson** (Portsmouth) who described genome sequencing of the virus isolated from patients over recent months. The speaker described the common occurrence of a D614G mutation which is associated with increased transmissibility of the virus but, thankfully, not with severity of the symptoms. The speaker's group is part of a UK consortium whose work informs infection-control procedures, with the aim of preventing a second wave. Next, **Maria Concistrè** (Southampton) described an advance in solid-state NMR, namely dynamic nuclear polarisation, in which the sample is spin-labelled and NMR spectra are collected with the excitatory microwave source both on and off. The following talk was given by **Emiliana De Santis** (National Physical Laboratory, Teddington, NPL) who described efforts to standardise bioengineered materials for gene, drug and vaccine delivery. The speaker outlined an interesting system of self-assembling synthetic capsids formed by disulphide-linked trimers of α-helical peptides, which have been studied by EM and CD.

## G-protein Coupled Receptors

G-protein Coupled Receptor (GPCRs) are targeted by more small molecule drugs than any other single protein family including natural compounds and 34% of FDA approved drugs[1]


1. Hauser AS, Attwood MM, Rask-Andersen M, Schiöth HB & Gloriam DE (2017) Trends in GPCR drug discovery: New agents, targets and indications. *Nat. Rev. Drug Discov.* **16**: 829–842

*Fig 4: The biological importance of GPCRs (not to be confused with GDPR, the well-known corporate legal headache) was emphasised by **Erik Landin** (Bristol).*

The final session, entitled *Enzymes 2*, was chaired by **Susan Crennell** (Bath) who introduced the first lecture, given by **Charlotte Colenso** (Bristol) on molecular dynamics studies of metallo-β-lactamases. The speaker described the application of a restrained dummy atom model to the zinc ligands to preserve key features of the active site during the simulation. The next talk was given by **Paul James** (Exeter) who outlined studies of an interesting transketolase from a hyperthermophilic archaeon, the gene for which is split across two open-reading frames (ORFs). The two halves of the gene were expressed separately in *E. coli* allowing the enzyme to be reconstituted in active form. Studies showed that the TPP cofactor is important for the enzyme's stability and work is ongoing to engineer changes in its specificity. The following talk was given by **Dan Mitchell** (Exeter) who spoke on measuring femto-Newton forces in enzymes by attaching them to gold nanoparticles and using an optoplasmonic sensor, which is currently under development, to measure the resonance frequency of the microsphere. Two transaminases and a glucanase of known structure have been selected for this project and molecular dynamics simulations of their different conformational states have been undertaken. Experimentally, the enzymes are attached to the nanoparticles by the use of a thiol-NTA linker bound to the gold which attaches to the enzyme's His-tag. Work to enhance the activity of the enzymes on the gold particles is in progress. The final talk was given by **Éilís Braggington** (ex-Bristol) who described work on a β-lactamase (OXA-57) from *Burkholderia pseudomallei*, the causative agent of the Southeast Asian disease melioidosis, for which there is no vaccine or effective therapy. The speaker described kinetic studies of the enzyme which has also been solved by X-ray crystallography with antibiotic substrates bound.

MβLs hydrolyse most β-lactam antibiotics

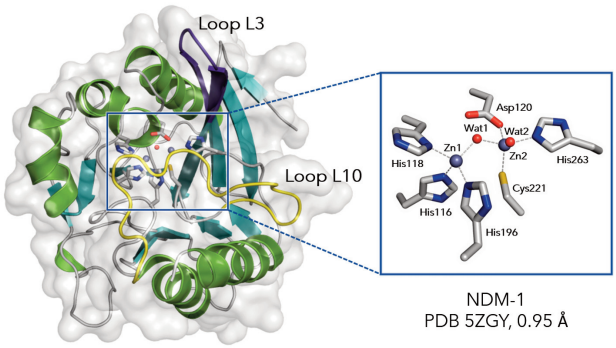
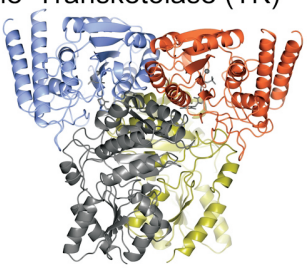



*Fig 5: A slide from **Charlotte Colenso's** (Bristol) talk.*

Thermophilic 'Split-gene' Transketolase (TK)

- *Carboxydothermus hydrogenoformans* (ChTK-F)
  - Reconstituted from two gene parts
- Sequence identity
  - 32 % *E. coli* enzyme (EcTK – PDB: 1QGD)
- Thermal Stability
  - ChTK-F
    - 100 % activity at 70 °C*
    - 50 % activity at 80 °C*
  - EcTK
    - 10 % activity at 60 °C*

*(for 1 hour)



PDB: 6YAK – 'Split-Gene' *Carboxydothermus hydrogenoformans* TK

*Fig 6: A slide from **Paul James's** (Exeter) talk..*

The meeting concluded with presentation of lecture prizes to **Emiliana De Santis** (NPL, Teddington) for early career research and to **Alex Lander** (Cardiff) for his postgraduate studies. This was followed by the poster prizes which were awarded to **Matthew Gaines** (Exeter), **Daniel Hinchen** (Portsmouth) and **Rachael Andrews** (Bath). **Mark Roe** (Sussex) received a special commendation as the social event quiz winner.

This concluded an excellent meeting for which the organising team, **Ivo Tews** (Southampton), **Charlie Collingham** and **Kim Watson** (Reading) were thanked by **John McGeehan** (Portsmouth) for their enormous efforts in bringing this virtual meeting together. The speakers and poster presenters were also thanked, along with the representatives of **CCP4** and **CCP4N** (**Vicky Higman** and **Ed Lowe**) who ran the early morning workshops. **Ivo Tews** (Southampton) must also be thanked for taking on the bulk of IT and administrative work, essential for ensuring that this virtual meeting ran as smoothly as it did.

**Jon Cooper**
UCL

# 69th Annual Denver X-ray Conference – A 2020 *Virtual* Conference

**THE COVID-19 pandemic has been a continuous challenge for the global community of scientists to work in new and different ways. As Chairman of the 2020 Denver X-ray Conference (DXC20) Organizing Committee, I am pleased to announce that the challenge was met by hundreds of scientists resulting in a successful virtual conference. The 69th Annual Denver X-ray Conference transitioned from a face-to-face meeting to a virtual format for the first time. The Conference Services team from the International Centre for Diffraction Data (ICDD) transformed the conference over a period of a few short months to an on-line platform available on a wide range of mobile devices, tablets, and desktop computers. The Organizing Committee focused on creating international participation. This meant that most workshops and session presentations were given as prerecorded videos, and the presentations were made available on-demand for the month of August. The content of over 150 videos and an additional 50 posters were produced by global scientists, many of them working from home in various time zones. During the conference, each video and poster had an active chat room that enabled viewers to ask questions, both during set period roll outs, and over the entire month. The conference included a virtual exhibit and many exhibitors offered their own videos as well as "live" video conferencing sessions to discuss their product offerings or view instrumentation or specimen preparation equipment. The conference was attended by ~ 380 scientists with attendees from 28 countries. The largest groups of participants were from the United States, Japan, Germany, Canada, and the United Kingdom.**

Attendees at the conference, and the global scientific community, have benefited from the tremendous advances in sources, optics, and detectors made over the past decade. Focusing optics, brilliant monochromatic sources, and detectors with both energy selectivity and wide dynamic range have created new capabilities that were highlighted at the DXC 2020. A combination of workshops and sessions worked to educate and train material scientists, from a wide range of disciplines and organizations, on advanced instrumental capabilities. There were 14 workshops and 18 sessions. Workshops on 2D detectors and X-ray optics were taught by a combination of scientists from the top manufacturers (XOS, Dectris, Malvern Panalytical, Bruker-AXS and Rigaku) and application scientists (Argonne NL, ICDD) with a focus on the fundamentals of how they work, and how they were developed. This was complemented by the session on New Developments in XRD and XRF Instrumentation. This session had 13 speakers and was the most viewed and attended session of the conference. Presentations by **Robert Redus**, Amptek, **Dubravka Sisak-Jung**, Dectris, **Moritz Schlie**, Incoatec, **Brian Jones**, Bruker-AXS, **Vlad Marion**, Mirion Technologies, **Christopher Own**, and Saku Tech./NASA, discussed the latest advances in new detectors at their respective organizations and highlighted the global nature of these developments. The ability of new optical devices to focus X-rays to nanometre range spot size of high brilliance has opened up a variety of new applications as diverse as space exploration, mining and cultural heritage analyses. The instrumental capabilities were highlighted in the New Developments session and technique applications were shown throughout the meeting in a variety of sessions.

The Denver X-ray Conference focuses on applied science and it was very interesting to see how the developments in sources, detectors and optics have not only influenced the traditional fields of powder diffraction and crystallography, but created new opportunities in microanalysis, tomography, thin film analysis, stress analysis, imaging science, and machine learning. The session on Machine Learning showed how new algorithms are taking advantage of new instrumental capabilities based on the ability to analyze large numbers of samples in a short period of time, with a variety of user-selected wavelengths and energy-selective detectors. The algorithms intelligently interpret this massive amount of data, while creating new experiments, proving new insights into the materials being analyzed. This wide scope of applications, shown in various presentations, is beneficial to all scientists, since it broadens the market and societal impact, spurring more development. In addition to the workshops cited above, there were also workshops on Polymer Diffraction, Thin Films, Stress Analysis, Micro XRF, Trace XRF and Multimodal XRF. Each workshop demonstrated a wide variety of applications based on advanced instrumentation while teaching attendees about the specific methods used in these fields.

*Figure 1: A behind-the-scenes tour of the Smithsonian by **Jeff Post** (left), highlighting the material science and analytical facilities of the museum (right).*

A highlight of the conference was a series of three plenary presentations provided by researchers from the Smithsonian Museums and Library of Congress (US). These presentations were made available beginning on the opening days of the conference and each presentation was the highest viewed of its day. The most viewed video of the conference was *"Investigations in the Smithsonian Gem and Mineral Collection: Challenges and Opportunities"* by **Jeff Post**, Department of Mineral Sciences (see figure 1). Jeff provided a fascinating tour of the Gem and Mineral collection, highlighting both important gems and the behind-the-scenes laboratory capabilities. Jeff provided many insights based on his expertise as a mineralogist and experience with both powder and single crystal diffraction, and with microanalysis techniques, all of which have been applied to study one of the world's largest gem and mineral collections. The next day featured the presentation, *"Cultural Heritage Science and the Material of Memory"* by **Lynn Bostoff** of the Library of Congress. Lynn's presentation focused on "the dynamic relationship between cultural memory and cultural heritage, where the value of individual objects lies

not only in their testimony to the past, but in their immense power to evoke vicarious experience". She used examples from the analyses of several valuable objects that have been studied in the Library of Congress collection, comparing physical evidence to written testimonies, the results of which often "enriches the cultural memory." The third presentation was a joint video by **Douglas Owsley** and **Timothy Rose** of the Smithsonian's Natural History Museum on *"Energy Dispersive X-ray Spectroscopy of 19th-Century Dental Fillings"*. This video followed their forensic investigations that tracked the development of dental techniques and materials in 18th century America and how these analyses can be used in bioarcheological examinations to study important historical events. In addition to being widely viewed, these three presentations were well received with numerous "likes", comments, and positive reviews. These presentations were complemented by an excellent session on Cultural Heritage with presentations from research teams associated with the Getty Conservation Institute (**Samuel Webb**), National Gallery of Art (**John Delaney**), Canadian Conservation Institute (**Maeve Moriarty**), and the Rijksmuseum (**Koen Janssens**).

Another session of mutual interest to material scientists and crystallographers was a session on Rietveld Analysis. Once again, diversity in application was very evident. **Jim Kaduk** gave a presentation on *"Crystal Structure of Large Commercial Pharmaceuticals"* that included new structural determinations of the active pharmaceutical ingredients in Lipitor®, Elidel, Rocefin and Valcyte®. **Tomče Runčevski** gave a presentation on *"In situ Crystallization of Model Minerals on Titan, Saturn's Moon"* which focused on understanding the unusual chemistry that has been identified through NASA satellite fly-bys. There were two presentations that focused on understanding environmental issues and trying to produce new green chemistries for industrial processes. **Marcelo Malagutti** discussed *"Challenges on the Microstructural Characterization of Nanocrystalline Alloys Produced by Mechanochemistry"* and **Herbert Pölleman** presented *"XRD-based Quantification Methods of $CO_2$-reduced Building Materials - Cements, Calcined Clay, Pozzolanes and Limestone"*. In both cases, the authors utilized Rietveld methods to structurally refine and quantitate new chemistries, based on more environmentally friendly methods in alloy and cement production. The remaining two presentations in the session focused on new method developments for quantitative phase analysis and nanomaterial crystallite size and microstructure characterization. They were presented respectively by **Hideo Toraya** and his colleagues at Rigaku, and **Alexander Moore** and research team at Sandia National Laboratory.

The conference sessions had many invited speakers that highlighted capabilities at international synchrotron facilities. At DXC, these talks typically highlighted beam lines dedicated to powder diffraction, imaging, X-ray spectroscopy and microanalysis, so they were distributed among dedicated sessions. Microanalysis capabilities at BAM (Bundesanstalt für Materialforschung) were highlighted in a session on Trace Analysis in an excellent invited presentation by **Martin Ratke**: *"Trace Element Analysis with Synchrotron Radiation Challenges – Applications – Results"*.

There was a dedicated session on Neutron Diffraction, where most of the presentations focused on structural characterization in cases where neutrons have an advantage due to preferred atomic scattering lengths in dynamic processes or the ability to measure magnetic structure. Two presentations were included on magnetic materials, *"Hydrogen Bonding in Layered Superconductors and Magnetic Materials"* and *"Neutron Powder Diffraction in Mixed Perovskites"*. The former was given by **Efrain E. Rodriguez** of the University of Maryland and the latter by **Florencia E. Lurgo**, University of Cordoba, Argentina. Dynamic measurement were shown in *"Crystal Structure of Uranium Monosilicide: A High Temperature Time-of-Flight Neutron Diffraction Study"* and *"Neutron Diffraction: A Unique Technique to Study Gas Adsorption in Functional Porous Crystalline Materials"*. The former was presented by **Tashiema L. Ulrich**, Los Alamos National Laboratory and the latter by **Hui Wu**, NIST. The final presentation in this session was *"Trindex – 3D Grain Mapping with Neutrons"* authored by an international collaboration of scientists at multiple sources, and was presented by **P. K. M. Tung.**

Awards were presented for best posters in both X-ray Diffraction (XRD) and X-ray Fluorescence (XRF) categories; for the complete list, see **http://www.dxcicdd.com** . Awards were also given to the top student posters as well as the 2020 Robert L. Snyder Student Awards. The Snyder Awards were presented to seven students from six countries. (**http://www.dxcicdd.com/20/students.htm**).

*Figure 2: Navpreet Kaur and Christian Lutz.*

Of particular note were **Navpreet Kaur** of the University of Minnesota, USA and **Christian Lutz** of Clausthal University of Technology, Germany who were awarded both the Snyder Student Award and best poster awards. Navpreet presented *"Partial Dehydration of Levothyroxine Sodium Pentahydrate in a Drug Product Environment: Structural Insights Into Stability"*, which won the student award for XRD. Christian presented, *"Laboratory-based XANES to Study Vanadium in Vanadium Redox Flow Batteries"*, and that was one of two student awards for the XRF Poster session.

Feedback from the attendees showed that they enjoyed the on-demand features of the virtual conference, noting that they didn't have to miss concurrent presentations in sessions or workshops. The conference did allow them to keep up with developments and still connect with colleagues.

**Tim Fawcett**
Chairman DXC Organizing Committee.

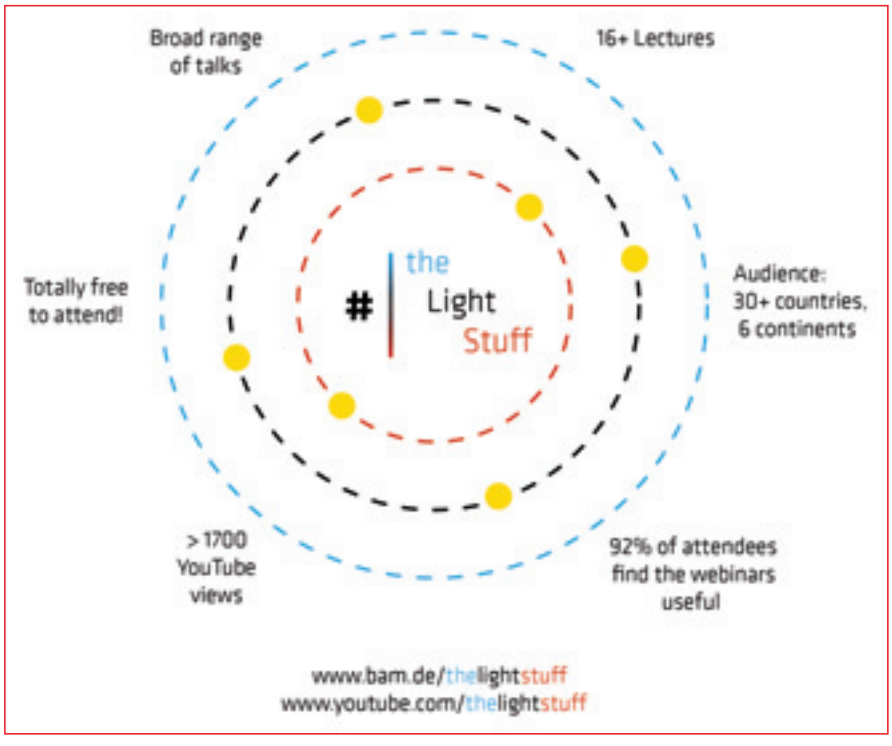
# #theLightStuff Lecture Series

**MODERN researchers, in general, rely greatly upon communication with other researchers. It creates a community, and with it, the desire to be actively involved within that community. Traditionally, conferences have been hugely important in facilitating these interactions, leading to new ideas, and the creation of new collaborations. However, with no realistic end date to the current pandemic in sight, and with standard venues and institutions for communication now largely inaccessible, alternative solutions have needed to be explored to facilitate the distribution of knowledge, and to further scientific conversations. This change has provided the opportunity to play around with the formula and possibly improve on the classical mechanics of scientific communication. Over the years, conferences have served a great purpose but have not necessarily been the most inclusive medium, with a financial barrier of entry (travel, accommodation, fees, etc.), alongside other personal stresses that can come from dedicating time away from home, or the thought of the environmental impact that travel to conferences has had.**

One approach to address these issues has been to explore the feasibility of online conferences and lecture series, the latter of which our team from the Bundesanstalt für Materialforschung und -prüfung (BAM) in Germany and Diamond Light Source in the UK have been doing since the start of lockdowns in March. In general, we find this to be a suitable and – in some respects – a much improved format for outreach and the distribution of information. Firstly, it removes many of the barriers for entry, the lectures are free to attend, require no pre-registration and can be accessed live from all around the world. These talks are also recorded, with permission of the speakers, and are made available on the #theLightStuff YouTube channel [https://youtube.com/thelightstuff], where they have since amassed over 1800 views. This means there is now an increasing library of talks online that provide an easy entry for curious scientists and crystallographers into the broad range of fields covered by the lecturers, regardless of available travel budgets.

By hosting one lecture a week, specifically on materials science using scattering and diffraction techniques, we have been able to facilitate over 18 lectures from speakers around the world. Our speakers have consisted largely of early career researchers, or young professors, based in materials science fields, and they have been able to share their research on a variety of topics including material transport in emulsions, planetary geology, metal alloys, nanoconfinement, gel structures, magnetic materials, fibres, battery materials, covalent organic frameworks (COFs), and microfluidics. This research has been made possible through the use of scattering and diffraction techniques, including high pressure crystallography, single crystal and powder diffraction, (grazing incidence) small-angle scattering and reflectometry, quasielastic neutron scattering (QENS), electron backscatter diffraction (EBSD), pair distribution function (PDF) analysis and NMR crystallography to name only a few.

The process of running an online lecture series has, of course, not been completely free of challenges. A conscious decision was made early on to keep the barrier of entry for the lectures low, with no (pre-)registration required, meaning that anyone is able to enter the lecture with no more than the Zoom link, which is publicly available on the website and (occasionally) in some announcement tweets. By making access simple and easy for those interested in attending these talks, it also does the same for "internet trolls". This became apparent particularly in the first lecture, held during the initial wave of lockdowns, and when the practice of "Zoombombing" became a popular pastime for some. This resulted in several trolls attending our first lecture and rapidly spamming the chat with offensive messages. Fortunately, we managed to quickly work out a system of removing them from the lecture to ensure our speakers and audience were not bothered by these mischief makers. This was helped by the fact that we were using the webinar plugin that separates the speaker and panellists/organizers from the audience, granting the latter reduced ways in which to negatively



disrupt the talks. We have since removed the ability for the audience to chat directly to attendees, and no further incidents have occurred.

Each talk is followed up with a Q&A session, so that the interaction between the speakers and attendees is maintained. This has produced great interaction between the speakers and attendees, with attendees asking a plethora of in-depth questions. These discussions have also helped to initiate new collaborations, in some way mimicking some of the most crucial elements that come from attending conferences. We have also been evaluating whether people enjoy the lecture series by running a short poll after each Q&A session. From this, we hope to be able to understand our audience, their background and their experience with diffraction and/or scattering better. The core results from these polls are presented in the figure: they are very positive and enthusiastic.

Finally, the challenge of balancing multiple demands on time with online meetings and other work commitments can make it tricky to actively engage with the scientific community. However, with most lectures available on YouTube, people can watch/re-watch the talks whenever is most convenient for them, and so far, the great work of our speakers has reached 30+ countries across 6 continents. We hope that you will take a look at the previous lectures available at **www.youtube.com/thelightstuff** and perhaps join us for a live lecture at **www.bam.de/thelightstuff**. We would love to see you there!

**Jenni Haberland**, **Brian Pauw** and **Glen Smales**, BAM
**Claire Murray**, Diamond Light Source

# Meetings of interest

**IN the continuing 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 .**

**6th Dec 2020 – 8th Dec 2020**
EMBO workshop on in situ Structural Biology – from Cryo-EM to Integrative Modelling
Virtual workshop.
**https://www.embl.de/training/events/2020/ISS20-01/index.html**

**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**

**17th Feb 2021 – 19th Feb 2021**
Reaction Mechanisms in Catalysis: Faraday Discussion
Virtual meeting.
**https://www.rsc.org/events/detail/36562/reaction-mechanisms-in-catalysis-faraday-discussion**

**22nd Feb 2021 – 26th Mar 2021**
HERCULES 2021 (Training course in Neutron and Synchrotron Radiation for Condensed Matter Studies)
Grenoble, France.
**http://hercules-school.eu/**

**29th Mar 2021 – 1st Apr 2021**
British Crystallographic Association Spring Meeting
Online conference.
**https://registrations.hg3conferences.co.uk/hg3/165/home**

**12th Apr 2021 – 14th Apr 2021**
Directing Biosynthesis VI
Edinburgh, UK.
**https://www.rsc.org/events/detail/39023/directing-biosynthesis-vi**

**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 Cryo-EM 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**

**23rd Jun 2021 – 25th Jun 2021**
MOFs for Energy and the Environment: Faraday Discussion
Manchester, UK.
**https://www.rsc.org/events/detail/40612/mofs-for-energy-and-the-environment-faraday-discussion**

**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/**

**7th Jul 2021 – 9th Jul 2021**
Challenges in Biological Cryo-electron Microscopy: Faraday Discussion
Sheffield, UK.
**https://www.rsc.org/events/detail/40005/challenges-in-biological-cryo-electron-microscopy-faraday-discussion**

**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**

**8th Sep 2021 – 10th Sep 2021**
Peptide-Membrane Interactions: Faraday Discussion
London, UK.
**https://www.rsc.org/events/detail/37143/peptide-membrane-interactions-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/**

**16th Dec 2021 – 17th Dec 2021**
Italian Crystal Growth 2021 - Crystal Growth: from Theory to Application
Torino, Italy.
**https://www.icg2020.net/**

**17th Jan 2022 – 22nd Jan 2022**
Third Pan African Conference on Crystallography
Nairobi, Kenya.
**https://pccr3africa.org/**

**23rd Aug 2022 – 27th Aug 2022**
Thirty Third European Crystallographic Meeting (ECM33)
Versailles, France.
**https://www.ecm33.fr/**

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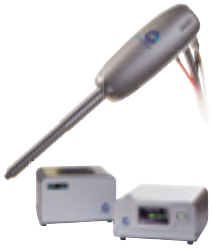
PheniX


Chimera


Cryostream

OxfordCryosystems