Crystallography News

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BCA Spring Meeting and CCP4 Study Weekend

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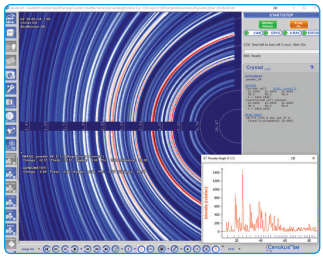
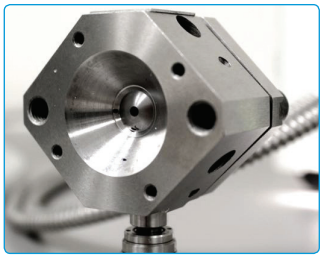
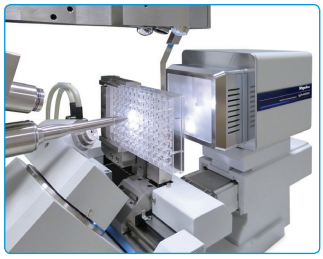
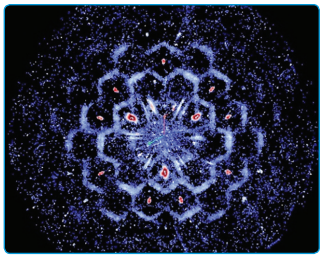
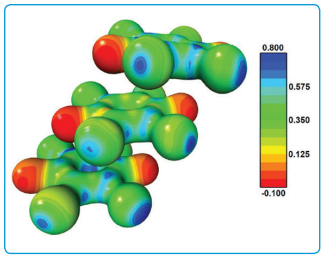

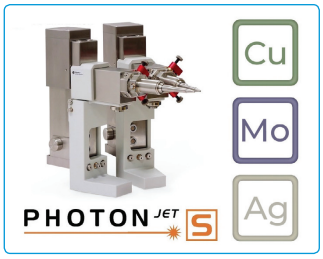

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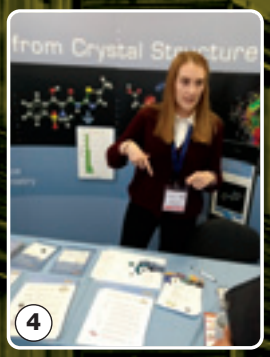
BCA Spring Meeting 2019



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This month's cover:

Spring Meeting venue, work and play; photos by Charlie McMonagle, Anuradha Pallipurath and CHS

From the President

I WRITE having just returned from my first BCA Spring Meeting as President. There were so many interesting talks on offer, that it was difficult to decide which sessions to attend. I was struck by the variety and reach of diffraction studies, and the way the meeting brought together people with widely different interests. We heard stories that stretched from plastic digesting enzymes, the control of protein degradation, the simulation of local structure in materials and how it produces those annoying diffraction intensities in between the Bragg peaks, the latest chemistry in battery technology, and a detailed description of why molecules crystallize in particular ways, to the latest in direct methods (and much more). A comprehensive account of the meeting appears elsewhere in this issue.

Sometime this summer, perhaps before this letter appears, we will learn whose picture the Bank of England has decided to use on the new £50 note. **Dorothy Hodgkin**, a BCA Founder Member, was a front runner in the online polling. Her work on penicillin and insulin are clear examples of how crystallography has helped to change people's lives. Her penicillin model in the Science Museum has been moved to a new spot in the Medicine Galleries, and the space vacated now houses a series of **Kathleen Lonsdale**'s structural models made from table tennis balls. I haven't been to see this myself yet, but it definitely looks to be worth a detour.

I spent a couple of months over the Christmas and New Year period suffering from an attack of shingles, an unpleasant disease resulting from reactivation of latent Varicella Zoster Virus (VSV) from an earlier dose of chickenpox as a child. Ever the crystallographer, I spent some of the time I was laid up looking at the literature in search of any crystallographic contributions to its treatment or elimination. I was being treated with Acyclovir (4g/day!), a guanosine analogue where the ribose ring has been replaced by a simple ether link. Viral enzymes process this to the equivalent triphosphate and incorporate it into the viral DNA they are busy replicating, but it stalls the replication process as there is no chemical handle for attaching the next unit in the chain. Acyclovir is a good drug from the synthetic point of view since it has no chiral centres. It crystallizes in space group $P2_1/n$ (i.e. the ever popular $P2_1/c$ but reindexed to bring β closer to 90° to reduce correlation issues in refinement). The structure is otherwise unremarkable, but nevertheless important.

It reminded me that most drug molecules do have chiral centres, perhaps the most notorious being Thalidomide, that caused terrible birth defects when expectant mothers were given the drug as a sedative in the 1950-60s. At the time, the drug was the best-selling sleeping pill in West Germany, and even available without prescription, but it was banned worldwide in 1962. The *(R)* isomer is a good sedative, but the *(S)* form is teratogenic (disturbs fetal development). It is clearly much easier to synthesize racemic mixtures, and for many drugs only one enantiomer would be active. The Thalidomide story made drug companies much more cautious. Purifying the *(R)* isomer sadly does not solve the problem as there is an enzyme in the liver that can racemise it, although it is now used in some circumstances. There are also several crystal structures of enzymes from VSV, including some complexes with Acyclovir and other antiviral drugs, but the best hope to vanquish shingles lies in highly effective new vaccines. An interesting anecdote about the discovery that shingles is just a re-awakening of latent chickenpox virus shows that you don't always need expensive equipment to make major scientific discoveries. When I was still at school, in the Gloucestershire town of Cirencester, my sister had a job as receptionist for a GP, Dr **R Edgar Hope-Simpson**, in a nearby village. She used to tell me that Hope-Simpson had done some important work, but I never knew the details. He, in fact, made the original proposition that shingles was caused by a reactivated chickenpox virus. He demonstrated this by teaching himself epidemiology, putting together a small team and running an extensive study of the isolated community on the Island of Yell in the Shetlands. This revealed the link. Hope-Simpson's obituary in the British Medical Journal judged this to be the most important discovery by a practising GP in the 20th century.

Members will have been saddened to learn of the death of **Stephen Wallwork**, a Founder Member of the BCA. A full obituary appears elsewhere in this issue. On a happier note, I would like to extend my congratulations to the newly elected Council members who have now taken office: **Simon Parsons** (Vice-President), **Alex Stanley** (Secretary) and **Anna Warren** (Ordinary Member).

I would also remind members that the Twenty-Fifth IUCr Congress and General Assembly in Prague in 2020, is looming on the horizon. The IUCr will elect the new members of the Executive Committee and the Commissions at the meeting, and is calling for suggestions for nominations for membership of the IUCr Executive Committee and the IUCr Commissions, with a deadline of 30 June 2019. The positions of the Executive Committee President, Vice-President, General Secretary and Treasurer, three Ordinary Members fall vacant in 2020 and the UK does not currently have a representative. It is important for us to be represented, so all members should consider whether they would like to propose someone for nomination, or indeed be considered for nomination themselves. Nominations will be submitted by the BCA so please send your suggestions for these posts to the BCA President and Secretary as soon as possible, to allow time for preparation of the submissions. The IUCr website shows the current membership of the Executive Committee and Commissions.

The UK has not hosted the IUCr Congress since the Glasgow meeting in 1999, and it would seem timely to consider it again. Lead times are very long, and a bid could be made for 2029 with a decision made at the 2023 IUCr Congress and General Assembly. I would call on BCA members who would consider leading a bid for an IUCr Congress in the UK in 2029 to contact the BCA Secretary or President. The current BCA Council members will not be in office in 2023, but can provide assistance and backup in the early stages of bid preparation. Note that the venue needs to be large enough to cope with the size of the Congress, such as conference centres in London, Harrogate, Birmingham, Manchester etc.

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BCA Council 2019

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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

I FULLY agree with our President's assessment of the recent BCA Spring Meeting as being very wide-ranging and very stimulating. In this issue you will find a good selection of reports and pictures of various aspects of the meeting. In itself this is a remarkable achievement because of the short time available between the conclusion of the meeting and the publication deadline. This was the consequence of an unavoidable chain of circumstances: through the inexorable operation of the Metonic cycle, Easter 2019 came late in April (not to be matched until 21 April 2030 in the Western calendar and surpassed on 25 April 2038). Therefore university vacations and the availability of facilities for BCA meetings were put back until mid-April. However, the print deadlines for *CN* are independent of the phases of the moon and the vernal equinox; and this year's deadline for submission of material to the Editor was the usual 25 April. Nothing daunted, our valiant contributors wrote their articles and sent in their pictures in double-quick time. They have my heartfelt thanks.

Once again our Exhibitors contributed importantly to the success of the meeting, both by paying for exhibition space and by demonstrating the advances they have made in instrument and software design. In this issue they are featured in a photo spread. We can take special pride that our meeting, although classified as a national meeting, attracted delegates from all over Europe and as far afield as Kansas and Brazil. There was an impressively large delegation from the University of Malta. Their motivation was clearly scientific, not touristic; just compare the average April high and low temperatures in Valletta (19.1 / 11.9°C) with what was to be expected in Nottingham.

One of the happiest moments in a Spring Meeting is the induction of new Honorary Life Members. According to the BCA website, the award of Honorary Life Membership recognises "significant contributions by the recipient to crystallographic science and to the work of the BCA", and the number is limited to two or fewer in any single year. This year's recipients of this accolade, **Sandy Blake** and **John Helliwell**, have admirably fulfilled these criteria. They have also given splendid service to the wider crystallographic community through the work they have done for the International Union of Crystallography, particularly in their senior editorial and policy-making roles for IUCr journals.

In my usual descriptions of BCA Spring Meetings I offer you ducks. This year I failed to spot any, even though other delegates did. However, as I was photographing "The Exchange", which was the venue for our meeting, I noticed two geese rapidly approaching and honking aggressively. They gave the distinct impression that they hated paparazzi, would drive them to a muddy splashdown in the lake if they could, and would withhold image rights from any commercial publication. I respectfully gave them room but snapped them anyway, confident that they would not object to appearing on the cover of such a worthy publication as *CN*. The geeky geese paused by the Computer Science building but then resumed their research on applied hydrodynamics.

One of our cover pictures was taken during our CCG Plenary lecture. presented by **Carl Henrik Görbitz**. Provided by **Anuradha Pallipurath**, it shows a rapt audience giving the lecture their undivided attention, including your Editor sitting in the front row indulging the habit of a lifetime by taking copious notes. Carl Henrik presented fascinating science. Also, with respect to the topic of the moment (Brexit), he gave us a light-hearted but perceptive account of what it was like to live in a country (Norway) that was closely aligned with the European Union but not part of it. Venturing into numismatics, he showed us the back of an original 2-euro coin with a map that appeared to endow Sweden with a North Sea coast, the *terra incognita* to its west having disappeared.

Our Spring Meeting wasn't the only one to fill participants with enthusiasm. Early in January CCP4 held its annual Study Weekend. The topic this year was "Molecular Replacement". I am grateful to **Mark Roe** (Sussex) for giving us such a comprehensive summary. The pictures have been chosen from a large selection, copyright of Science & Technology Facilities Council and kindly made available by **Karen McIntyre** (STFC).

No sooner does one meeting finish, then planning for the next one commences. The Programme Committee for the 2020 Spring Meeting in Leeds met over breakfast on Thursday morning the 18th in Nottingham, at a time when many other delegates were still recovering from the conference dinner and ceilidh. Of course, you don't have to wait a whole year for a stimulating meeting. Planning is well advanced for the autumn / winter meetings of our Groups. Even sooner, our Industrial Group will hold its XRF meeting at Sheffield Hallam University on 12th June, starting with registration and coffee at 09:30. You can still book a place if you hurry, since registration closes at 23:59 on Thursday 6th June 2019. As the programme takes shape, you can follow it at https://sites.google.com/site/bcaxrf/meetings/12-june-2019. Already it makes clear that the meeting will provide both advice about how to keep your lab and its equipment running with maximum efficiency, and examples of successful application of XRF.

I draw your attention to CIFiesta, to be held in Naples 29 August – 3 September. Although it is too late to apply for a bursary, regular registration is open until 14 June. Unlike most schools, this one offers an intensive course in Crystallographic Information. The organisers aspire to making it the start of a series.

Crystallographers will await a Blessed Event this summer almost as eagerly as expectant parents await theirs: the accession of the millionth crystal structure to the Cambridge Structural Database. You can check the countdown odometer on the CCDC website and learn about the special commemorative events that are planned. I hope that it will be a BCA member's structure that will be awarded the magic number, and I wish that the "very special baby" may be yours!

Carl Schwalbe

BCA Corporate Membership

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

- Up to 10 free BCA memberships for your employees.
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For current rates, and to join, please see **www.crystallography.org.uk/membership/**

Puzzle Corner

IN this Year of the Periodic Table our Programme Committee succeeded in constructing our society's initials out of element symbols. With the order changed and a number added, CaB_6 is a fascinating material with high electrical conductivity, hardness and melting point. It is a black, lustrous, chemically inert powder with a low density. It exhibits unusual high-temperature ferromagnetism. Its structure is cubic.

Can you make the following sets of initials of some of our sister crystallographic societies out of element symbols? Identify the country as well. You may find this IUCr website helpful: https://www.iucr.org/resources/other-directories/organizations .

ACA
AFC
CSCA
DGK
ICA
ICRA
NVK
PTK
SGK
SMCr

Answers to March Puzzle Corner

THROUGH the inexorable increase of entropy, the letters have become scrambled in the names of the cities where recent and prospective meetings have been held or will be held. Maxwell's Demon has now put them back together the right way, maybe not always as much fun.

Nhotmating	Nottingham
Elfbats	Belfast
Nnaive	Vienna
Donnol	London
Convoting	Covington
Murdah	Durham
Abonding	Abingdon

BCA Spring Meeting 2019 Group Reports

Speakers from the first session of the YCG (L-R) ***Pollyanna Payne*** *(Bath),* ***Hristo Gonev*** *(Diamond),* ***John McGeehan*** *(Portsmouth),* ***Angus Cowan*** *(Walter and Eliza Hall Institute, AUS).*

THE meeting began with the Young Crystallographers' Satellite Meeting and continued with the Lonsdale Lecture, leading into the main meeting, which generally ran in 3 parallel sessions. The write-ups will follow this order: YCs first, then Lonsdale Lecture, main meeting session summaries arranged by groups alphabetically, and the BCA Prize Lecture.

YCG Report

THE YCG satellite meeting followed a slightly different format this year. As usual we started by giving early career researchers the chance to present their work, but then instead of continuing this into the Tuesday morning, we dedicated the final session solely to public engagement and outreach.

The YCG committee for 2019.

The meeting began with an excellent plenary lecture by Dr **John McGeehan**, describing how crystallographic studies provided valuable insights into the understanding and development of plastic eating bacteria. This work was very exciting and with a bit of luck it won't be the last we hear about it. The biological theme then continued as our first YCG speaker **Angus Cowan** took the stage, discussing several new crystal structures of BAK core homodimers with bound lipids, and thereby developing the understanding of the behaviour of BAK proteins in cell death by apoptosis. **Pollyanna Payne**, who was later awarded the IG prize, then switched to chemical crystallography, discussing her search for co-crystals of the tuberculosis drug isoniazid. Isoniazid normally forms needles, which are typically hard to process, but by combining the drug with a co-former she was able to show changes to the morphology. **Ali Ebrahim** then discussed how you can minimise radiation damage when collecting data at the synchrotron, before the session's final speaker **Hristo Gonev** reported on the effects of additives on crystal growth in $CaCO_3$, building on I11's project M.

The diversity of topics continued into the second session which covered a range of highly complicated techniques. **Eleanor Dodd** began by with some detailed charge density studies, identifying an intermolecular H-F interaction in a series of fluorine substituted ring compounds and discussing its effect on the crystal packing. **Katherine Rowlinson** moved on to complementary techniques, combining X-ray, NMR and DFT to understand the disorder observed in inclusion compounds. **Aly Abdeldaim** used highly detailed neutron powder diffraction studies in combination with magnetic susceptibility measurements to understand the magnetic properties of $BaMo(PO_4)_2$, and **Rosemary Young** finished this second session with some impressive *in situ* crystal structures, monitoring CO release from carbonyl complexes in an extended metal-organic framework material.

The final research session began with a highly educational talk on auxetic crystals by **James-Nicholas Grima-Cornish**, using both slides and props to demonstrate how stretching a material can actually make it wider, before presenting a series of DFT calculations to predict this behaviour in known inorganic crystalline materials. **Demetris Bates** then returned to the field of magnetism, reporting on the magnetic bistability of a heterocycle radical and the first experimental evidence of dimerization through a previously predicted σ -bonded motif. Finally the YCG research talks were concluded by **Kenneth Freeman** who presented some highly detailed customised Rietveld refinements on high pressure BiTe compounds, gaining insight into the partially ordered guest atoms.

After the research talks the YCG held its annual AGM and a 30 second flash poster presentation session. **Natalie Pridmore** gave an excellent intro to her poster on the spin crossover properties of iron(II) phosphine complexes and was later awarded the flash presentation prize.

Tuesday's outreach session meanwhile was kick-started by **Hamish Yeung**, the recipient of the Parkin award lecture, who discussed his recent engagement activities relating his MOF research to commonly found minerals to audiences at the natural history museum. **Caroline Davies** then discussed the CCDC's exciting *internal year of the Periodic table* project, where their website would feature each element with both an overview and a focal crystal structure. Keynote lecturer **Christine Beavers** gave the audience a run-down of all the different social media platforms, encouraging us all to share real scientific experiences with the world, and last but not least, **Tim Easun** gave his plenary lecture on a host of public engagement activities he had done using Poetry, 3D Printing, Plastic toys and even Virtual reality set-ups. Tim was also kind enough to bring this virtual reality set-up along with him, giving everyone the chance to explore inside a crystal. The meeting ended with an open discussion lead by **Simon Coles** and **Elliot Carrington** where we tried to address what the best ways to get involved with outreach were.

(L-R) Tim Easun, Hamish Yeung, Alex Tansell.

Thanks to everyone who came; it was a really great meeting. We look forward to seeing everyone again next year!

The YCG Committee

Lonsdale Lecture

THE Lonsdale Lecture provides a bridge between the Young Crystallographers' Satellite Meeting and the main meeting. As such, it should incorporate some teaching and also present recent advances in an area of crystallography. In his lecture entitled "SHELXT – dual space structure determination using the phases to determine the space group" George Sheldrick admirably fulfilled this dual remit. For those "born later than direct methods" as well as old-timers like me he surveyed the high points in the development of methods for phase determination. With typical generosity of spirit he did not confine himself to SHELX(…) software. He described the MULTAN era (1969-1990). This software was user-friendly and highly effective, but it suffered from the risk of getting a "uranium atom" solution (all phases zero) in the absence of translational symmetry. Negative quartets then provided a way to detect and avoid this. The next major advance was dual space recycling, implemented in "shake and bake" and later SHELXD. The real space part of the cycle imposes a strong atomicity constraint. We learned about "the other double helix", the parallel double helix structure brilliantly predicted for poly (rA) by Rich, Davies, Watson & Crick (1961). More than 50 years later SHELXD, run for a week on an 8 CPU computer, showed it was remarkably accurate.

(L-R) Simon Philips and George Sheldrick.

We are used to getting the space group by establishing the Laue class and lattice type, but phases are more powerful. Assuming that the Laue class is known, we average equivalent intensities, expand to P1 and solve in P1. The Patterson superposition minimum function should provide a double image of the structure, which is treated as a starting point for dual space recycling. Random OMIT maps leave out a different ≈30% of peaks each cycle, and the remaining atoms (masked to a Gaussian peak shape) can be used to calculate phases. Methods for obtaining the origin and space group from the phase information developed by Giacovazzo and by Palatinus both work well. After further dual-space recycling, elements can be assigned to best fit the integrated peak densities. For non-centrosymmetric structures an initial estimate is also given of the Flack parameter and, where appropriate, the correct enantiomer is chosen.

Carl Schwalbe

continued >>>

BSG Reports

Novel Data Collection Strategies

Tuesday, 16 April

(L-R) Jeremy Sinoir (Keynote), Sam Horrell, Emma Beal, Agneta Butryn, Ramona Duman (chair).

J Sinoir (EMBL Grenoble)
Opening the shortest path from crystal to data with CrystalDirect and NewPin

The CrystalDirect system was designed at EMBL, Grenoble, to fulfil automated crystal harvesting from 96 well plates, thus eliminating the slow and error-prone manual task of sample preparation, which often damages protein crystals. Crystallisation is performed on ultra-thin, low x-ray background film, which becomes the sample support through the laser photo-ablation process used to extract crystals from their crystallisation drops. Complete removal of mother liquor surrounding the crystals, in most cases, eliminates the need for cryo-protection. Ligand binding, room temperature data collection, as well as crystal dehydration experiments are also within the scope of the instrument. The system can be used off-line for sample preparation before beam time. Prior characterisation of the sample positioning on the laser-cut film, in advance of beam-time, improves efficiency of data collection and usage of beam time. Incorporation of the CrystalDirect instrument into the beamline environment at ESRF beamline ID30B has successfully shown that a completely automated pathway from crystal production to structure solution is achievable.

E Beale (Diamond)
VMXm: A new micro/nanofocus macromolecular crystallography beamline at Diamond

X-ray diffraction data collection from micrometer and nanometer-size crystals requires a complex and specialised experimental setup. Beamline VMXm at Diamond Light Source is pushing the limits of micro-crystallography by combining an in-vacuum sample environment, sample visualisation with a scanning electron microscope and high precision goniometry, which can achieve rotation data collections from sub-micrometer protein crystals. Sample preparation makes use of electron microscopy grids and cryo-cooling is achieved by plunge-freezing in liquid ethane. The beamline has recently had a very successful First User experiment and early results were presented highlighting its experimental capabilities, notably, the 0.4 µm x 2.8 µm beam size, measured at the sample position, and the high resolution, low background diffraction data from 2 μm^3 cytoplasmic polyhedrosis virus polyhedrin crystals.

Agata Butryn (Diamond)
Dynamic structural biology at Diamond and XFELs

Measuring room temperature serial crystallography data at XFELs brings information on the dynamic behaviour of protein targets. The XFEL Hub team at Diamond Light Source focuses on helping the structural biology community with all aspects of the application process for XFEL beamtime and optimizing the sample preparation, to enable users to get the most out of their XFEL experiments. The presentation focused on sample delivery methods for serial crystallography experiments optimised by the XFEL Hub team in collaboration with users, such as the lipid extruder and the acoustic injector. Details were presented of 'on-demand methods', using the acoustic injector and conveyor belt, geared to match sample delivery to the pulse frequency of XFEL sources. Such methods eliminate sample waste, while enabling a host of experiments like flexible laser pump schemes, ligand-binding and chemical reaction chambers.

S Horrell (University of Hamburg)
No goniometer? No problem. Novel Data Collection methods at P14 T-ReXX

A new end-station (T-ReXX) attached to beamline P14 at EMBL, Hamburg, tailored for time-resolved crystallography experiments, enables serial data collection from microcrystals. The setup is equipped with a Hadamard sequencer combined with detector gating to achieve a variety of time resolutions. This enables capturing data that can resolve protein dynamics within microsecond to millisecond timescales. Fixed target silicon chip are currently the main sample delivery method, however, the installation of the experimental table has built-in flexibility to allow for a variety of delivery setups, including flow-focused microfluidics and droplet injectors. Early results were presented showing the impressive potential of this instrument.

Ramona Duman
Diamond Light Source

Complementary Structural Biology Techniques

Tuesday, 16 April

(L-R) Ewan Main, Dimitri Svergun (Keynote), Chris Waudby, Joao RC Muniz, James Garnett (chair).

This session entitled "Complementary Structural Biology Techniques" focussed on alternative approaches that can supplement high-resolution structural data or provide insight

when high-resolution structures are not available. The session began with the keynote lecture given by **Dmitri Svergun** from the EMBL on "Small-angle scattering on macromolecular solutions: progress and perspectives". He gave an excellent overview of SAXS in studying biological systems and recent advances in the field. The second talk was by **João Muniz** from the University of Sao Paulo on "The use of biophysical techniques applied to the structural characterization of carbohydrate-active enzymes with biotechnological applications". He gave examples of how structural and biophysical techniques (SAXS, CD, DLS, DSF) can be coupled with homology modelling to study the structure/function of bacterial hydrolases. The third talk was given by **Ewan Main** from Queen Mary University of London on "Scalable geometrically designed protein cages assembled via genetically encoded split inteins". This talk described a novel strategy to create synthetic recombinant protein cages and the use of SAXS to model their structure. The final talk was given by **Chris Waudby** from University College London on "Dissecting the interactions of emerging nascent chains with the ribosome surface using NMR spectroscopy". This talk took a different angle and first gave an overview how NMR can be utilized to study biological problems, including solid, solution and in cell samples. He then described the use of NMR to study residue-specific interactions between nascent polypeptides and the ribosome during co-translational folding.

James Garnett
King's College, London

Novel Crystallisation Strategies

Wednesday, 17 April

*(L-R) **Wangshu Jiang**, **Claire Naylor** (chair), **Chia-Ying Huang**, **Apirat Chaikuad** (Keynote).*

This lovely session provided interesting and novel examples of protein crystallisations. The keynote speaker was Dr **Apirat Chaikuad** of the SGC Frankfurt. He described his efforts at SGC Oxford and Frankfurt to optimise crystallisation strategies to maximise successful crystallisations while minimising workload and expense. High throughput is integral to their method – but experimental design is vital as there are too many parameters to cover. This has led to the design of several screens that broaden the chemical space explored in the confines of a single plate, and a protocol that optimises protein composition and includes multi-drop plates and two temperatures. Dr Chaikuad's latest investigations are into the possible use of branched PEGs as crystallisation agents. Dr **Chia-Ying Huang** (Paul Scherrer Institute) described the use of IMISX, an *in situ* sandwich plate system with 3D-printed holders for LCP crystallisation, which they have developed. In addition, the group has developed software for rapid scanning of the mounted crystallisation drops to identify drop position and automate data collection and processing. Dr Huang described the first *de novo* structure solution using IMISX, BacA, an enzyme involved in peptidoglycan synthesis. She finished with a description of the use of IMISX at the SwissFEL, for which they designed a plate with thinner film and spacer to reduce background. The structure was solved to 3.0 Å using data from 471 10 µm crystals in 8 wells. The session ended with a presentation from Dr **Wangshu Jiang** of Uppsala University, who described the crystallisation of the proteins involved in the production of spider silk. These fascinating proteins are made of two domains, and Dr Jiang crystallised the NT domain associated with amyloid fibril formation at low pH. She could crystallise in a wide range of pH using seeding, with the protein always being dimeric. There was a rare C2 crystal form with two different dimers. The dimer interface included pH sensitive residues. She also described the structure solution of fimbrial adhesins from *P. mirabilis*, a bacterium involved in urinary tract infections. This protein crystallised via interactions with the His-tag, but to get reproducible crystals thermostability screening and *in situ* proteolysis with subtilisin was required. Dr Jiang's take home messages were that there are many considerations for successful screening, including His-tag, seeding and thermostability screening.

Claire Naylor
Molecular Dimensions

Early Career Prize:

Dr Paul Elliot (University of Oxford)

Dr **Paul Elliot** has recently moved to the Department of Oxford with a Career Development Award to continue his researches into ubiquitin-regulated signalling pathways. This continues work started while studying for his PhD at the University of Leicester and later at the University of Liverpool and the MRC Laboratory of Molecular Biology, Cambridge. He gave an interesting talk reviewing his work on Ubiquitin, a small protein that acts as a post-translation modification to proteins. This small protein attaches to lysine, but contains many lysines, so that chains may be attached to proteins. It is essential that the type, length and time of ubiquitination is right to avoid disease. Dr Elliot described his work using structure and point mutations to interrogate complex signalling pathways. He described the way that writers (proteins that add ubiquitin), readers (proteins that sense ubiquitin's presence on a protein) and erasers (proteins that remove ubiquitin) all act together with their regulators to tightly control protein behaviour and cell-signalling outcomes. He illustrated this with a detailed description of Met1 ubiquitination which is involved in inflammatory signalling. He showed how structures and mutations revealed how the readers, writers and erasers acted in concert, and often as regulators for each other, to produce finely tuned signalling responses.

Claire Naylor
Molecular Dimensions

Computational Structural Biology
Wednesday, 17 April

(L-R) Arianna Fornili, Gianni de Fabritiis (Keynote), Sameer Velankar, Gianni Botteoni, Shozeb Haider (chair).

The session was chaired by Dr **Shozeb Haider** (University College London), who introduced the speakers. The session started with the keynote lecture by Prof **Gianni De Fabritiis** (CEO Acellera and Professor at GRIB Barcelona). He spoke extensively about his new web application – Playmolecule (www.playmolecule.org) and how it could benefit structural biology research. The main focus was on model, ideas and hypothesis that he has been pursuing recently. Other web applications discussed were (1) Parameterize, which involved quantum machine learning algorithms to accurately predict force field parameters; (2) Deep site to calculate the binding affinity of ligands. The lecture concluded with example cases and benchmarks from Trypsin-Benzamidine binding simulations.

The second lecture was given by Dr **Giovanni Bottegoni** (University of Birmingham) on the polypharmacology of Dopamine D3 receptor modulators. The general idea presented was how one chemical compound can be modified to bind to two different targets simultaneously and modulate the activity of both targets. A comparison was made between D3R-GSK3beta kinase and D3R-fatty acid amide hydrolase. Novel synthesis of the chemical entity was also presented.

The third talk was given by Dr **Arianna Fornilli** (Queen Mary University of London) on Mechano pocket formation in proteins. The lecture discussed how pockets form as a result of mechanical stress in Myosin binding protein C in sarcomere cardiac muscle. The methods involved applying mechanical stress with varied frequency and studying the dynamics of the protein under stress. In case of low forces, steered molecular dynamics was employed. The conformation of the protein was searched for pockets arising as a result of this stress. The druggability of the pockets formed was studied computationally by flooding the pockets with virtual fragments. Similar comparisons were made in homologous proteins and a comparison made if mechanical pockets can be used as a potential drug target.

The final talk was given by Dr **Sameer Velankar** (European Bioinformatics Institute) on their latest one-stop annotated knowledge database. PDBe-KB is an integrated resource of macromolecular structures that is community driven and aims to promote basic and applied research. The example of how to use PDBe-KB was illustrated using CREB-binding protein. The database can be accessed using a PDB code, which then displays data with novel aggregated views. The annotations is interconnected with other annotated databases with PDB entries. The ultimate aim is to provide better visibility for macromolecular structures and provide better web services.

Shozeb Haider
University College London

BSG Plenary
Thursday, 18 April

(L-R) Vidya Chandran Dabari (chair), Liz Carpenter.

Prof **Liz Carpenter** delivered the BSG plenary session for the BCA Spring Meeting 2019. Prof. Carpenter is the Principal Investigator for the Integral Membrane Proteins group at the SGC, Oxford, and introduced the workflow adopted for determining the structures for challenging membrane proteins important for various disease conditions using various examples. She emphasised the importance of functional studies in combination with the structural studies to understand the mechanism of action and possible future exploitation of the high-resolution structures for intervention. She presented the structure of DPAGT1, an enzyme involved in the first committed step required for N-glycosylation, missense mutations in which causes myasthenic syndrome. The threshold of symptoms and increasing disease severity varies between no disease at 50% activity of DPAGT1 protein to severe disease when activity drops to 5%–10%. Structures of DPAGT1 in complex with tunicamycin, an off-target inhibitor, and substrate UDP-GlcNAc were presented. Using this example, she explained why active site mutations supported by structures might not always explain the diverse effects in activity they cause. The structure of Polycystin-2 (PC2) determined using Cryo-electron microscopy in collaboration with Prof **Juha Huiskonen** was also presented. This structure was also supported by crystal data from LCP crystallisation and detergent-based crystallisation.

Vidya Chandran Dabari
Queen Mary University of London

Multi-techniques for solving large macro molecular structures
Thursday, 18 April

(L-R) Christos Savva (chair), Aravindan Ilangovan, Mohinder Pal, Carolyn Moores (Keynote), Louise Fairall

This great session featured speakers using multiple

structural techniques to answer important biological problems. Our keynote speaker, Prof **Carolyn Moores** from Birkbeck College, told us about her research working with Microtubule Associated Proteins and using cryo-EM to solve the structures of doublecortin bound to microtubules which allowed the observation of the conformational changes occurring at different stages of GTP hydrolysis. Dr **Mohider Pal** from University of Sussex gave a lovely talk about his work on solving the Cryo-EM structures of HSP90 binding partner R2TP from yeast and humans. Dr **Louise Fairall** from University of Leicester talked about the structural determination of the MiDAC chromatin remodelling complex using X-ray and Cryo-EM and how she managed to tackle sample instability to obtain a 4Å structure of this complex. Finally Dr **Aravindan Ilangovan** from Queen Mary shared his wonderful research studying the structural basis of bacterial conjugation by the relaxase multi-functional protein.

Christos Savva
University of Leicester

BSG (joint with RaMP): EU Network for rationalising membrane protein crystallisation

Thursday, 18 April

*(L-R) **Sam Hjorth-Jensen, Cristina Cecchetti** (Imperial College) (co-chair), **Adrian Goldman** (Keynote), **Jannick Strauss, Claudia Stohrer** (University of Leeds) (co-chair).*

The session opened with a short presentation (5-10 minutes) from **Claudia Stohrer** (University of Leeds) about Innovative Training Network- Rationalising Membrane Protein crystallisation (ITN-RAMP). ITN-RAMP is a network that comprises 12 ESR positions (9 beneficiaries and 6 partner organisations) funded under a MSCA action- Horizon 2020. The scientific objectives are to understand the physical/chemical basis of the crystallisation process, explore new crystallisation techniques and products, rationalise new crystallisation methods, improve crystal size and handling and solve structures of novel membrane proteins taking advantage also of the techniques and methods developed. Dr **Adrian Goldman**'s (University of Leeds) keynote talk reviewed his work on Pyrophosphatases, essential enzymes found in all organisms and responsible for crucial mechanisms. He provided an overview of his team's investigation into the mechanism of the membrane-bound pyrophosphatases (mPPases). They couple H^+/Na^+ transport to pyrophosphate synthesis/hydrolysis and play an essential role in the infectivity of protozoan parasites. Validated also via molecular dynamics, this is the first time that this mechanism had been observed for any protein belonging to the pyrophosphatases family. MPPases are found in plants, archaea, bacteria and protozoan parasites but they are absent in humans, making them a promising drug target. The second half of the talk was focused on the design and development of novel mPPase inhibitors along with investigation into the binding of the latter to the mPPases. **Jannik Strauss** (University of Leeds) gave more details on MPPases. The talk presented a novel computational prediction pipeline called IMPROvER, which improves the efficiency of initial selection of stabilising mutants and doing so, reduces the costs and workload. The validity of this approach was investigated by designing 43 mutants of mPPase from *Clostridium leptum with* IMPROvER, and testing via GFP-based thermostability assays. Twelve stabilising mutants were identified, a success rate of about 28%. The best mutant increased the apparent melting temperature by about 13C when compared to the WT and all the mutants in general retained catalytic activity. **Samuel J Hjorth-Jensen** of Aarhus University talked about the sarco/endoplasmic reticulum Ca^{2+}-ATPase (SERCA) which transports calcium and protons in opposite directions across the membrane. The aim of this project is to determine the molecular mechanism of proton countertransport in SERCA by using the hydrogen maps obtained via neutron crystallography. Very large crystals are necessary (1 mm^3) for this. The talk focused on the different approaches and techniques to improve the crystal quality and size. Several different formats were explored such as hanging- and sitting-drop vapour diffusion with different drop size, dialysis and capillary. An initial room-temperature X-ray structure at 3 Å of SERCA was presented. The crystals were produced via batch crystallization within capillaries.

CCG Reports

CCG Plenary

Tuesday, 16 April

Prof Carl Henrik Görbitz.

The CCG plenary was given by **Carl Henrik Görbitz**, the godfather of amino acid structure chemistry. For this highly entertaining plenary Carl Henrik gave us a crash-course in Norwegian before taking us on a journey into the structure and temperature-induced phase transformations in the

hydrophobic amino acids, norvaline and norleucine. “Slippery when hot: temperature-induced sliding phase transition in amino acid crystals” explored the packing of the molecules and rationalised the phase transformations by highlighting the different conformations that the molecules adopted in each of the phases whilst remaining in their bilayers. Carl Henrik used simplified 2D shapes and cascading domino effects to help aid explanation of why the slip transitions occur which made the talk accessible to all present. He concluded by presenting some computational work that starts to explore the disorder present in the structures by using Monte-Carlo simulations of 48x48x48 block of unit cells. He was able to reproduce the diffuse scattering observed in the experimental data and a staggering 2000 defects were observed to yield such a diffraction pattern. It was an excellent start to the main BCA meeting.

Iain Oswald
University of Strathclyde

I didn’t know CCDC Mercury could do that!

Tuesday, 16 April

(L-R) Luke Frendo, Jonathan Pickering, Carl Henrik Görbitz, Helen Blade, Elna Pidcock, Matt Reeves.

The first CCG session, ‘I didn’t know CCDC Mercury could do that!’, chaired by Dr **Anuradha Pallipurath**, had several interesting talks which touched upon various aspects of the Mercury software. The keynote lecture was given by Dr **Helen Blade** from Astra Zeneca. She gave everyone an insight into how solid form research is aided by the use of tools in the Mercury software and how it is vital to understand the crystal structure and the molecular interactions in them, for controlling crystallisation, predicting morphology, developing manufacturing processes and getting regulatory approval. The second keynote lecture was given by Dr **Elna Pidcock** from the CCDC. She educated an attentive audience about several shortcuts and new features in the software that not only improve the visualisation of structures but makes analyses of these structures easier. For example, tools like the full interaction maps make use of the wealth of information in the Cambridge Structural Database to inform possible new interactions that can be achieved through crystallisation. By request from delegates, the illustrations for this talk have been made available at https://www.ccdc.cam.ac.uk/support-and-resources/ccdcresources/f6a416d9d1f2431a8085738b5d696a57.pdf. Dr **Jonathan Pickering** from the University of Leeds showcased ADDoPT project’s new feature called ‘Visual Habit’ that will be part of the next release of the Mercury software. Visual Habit makes use of lattice energy calculations to identify the different interactions in a crystal and their strengths to better predict experimental morphologies of crystals. Mr **Matt Reeves** from University of Edinburgh enlightened everyone on the use of the python module to do data mining into the CSD, to give information above and beyond what is available through features in Mercury. Our final speaker **Liana Vella-Zarb**’s talk was given by her student **Luke Frendo**, who explained how the small molecule-solvent interactions in a solvate structure can be studied using the statistical analysis tools in Mercury.

Anuradha Pallipurath
University of Leeds

Neat structures

Tuesday, 16 April

(L-R) Ben Williams, Marc Little, Michaele Hardie, Mairi Haddow, Lucy Saunders (chair), Helena Shepherd.

This year we got back to basics in the CCG ‘Neat structures’ section, celebrating all things structural from those in our community. **Michaele Hardie** from the University of Leeds opened the session with her excellent keynote lecture ‘Metallo-supramolecular assemblies from cavitand ligands’. Michaele showed us how these coordination cages are far from being square, formed of complex knots and entangled rings and having interesting guest uptake behaviour revealed by her team using Raman techniques.

Mairi Haddow from Heriot-Watt next took us into the world of coordinated lanthanide complexes that have varied ligand geometry affected by temperature and where agostic type M… H interactions contribute to stabilisation. **Marc Little** from the University of Liverpool complemented the keynote with his presentation about organic cage clathrates that are built around photo-luminescent guests for improved properties. **Helena Shepherd** from the University of Kent continued the theme of functional discrete units, presenting her research into spin crossover materials which works to understand their actuator like behaviour. **Ben Williams** from Diamond Light Source ended the session with his presentation about software screen19 implemented on Diamond beamline i19 to help scientists to access these neat structures.

Lucy Saunders
Diamond Light Source

Chemistry of Voids

Wednesday, 17 April

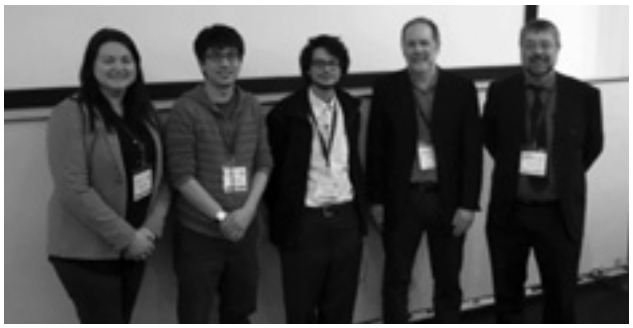
(L-R) Sophie Hodgkiss, Francesca Firth, Kim Jelfs, Petra Bombicz, Hamish Yeung (chair).

The CCG "Chemistry of Voids" session started off with a keynote lecture by Dr **Kim Jelfs** (Imperial College London), entitled "Computational Discovery of Porous Molecular Materials". Kim took the audience on an exciting journey through a range of computational approaches to the creation of new organic materials with intrinsic and extrinsic pores. **Francesca Firth**'s (University of Cambridge) presentation on "Using Defect Engineering to Create New Crystallographic Phases of UiO Family MOFs" followed, elegantly illustrating how synthetic conditions can alter defects and phase selection of metal-organic frameworks. The third talk, "Conditions of Ionic Hydrogen-bonded Organic Framework Formation" by Dr **Petra Bombicz** (Hungarian Academy of Sciences), took a turn towards catalytic materials design, involving fine control over molecular flexibility and intermolecular interactions. The session was brought to a close by **Sophie Hodgkiss** (University of Liverpool), whose talk, "Developing Rapid Powder Diffraction Analysis for Efficient Characterisation of New Materials", tackled the computational challenges of analysing large quantities of high-throughput and synchrotron XRD data. Overall, the session was a great success. The talks covered a wide range of topics in which crystallography plays a major part in and beyond porous materials design and the discussion after each one showed a high level of audience engagement.

Hamish Yeung
University of Oxford

Crystallography in chemical research

Thursday, 18 April



(L-R) Helena Shepherd, Hamish Yeung, Duncan Micallef, Lee Brammer, Jeremy Cockroft.

The CCG session entitled "Crystallography in Chemical Research" was chaired by Dr **Helena Shepherd** from the University of Kent, and featured a number of fascinating talks describing how crystallographic techniques can help address wider questions in the chemical sciences. Prof **Lee Brammer** from the University of Sheffield gave a superb keynote lecture entitled "Crystallography as the central pathway for chemical research". He used it to showcase a wide range of examples in which structural information has allowed chemists to advance their research. This was followed by Dr **Jeremy Cockroft** from UCL describing how both powder and single crystal X-ray diffraction can allow insights into materials with phase transitions and other puzzling situations in a talk entitled "Tackling challenging problems in chemical crystallography". Dr **Hamish Yeung** from the University of Oxford presented his work on "Pressure-induced metallicity, metal-metal bond formation and negative linear compression in a single component molecular conductor", showing how structural deformations can significantly impact the useful properties of metal complexes. The session was concluded by **Duncan Micallef** from the University of Malta describing a "A study on the structure and chemistry di-$\lambda^5\sigma^4$-phosphorane compounds", where he showed a number of interesting chemical and crystal structures of these main group molecules.

Helena Shepherd
University of Kent

IG Reports

Surfaces

Tuesday, 16 April

(L-R) Tony Bell, Paul Bingham, Lewis Owen.

The Industrial Group sessions on the theme surfaces got off to a fantastic start with a talk from **Paul Bingham** (Sheffield Hallam University) in a joint session with PCG on structures of alloys and glasses, chaired by **Tony Bell** and **Lewis Owen** (Sheffield Hallam University and University of Cambridge). An enlightening talk was given on advanced spectroscopy of glasses for radioactive waste immobilisation, to support the technical challenges associated with safely storing the glasses for very long periods of time.

continued >>>

IG Plenary

Wednesday, 17 April

Prof Kevin Roberts.

The plenary lecture, chaired by **Helen Blade** (Astrazeneca), was given by Prof **Kevin Roberts** (University of Leeds). Kevin gave an insightful talk on the challenging field of understanding the structural pathway underpinning nucleation and the crystal growth of organic crystals Examples were given detailing factors effecting nucleation, particle size, crystallinity, polymorphic form, crystal growth and surface properties.

(L-R) Tony Bell, Linda Seton, Anuradha Pallipurath, Mike Anderson.

Next, **Linda Seton** (Liverpool John Moores) gave a captivating talk on the crystal growth at surfaces, and how the chemistry of the surfaces can be modified to affect the growth and that challenges associated with characterising the surfaces. Then **Mike Anderson** (University of Manchester) talked through how it was now possible to both simulate and study crystal growth. Applying AFM techniques to obtain crystal habit and surface topology, that could be simulated and assessed. Finally, **Anuradha Pallipurath** (University of Leeds) rounded off the IG's sessions on surfaces with a talk on the chemical understanding of organic crystal surfaces, via a polarised Raman and computational study.

This year's industrial group poster prize went to **Pollyanne Payne** (University of Bath). Pollyanne presented a fantastic poster on how to control solid form and particle morphology using additives and crystallisation conditions. The poster was selected for the IG prize due to the direct applicability of the research to industry.

Helen Blade
Astrazeneca

PCG Reports

Local structure probes

Tuesday, 16 April

(L-R) Helen Playford, Emma Wolpert, Karen Johnston, Moreton Moore, Tobias Bird.

The first PCG session of the main meeting was on "Local structure probes" with a brilliant keynote talk from Dr **Karen Johnston** (Durham University; "Probing ion mobility mechanisms in solid electrolytes using solid-state NMR spectroscopy") to open the session. Karen's group works on understanding structure – property relationships in functional materials for energy storage and she gave us a glimpse of this by guiding us through their work on lithium-rich antiperovskites. Starting from the synthetic challenges they overcome, she showed how they've been able to use ssNMR (complemented by DFT calculations) to understand how a deeper understanding of the structure allows them to explain the changes in conduction as a function of temperature.

This was followed by a talk on X-ray diffraction topography studies of diamond from Prof **Moreton Moore** (Royal Holloway University of London; "My fifty years of diamond diffraction") revealing the defects in diamond. Moreton's presentation not only contained beautiful images of diamond, but was complemented by very effective models and props!

Tobias Bird (University of Warwick, "Understanding negative thermal expansion in ScF_3 and $CaZrF_6$ from local structure") spoke about his work understanding the complex structural distortions of two perovskite-related phases which was fascinating, and showed how possible distortions might be related to the thermal expansion behaviour of these materials.

Emma Wolpert (University of Oxford, "Understanding structural disorder in nickel cyanide using 1D statistical mechanical models") ended the session with a beautiful talk, gently introducing us to quaternions and illustrating how the stacking in layered Ni(CN)2 can be modelled analogously to an Ising magnetic system.

This session gave a great overview of techniques and approaches used to understand structure on a more local length scale, but also the important insight this gives to physical properties, a theme emphasised again by Dr **Igor Levin** (NIST, US) later that day in the PCG plenary lecture.

Helen Playford
The ISIS Facility

Structures of glasses and alloys

Tuesday, 16 April

*(L-R) **Tony Bell** (co-chair), **Paul Bingham**, **Lewis Owen** (co-chair).*

The keynote lecture was given by Prof **Paul Bingham** (Sheffield Hallam University) who, inspired by the YCG sessions that morning, began in "outreach" style to impress on the audience the importance of managing radioactive waste. This was really effective at putting the work in context and communicating the scale of the challenge we face. He went on to explain how his work on glasses is starting to address this. Whilst waste can be vitrified, the challenge of maximising the waste content within the glass whilst managing the effects of radiation damage is difficult. Paul showed how his group rely on several techniques to characterise the materials to understand the effects of radiation damage, and this work generated much discussion.

PCG Plenary

Tuesday, 16 April

Dr Igor Levin.

We were pleased to welcome Dr **Igor Levin** from NIST as this year's PCG plenary lecturer. Igor started his plenary lecture by highlighting that to understand physical properties such as piezoelectricity and ferroelectricity, understanding the structure at local length scales is important – and is increasingly being recognised as such by materials science research communities. Although we can try to understand the role of nanoscale defects or heterogeneities by molecular dynamics simulations, experimental studies on this are needed. Igor went on to explain the approach taken by the RMCProfile code, of which he is a co-developer, to gain an understanding of local and long-range structures by making use of total neutron and X-ray scattering data, as well as single crystal diffuse scattering data and EXAFS. He showed how powerful this approach is by sharing results on the room-temperature ferroelectric $K_{½}Bi_{½}TiO_3$ and on the relaxor ferroelectric $PbMn_{⅓}Nb_{⅔}O3$.

Igor ended this fascinating lecture by challenging the audience to use the technique more widely, not only to uncover more about local structure in an increasingly wide range of materials, but also in order to continue to develop the technique itself.

Energy materials

Wednesday, 17 April

*(L-R) **Anthony Powell**, **Paz Vaqueiro** (chair), **Eddie Cussen**, **Tony West**, **Josie Auckett**.*

Following on from work on functional and energy materials in earlier PCG sessions, Dr **Paz Vaqueiro** (University of Reading) chaired an excellent session focused on energy materials. Dr **Eddie Cussen** (University of Sheffield) got the session off to a great start with his keynote lecture ("Synthesis, characterisation and optimisation of new fast ion conducting phases as battery materials") looking at Li^+ mobility in the solid state, and in particular, materials for solid electrolytes. One highlight for me was Eddie's work on Li-stuffed garnets which showcased the range of techniques employed to understand and optimise materials, including microwave synthesis, neutron powder diffraction, EXAFS, impedance spectroscopy and muon spin rotation. Together, these allowed Eddie and his group to understand both the local and average structures and to relate these to the conductivity and to propose strategies to optimise performance.

Josie Auckett (Durham University, "Implications of disorder for oxide-ionic conductivity in $Ba_3NbMO_{8.5}$ (M = Mo, W)") followed with a fascinating talk which really highlighted the importance of disorder for understanding the oxide ion conductivity of this complex oxide system. It was also interesting to hear about the challenges in preparing single crystals via the floating zone method and the various strategies Josie is employing to optimise this process. Moving away from ionic conduction, **Anthony Powell** (University of Reading, "Structures and properties of Kesterite-type quaternary chalcogenides") gave a great discussion of sulfide-rich earth abundant minerals as thermoelectric materials and the challenges of differentiating between related structures. Using both neutron powder diffraction and DFT calculations, Anthony was able to understand the cation distribution and differentiate between similar materials. Building on this, his group went on to tune the composition to hole-dope the materials and optimise the thermoelectric properties. **Tony West** (University of Sheffield, "Redox-active oxides in yttria-stabilised zirconia") rounded the session off by looking at the well-known oxide-ion conductor yttria-stabilised zirconia (YSZ). Despite YSZ being generally considered as an electronic insulator, Tony explained circumstances (in an applied DC bias, or depending on pO2) in which it can behave as a mixed conductor showing some electrical conductivity. These

experimental results imply the presence of O^- ions near the surface of the material; although this at first seems a surprising hypothesis, it's borne out by experimental observations on a range of materials including Li ion battery materials and acceptor-doped $BaTiO_3$. This session highlighted the range of crystallographic and complementary techniques that can be applied to energy materials. Together, they give insight into both the average and local structures, which is essential to understand and then optimise physical properties and materials performance.

Paz Vaqueiro
University of Reading

Magnetic structures

Thursday, 18 April

(L-R) Paul Saines, Matthew Cliffe, Sian Dutton, Kate Tustain, John Claridge (chair).

The final day of the Spring Meeting included a fascinating session on Magnetic structures, chaired by **John Claridge** (University of Liverpool). **Sian Dutton** (University of Cambridge, "Magnetic and magnetocaloric properties of lanthanide garnets") began the session with her keynote lecture on solid state cooling by the magnetocaloric effect. Sian showed very elegantly how substituting magnetic ions onto some of the non-magnetic octahedral sites can be used to tune the magnetic order on the Ln^{3+} array. Beyond the academic interest of these complex materials, Sian and her group have been able to apply this understanding to prepare functionally-graded low temperature magnetocaloric materials more tuned to applications.

Matthew Cliffe (University of Nottingham, "Magnetic structures of thiocyanate frameworks") followed this by introducing us to the magnetic diversity of halides and explained how thiocyanates might provide analogous systems for study. He and his group used a range of complementary techniques (neutron powder diffraction, inelastic neutron scattering, DFT, magnetic susceptibility measurements, 13C NMR) to understand these fairly low dimensional materials.

Kate Tustain (University of Liverpool, "Nuclear and magnetic structures of the frustrated quantum antiferromagnet barlowite, $Cu_4(OH)_6FBr$") gave us a great introduction to quantum spin liquids (QSLs) and the mineral Herbertsmithite which has a ground state closely-related to a QSL. Her work on closely-related Barlowite has revealed changes in the structural chemistry on cooling which helps explain the magnetic behaviour. Having understood the structural chemistry, the group have succeeded in tuning the physical properties by Zn-substitution on the Cu site.

Paul Saines (University of Kent, "Magnetic structure of $LnOHCO_3$ frameworks: optimising magnetocaloric properties through magnetic interactions") rounded the session off returning to the topic of magnetoelectrics, but looking at coordination frameworks and looking beyond Gd systems. One focus of Paul's work was to understand the paramagnetic phases (in which the magnetocaloric effect occurs) from fitting magnetic diffuse scattering in neutron powder diffraction data.

John Claridge
University of Liverpool

PCG/YCG "In situ methods"

Thursday, 18 April

(L-R) Charlie McMonagle, Hamish Yeung (co-chair), Steve Hull, Anthony Phillips, Lois Wayment, Tom Wood (co-chair).

The joint PCG/YCG session on "In situ methods" featured talks on a range of experimental techniques for performing crystallographic experiments under non-ambient conditions. The keynote lecture was given by **Steve Hull** (ISIS Neutron and Muon Source), entitled "Neutron diffraction studies of energy materials", which covered the many sample environments available at ISIS, for investigation of batteries, thermoelectrics, fuel cells and hydrogen storage materials. This was followed by **Lois Wayment** (University of Bath / Diamond Light Source), talking about the insights and challenges of monitoring polymorphism using "In situ X-ray diffraction analysis of continuous segmented flow crystallisation at Diamond Light Source". The session's third talk turned to phase transitions and new mechanical behaviour under high pressure, with **Anthony Phillips**'s (Queen Mary University of London) fascinating presentation, "Formate frameworks under pressure: decoupling topology and coordination geometry". Finally, **Charlie McMonagle** (Newcastle University) spoke about "Reducing the background of ultra-low temperature X-ray diffraction data through new methods and advanced materials", in which he described some ingenious advances in laboratory instrumentation that yield high data quality down to 2 K. Overall, the session showed off an exciting breadth of crystallographic techniques and insight that is possible away from ambient conditions, and the audience was kept entertained and engaged throughout.

Hamish Yeung
University of Oxford

Topologically interesting materials

Thursday, 18 April

(L-R) Alex Gibbs (chair), Fernando Pomiro, Maia Vergniory, Quinn Gibson, Jian Rui Soh).

The final session of the day focused on topologically interesting materials, chaired by **Alex Gibbs** (ISIS). **Maia Vergniory** (Donostia International Physics Centre, "Realisation of topologically protected magnetic fermions in materials") gave a fantastic tour through the theoretical investigation of fermions based on higher-order nodal crossings at high symmetry points in semimetals. She outlined the extension of this idea to magnetically ordered systems which may host new fermions and discussed potential realisations of these in materials, with insight into the experimental challenges that are faced in compounds such as PtFeSb.

Jian Rui Soh (University of Oxford, "An ideal Weyl semimetal induced by magnetic exchange") gave a great introduction to the search for an ideal Weyl semimetal (which would have a single pair of Weyl nodes in proximity to the Fermi energy, and no overlapping bands). He focused on magnetically ordered $EuCd_2As_2$ as a candidate in its ferromagnetic phase under applied field, outlining the results from experimental probes such as REXS and ARPES which have been used to investigate this.

This was followed by **Quinn Gibson** (University of Liverpool, "Chemical concepts and building blocks for topological materials") giving a fascinating insight into how chemical principles can be used to try to rationally design and manipulate topological materials. He discussed several key materials criteria and the ways in which problems such as structural instabilities to e.g. Peierls distortions can be prevented through analogy with radicals in organic chemistry.

Fernando Pomiro (University of Warwick, "Phase transitions in the hybrid improper ferroelectric $Ca_{2.15}Sr_{0.85}Ti_2O_7$ Ruddlesden-Popper perovskite") ended the session by taking us through the intriguing series of phase transitions in $(Ca,Sr)_3Ti_2O_7$, a hybrid improper ferroelectric. He outlined the results of his detailed investigations into the octahedral tilting patterns as a function of temperature, based on symmetry analysis of high resolution synchrotron x-ray data.

Alex Gibbs
ISIS

BCA Prize Lecture

Prof Clare Grey.

Global warming and demonstrations about it were much in the news while we attended the Spring Meeting. Plainly we need to make more use of renewable energy sources; but these tend to be intermittent, and efficient storage technology is required. Therefore the BCA Prize Lecture by Prof **Clare Grey** (Cambridge) on "Developing and optimising the function of Li-ion and 'beyond Li' batteries and supercapacitors by advanced characterization methods" could not have been more topical. Clare reminded us that the Li-ion battery has powered the revolution in portable electronic devices. Nevertheless, there can be problems: electrolyte that is only metastable when the battery is fully charged, multiple degradation products, formation of a surface electrolyte film that sequesters Li from the cell, and a fire hazard from Li-plating upon excessively rapid charging.

Research has attempted to push current Li technology by replacing C with Si or Sn in the anode. More ambitiously, moving beyond Li to Mg would increase the capacity due to the 2+ charge. Using Na instead of Li would provide the advantage that Na can be used with Al, leading to the reassuring safety of an all-solid-state device. Before we can rely on such batteries, we must understand their mechanisms, including the nature of metastable intermediates or structures that may not survive disassembly. NMR is a useful probe, but it cannot penetrate a battery in a metal can. "Plastic bag" batteries made using food industry laminators circumvent this difficulty. PDF analysis gives information about the structures of amorphous and disordered Li and Na anode structures. DFT calculations and *in situ* diffraction measurements provide further validation.

Carl Schwalbe

BCA Spring Meeting 2019 Bursary Reports

WHAT was the highlight of the BCA spring meeting 2019? An unforgettable demonstration by Dr Tim Easun. From being sat in the lecture theatre, myself and the audience were transported inside a 3D metal organic frame work (MOF)! In this alternate world benzene rings were used as tennis rackets, small molecules as balls and the observer had free rein to grab, throw and play in what looked like virtual heaven for a crystallographer. The activity demonstrated how MOFs are able to separate molecules, an experience I will never forget. It was an excellent virtual reality activity that linked scientific research with outreach.

I was looking forward to coffee fuelled days filled with silly crystallography puns, influential keynote speakers and meeting a network of amazing people. I was not disappointed. The conference started off on a beautiful sunny day, the blue skies were never ending and the young crystallographers group satellite meeting (YCG) began. The young faces of PhD and master's students ignited interest with flash presentations for the poster exhibitions that were held throughout the event. The exhibitions provided a great opportunity to chat to other students, academics and industrial partners about research and get to know the global community that attended.

The main meeting contained many intriguing speakers including; Dr **Christine Beavers**, who taught us to be ourselves in order to humanise science and leave behind the stereotypical public view on what a scientist is and looks like. Prof **George Sheldrick**'s detailed overview of SHELXT: for a daily SHELXT user the talk was inspirational, a great opportunity. Prof **Kevin Roberts**, gave a talk that imparted a physics perspective to crystal engineering, an outlook that I particularly enjoyed as a chemist.

Scheduled networking events ensured plenty of time to socialise with guest speakers and other students about their research careers as well as my own. The spring meetings award ceremony and conference dinner wrapped up the event nicely and was a great opportunity to celebrate everyone's hard work. It was a lovely surprise to be awarded the Chemical Crystallography Group RSC CrystEngComm poster prize!

Overall the conference was stimulating with lots of coffee and biscuit breaks keeping my caffeine and sugar levels up. The four days covered an exciting range of research areas from learning all the hidden secrets of what the CCDC Mercury can do to a detailed analysis of what we can learn from crystal surfaces. I very much look forward to the next BCA meeting!

Aneesa Al-Ani
Centre for Sustainable Chemical Technologies.
The University of Bath.

I ATTENDED my first BCA Spring Meeting at the University of Nottingham's Jubilee Campus during an unseasonably warm period, in mid-April 2019. I knew it had a reputation as a friendly and interesting conference and was looking forward to experiencing it first-hand.

My week kicked off on Monday the 15th with the Young Crystallographers' Satellite Meeting, which opened with a fascinating talk by Prof **John McGeehan** about engineering enzymes to break down PET plastics and also included the way the work was reported on, with variable quality, by the world's media. Many high quality talks by young researchers followed throughout the rest of the day and I felt honoured to have the opportunity to present my own research among such an impressive line-up! The following morning wrapped up the Young Crystallographers' portion of the conference with talks on the topic of outreach. Each speaker tackled different areas of outreach ranging from how to use social media, to using VR to explore the inside of a MOF. There was a sense of excitement about getting involved in outreach following the talks and it certainly opened my eyes to the rewarding nature of getting the public involved in science.

The main meeting then opened with a talk by the legendary Prof **George Sheldrick**, who spoke with great humour and humility about his work creating and developing SHELX. I now have a newfound respect for the effort that went into the software I use on such a regular basis!

The next three days were filled with talks on topics ranging from materials for use in batteries, to porous organic materials and tips on using Mercury, among many others. One of my personal highlights was a talk about phase transitions in amino acid crystals by Prof **Carl Henrik Görbitz**, which included not only great science, but also some top tips for visiting Norway! Also of interest were the wide range of techniques utilised in people's research, in addition to crystallography. A few examples include neutron scattering, NMR and computational simulations, which highlighted the multidisciplinary nature of modern science and the key part crystallography still has to play in it.

The conference also offered plenty of opportunities to meet other delegates in a relaxed environment, including several poster sessions and the conference dinner – topped off by the famous ceilidh!

The BCA spring meeting showcased crystallography within a wide range of scientific areas and opened my eyes to the ways it can be supplemented by other work to provide incredible insights into the world around us. I found the conference highly interesting and stimulating and will take everything I learned into my work in the remaining year and a half of my PhD, which I will hopefully be able to discuss at next year's meeting!

Demetris Bates
University of Liverpool

THE BCA Spring Meeting 2019 was held in Nottingham this year on the beautiful Jubilee Campus of the University of Nottingham. It was a lovely sunny day when I arrived and pleasant to see the ducks swimming in the lake behind the Exchange building where the conference was held.

The first day of the conference started with the Young Crystallographers conference. There was a great plenary talk from **John McGeehan** about his research on the PET-ase enzyme. The application and science behind this discovery was extremely interesting. This was followed by a wide range of talks from other young crystallographers on their PhD research. I was pleased to be given the opportunity to be a part of this session and give a talk about some of my research to other PhD students. A great addition was a flash presentation session to give an overview on the posters the YCG members would be displaying. This was followed by an opportunity to have some food, drinks and network with the other students.

The next morning consisted of some outreach talks, a particular passion of mine. I found the talk from **Christine Beavers** to be really engaging and thought provoking. Her talk *'Scientists, science communication and social media: is it all worth it?'* discussed the skewed and stereotypical view of 'scientists' on the internet and encouraged those present to appear human online and not 'a scientist imitating a human'. I felt this was a really important message given the mistrust a large portion of the general public have for science at the moment, particularly surrounding topics such as global warming.

The rest of the week had talks on a wide range of topics, covering everything from chemical crystallography to *in-situ* diffraction methods. I particularly enjoyed the session covering uses for the CCDC software. The industrial group plenary lecture by **Kevin Roberts** was an interesting listen. His talk focussed on computational modelling to predict the growth mechanisms of para amino benzoic acid and, therefore, the final morphology of the crystals. This is very closely related to my PhD research and was nicely followed by a talk from **Linda Seton** in the next session explaining some of her work on crystal growth surfaces throughout her career.

There was plenty of opportunity to network throughout the conference. A main meeting poster session on the Tuesday night, again during dinner, gave us the chance to question delegates who didn't give a talk about their research interests. During coffee breaks there were trade exhibition stands where we would talk to companies about their up and coming technologies.

On the final night of the conference there was a celebration dinner followed by a ceilidh. This was another brilliant opportunity for networking and thoroughly enjoyed by all who attended. Prizes were awarded for the best posters, a nice way to acknowledge the good work being done by those who didn't give a talk. I was honoured to receive the Industrial Group poster prize. Overall I thoroughly enjoyed this conference and look forward to hopefully attending again in the future.

Pollyanna Payne
University of Bath

THE venue for this year's BCA Spring Meeting was Nottingham University Jubilee campus, with all the sessions in the Exchange building. Nicely situated next to a body of water, it is a very idyllic and calming place to set about the conference. The poster session offered a relaxed environment for discussion around posters, which was well attended by all the delegates and therefore offered a wide audience. I found the poster session really helpful in terms of discussing where my research is now and where it could go. The variety of different exhibitors also offered a great range of information about their new and existing products to help attendees with their research.

Networking opportunities were available throughout the whole conference with a great range of places to congregate and exchange ideas. In particular, the conference dinner offered a fantastic opportunity for all attendees to mingle and then after a few glasses of wine (with kind thanks to Malvern Panalytical) dance at the Ceilidh.

The Young Crystallographers' satellite meeting was split into two main sessions, the first including a diverse selection of research talks given by early career scientists followed by the second session focussing on outreach and social media in science. The meeting kicked off with a great talk from Prof **John McGeehan** about his work on protein engineering a PETase, originally identified from a micro-organism isolated from a recycling plant. His talk was a particular highlight for me as it was a great example of how research can take you in unexpected directions and how embracing what the data shows can result in high impact publication and worldwide publicity. The other fantastic thing about the Young Crystallographers' satellite meeting is that it offers attendees research talks from all groups of the BCA (CCG/ PCG/ BSG/ IG), which provides a different perspective on your research and science in general. I think this meeting is fairly unique in this respect.

The main meeting started with the Lonsdale lecture given by Prof **George Sheldrick**, a founding member of the BCA, whose work has undoubtedly aided most crystallographers at one time or another. The BSG sessions across the whole meeting were well organised and offered insights into a great diversity of research topics. It was fantastic to see a session included on complementary techniques for crystallography, an easily overlooked area, which is key for getting the most out of any macromolecular crystallographic data. There was also a nice balance of new data collection strategies looking at a variety of different beamlines (VMXm)/ end stations (T-ReXX) and new computational strategies (Playmolecule) as well as databases (PDBe-KB). Another highlight of the conference for me was this year's early career prize lecture for the BSG by Dr **Paul Elliot** from the University of Oxford, on his work into the regulation of ubiquitination control.

All in all, I left the BCA Spring Meeting with a much greater knowledge of what is being developed in the field and great ideas about how best to progress my own research.

Rachael Wilkinson
University of Oxford

BCA 2019 Poster Prizes

The BSG ECR prize talk was awarded to Dr **Paul Elliot** (University of Oxford). This was sponsored by *Rigaku*, presented by **Marcus Winter** and chaired by Dr **Claire Naylor** (Molecular Dimensions).

CCG/CCDC poster prizes prize sponsored by *CrystEngComm* were awarded to:

- **Aneesa Al-Ali** (University of Bath), ***"Engineering a new access route to metastable polymorphs with electrical confinement for enhanced pharmaceutical properties"***.
- **Georgia Scurfield** (University of Oxford), ***"Furthering our understanding of modulation in molecular crystal structures"*** (presented by Dr **Iain Oswald**).

IG poster prize awarded to **Pollyanna Payne** (University of Bath), ***"Control of solid form and particle morphology using additives and crystallisation conditions"***, presented by Dr **Helen Blade** (AstraZeneca).

PCG-related poster prizes presented by Dr **Anthony Philips** (Queen Mary University of London):

PCG poster prize awarded to **James-Nicholas Grima-Cornish** (University of Malta) ***"Auxeticity in boron arsenate"***.

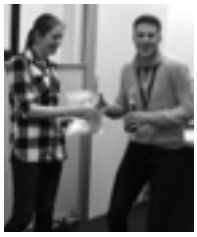
RSC's Solid State Group poster prize awarded to **Kenneth N Freeman** (University of Edinburgh), ***"Host-guest structures in Bi – Te compounds at high pressure"***.

BSG poster prize sponsored by *PDBe* awarded to **Angus Cowan** (Walter and Eliza Hall Institute, Melbourne, Australia), ***"The first crystal structures of BAK in complex with lipid offer novel insights into oligomerisation and membrane permeabilisation"***.

"MDPI Crystals" sponsored poster prize awarded to **Thomas Roseveare** (University of Sheffield), ***"Exploring the dynamic gas adsorption behaviour of a family of coordination polymers through in situ diffraction techniques"***, presented by Prof **Simon Philips**.

ACA Judy Flippen Anderson Journal of Structural Dynamics sponsored poster prize awarded to **Katherine Rowlinson** (University of Oxford), ***"Disorder in deoxycholic acid inclusion compounds: a solid state NMR and crystallographic study"***, presented by Prof **John Helliwell** (University of Manchester).

Rigaku sponsored poster prize awarded to **Eliott Carrington** (University of Liverpool), ***"When crystallography needs some help: gaining insight through computational approaches"***, presented by **Marcus Winte**r (Rigaku). *(This was judged by the programme committee (two members of it) for a poster that used complementary techniques.)*



YCG prize for best flash presentation awarded to **Natalie Pridmore** (University of Bristol), ***"Spin crossover properties of iron(II) phosphine complexes"***, presented by **Stephen Dodsworth**.

CCP4 Study Weekend Report 8-10 January 2019

THE theme of this year's Study Weekend was Molecular Replacement organised by Isabel Uson, Randy Read and Ronan Keegan. The meeting started with an overview and history of MR given by Eleanor Dodson (York) where she outlined the four steps of MR, namely (i) what have you crystallised, (ii) what is your lattice, (iii) can you position a known model and (iv) can you bootstrap to a solution. Airlie McCoy (Cambridge) followed up with an introduction to Phaser – the next generation and the tools inside including data analysis (anisotropy, tNCS, twinning), data guided model generation and search improvements (gyre/gimble and coordinate refinement, LLG pruning). The first session was completed by Bjorn Wallner (Linköping, Sweden) who gave an introduction to ProQ which is a program to estimate which parts of your model are good or bad. ProQ uses machine learning to assess secondary structure, surface accessibility, atom-atom and residue-residue contacts to predict model quality. ProQ2 and ProQ3 use Rosetta energy functions and deep-learning algorithms respectively to enhance the assessment.

The second session was supposed to be started by **Deborah Marks** (Harvard) with a talk on Evolutionary Covariance, but she was unable to attend due to ill-health. **Dan Rigden** (Liverpool) then gave a talk on the AMPLE pipeline which is designed to use bioinformatics techniques to extend the reach of MR. AMPLE can generate many search models through Rosetta or Quark, use NMR solutions or generate ensembles through normal mode analysis. These are then clustered into structural ensembles and can be truncated to give many search models of different sizes. The next talk was from **Adam Simpkin** (Liverpool) on his program SIMBAD. This tries to solve your MR problem even in the absence of a protein sequence (and therefore a model). It uses the domains present in the MORDA database in an AMORE rotation search to identify promising leads. If the resolution is high enough, these may be good enough to bootstrap to a solution. The program is also used to check against a list of known contaminants that tend to crystallise easily – sometimes what you have crystallised is not what you think!

After lunch on the first day, instead of the usual lunchtime bytes, the organisers ran a MR clinic. Datasets that people were having trouble with were sent in to be analysed by the experts, who then showed how they had made progress and what lessons could be learned in each case.

The afternoon session was kicked off by **Andrew Senior** (DeepMind) who showed how DeepMind's AlphaFold program was using deep-learning to predict protein structures de-novo. The structures were constructed using distance predictions generated from co-evolutionary data (increasingly better due to the explosion of sequencing) and then optimised with gradient descent refinement. Andrew showed that AlphaFold was doing very well in the bi-annual CASP tests, coming first in the best-of-5 ranking. **Massimo Sammito** (Cambridge) then showed how fragment based MR was dependent on the quality of the fragments used. He introduced ALEPH which generates many very small, but accurate partial models (Local Folds) from an ensemble of models taken from the PDB. Arcimboldo is then used to solve the structure. The next talk was given by **Andrey Lebedev** (STFC) on how the selection and preparation of models is key to a successful solution. MrBUMP generates models from ensembles of homologs which are then variously cropped based on the variance in the ensemble to achieve better models. **Regine Herbst-Irmer**

continued >>>

Andrew Senior (Google DeepMind)

Regine Herbst-Irmer (Göttingen)

Carmelo Giacovazzo (Bari)

Alan Roseman (Manchester)

Randy Read (Cambridge)

Kevin Cowtan (York)

(Goettingen, Germany) then explained the difference between (pseudo-)merohedral (overlapping spots) and non-merohedral twins (overlaps, partial overlaps and split spots) and showed how SHELX can still solve and refine structures (small molecule and protein) that have twinning and gave an example of a twinned Insulin crystal that they had solved. The last talk of the session (and day) was given by **Iracema Caballero Muñoz** (Barcelona, Spain) who explained the various forms of translational non-crystallographic symmetry (tNCS), the effect they have on the recorded data, how they cause problems in MR and how to deal with them. She showed results from published data in the PDB to show that Phaser is accounting for the tNCS correctly. The dancing at the post-dinner ceilidh was led by **Elspeth Garman** (as usual) and fun was had by all who participated!

Day two was kicked off by **Carmelo Giacovazzo** (Bari, Italy) who spoke about how to get to a full structure from a partial MR solution. He showed that by cycling density modification and automated model building, one could get to much better completeness automatically. **Claudia Millān** (Barcelona, Spain) introduced the program ALIXE which can be used to better discriminate between true and false solutions in the case of small fragments as used by Arcimboldo. It has proved especially useful in the case of Arcimboldo-Shredder, which generates fragments from distant homologs. **Rafael Borges** (Barcelona, Spain) showed how solutions can be improved for lower resolution data sets, by adding side chains to correct fragments to allow further autobuilding of the solution. Sequence_Slider tests all possible sequences for each fragment and selects the best. This can be cycled with autobuilding to improve model completion. The next talk was given by **Kaushik Hatti** (Cambridge). He explained the need for a good estimation of the rmsd of the model to provide an accurate eLLG, which is required to be able to rank solutions correctly. Kaushik introduced a new algorithm for predicting the eVRMS which slightly improves the estimate for X-ray models, but is much better for NMR-derived models. The last talk of the session was given by **Alan Roseman** (Manchester) who showed how to dock and refine known fragments into electron density – either from X-Ray or EM data – to produce contiguous chains.

After coffee, **Randy Read** (Cambridge) gave an explanation of LLG, eLLG and how these relate to information content and showed how the information content of a problem and be used to determine the resolution limit for useable data. **Kevin Cowtan** (York) then followed up with an explanation of shift field refinement, which allows for large shifts of secondary structure in a coordinated manner, which can be very useful after MR solution to automatically improve the model. The last talk in the session was given by **Grzegorz Chojnowski** (EMBL Hamburg, Germany) on the improvements in ARP/wARP 8.0 that allow for better automated model building after MR. These include a new side-chain algorithm, homologs to help build loops, resolution extension through 'free lunch' and sequence free model building. The update allows better building at lower resolution – down to 3.5Å.

The final session started with **Paula Salgado** (Newcastle) giving a personal perspective of MR and several practical examples of MR where non-routine strategies were required, including a Type IV major pilin protein, eventually solved by Arcimboldo. The next talk was by **Jennifer Miao** (UCLA, USA) on micro-electron diffraction (microED) which involves collecting electron diffraction data on micro crystals (<0.5um) in a cryo-electron microscope. Due to the electron wavelength, good resolution can easily be obtained (~1.7Å) and the structure can be solved by MR. The next talk was given by **Monserrat Fàbrega-Ferrer** (Barcelona, Spain) who showed how partial models built in EM density could be used to phase x-ray low resolution diffraction data and gave an example of a bacteriophage protein complex, where 8Å cryo-EM phases could be used to phase a 3.8Å X-ray data set. The final talk was given by **Owen Davies** (Newcastle) who explained how coiled-coil structures could be very hard to solve by MR, but by using non-standard approaches (Arcimboldo, AMPLE) the structures could be solved. He also described efforts to improve initial models of the coiled-coils by using Rosetta modelling.

Mark Roe
University of Sussex

Greg Chojnowski (Hamburg)

Jennifer Miao (UCLA, USA)


Owen Davies (Newcastle)


Dave Brown (President of CCP4, Kent)


Lunchtime Bytes


Fun at the Ceilidh

The pictures have been chosen from a large selection, copyright of Science & Technology Facilities Council and kindly made available by **Karen McIntyre** (STFC).

African Adventures

IT was with much excitement that Amy Sarjeant and I headed off to the second Pan African Conference on Crystallography (PCCr2) in Ghana at the end of February on behalf of the Cambridge Crystallographic Data Centre (CCDC).

Africa is one of the largest continents on the planet with a population of 1.29 billion, but it has been reported that as little as 1% of the world's research output is produced in Africa[1]. Last year we started capturing crystallographer details during deposition and these details include country. This means we can look to see how many structures have been both deposited and published since then with a crystallographer from an African country added during deposition.

Map showing the number of structures added to the CSD that have an African crystallographer listed that were deposited since 2018. The total number of structures from Africa will be much higher and from a wider variety of countries!

Although we have seen the number of structures from Africa rise slightly in recent years, helped by initiatives such as the IUCr-UNESCO OpenLabs and the PCCr, you can see that there is still lots of opportunity for further growth. From presentations and conversations at the meeting in Ghana I am confident that over the next few years this map will become much more populated, and it was also good to hear about research using the CSD in institutions where diffractometers are not available.

This time the PCCr2 conference partnered with The African Light Source (AfLS2) and the theme of the meeting was 'Crystallography, a tool for sustainable development in Africa'. This conference turned out to be one of my personal highlights of my time at the CCDC.

After a vibrant opening ceremony, Amy and I started our part of the conference by hosting a workshop on how participants could use the CSD for research and education. It was great to see so many engaged participants; I think we even had the youngest ever participant to a CCDC workshop!

Some of the participants at the CSD workshop at PCCr2, including the youngest ever CSD workshop attendee.

The following day we attended the Crystal engineering/ Structural chemistry session. The session started with **Aurora Cruz-Cabeza** and **Alessia Bacchi** giving engaging and thought-provoking talks on turning liquid active ingredients into crystals and polymorphism in molecular crystals, respectively. The highlight for the session for me though was hearing **Dzesse Tekouo Christelle**, whom we had first met at the PCCr meeting in Cameroon, speak about single crystal to single crystal transformations in metal-organic frameworks. It was a pleasure seeing some of the research that has happened in Africa since the first PCCr meeting.

In the afternoon session Amy and I both spoke in the Chemical Databases session chaired by **Simon Coles**. Between us we gave an overview of the CSD and hopefully provided participants with a flavour of how the CSD can be used in a variety of ways in both education and research. A real stand-out talk in the session was by **Samuel Tetteh**. I first met Samuel back in 2016 at a workshop in Kumasi and since then he has gone onto apply for the CCDC's FAIRE Programme and use the CSD in both research and education at the University of Cape Coast in Ghana.

Samuel Tetteh speaking about how he has been using the CSD at the University of Cape Coast in Ghana

Over the course of the meeting we attended many more interesting lectures on topics ranging from inorganic and industrial materials to large facilities for emerging countries. It was also encouraging to hear about efforts to establish both an African Crystallographic Association and an African light source.

We are already looking forward to the next African meeting and I know discussions are already underway to decide the location. Back at the CCDC we are hopeful that many more of the attendees will go on to benefit from the CCDC's FAIRE programme, which was established to support structural chemistry research and education in developing countries through use of the CSD. Who knows, maybe the millionth structure in the CSD will be from the African crystallographic community too!

1. https://www.theguardian.com/global-development-professionals-network/2015/oct/26/africa-produces-just-11-of-global-scientific-knowledge

Suzanna Ward
CCDC

Obituary

Stephen C. Wallwork: 1925-2019

Photograph from the BCA Spring Meeting in Nottingham in 2016, where Stephen and his wife Marion were guests of honour.

THE BCA has lost a great friend, staunch supporter and a true crystallographer, in the passing of Stephen Wallwork earlier this year. Stephen would have been 94 in May – a tremendous record in our subject.

Stephen was educated at Manchester Grammar School and Brasenose College, Oxford. In 1949 Stephen was appointed to an assistant lectureship in physical chemistry and prior to applying for the job, he had checked with the head of chemistry, Professor **F.E. King** that, if appointed, he would be able to continue research in crystallography. Thus chemical crystallography started at Nottingham. Professor King had enquired how much it would cost to set up a crystallography laboratory and Stephen estimated that it could be achieved for about £1000. In the event, a sealed X-ray tube, a generator, a Unicam single crystal goniometer, a polarising microscope, a desk adding machine and a set of Beevers-Lipson strips for Fourier calculations did cost about £1000! The laboratory, about three metres square, also served as Stephen's office and later when, on the permanent staff as a lecturer, he was able to have two research students, they also initially shared the same office. Health and Safety regulations would certainly not permit that today! The main structural research in those days was the investigation of charge-transfer and hydrogen-bonded organic complexes but several structure determinations were also carried out for the inorganic chemists at Nottingham. After a few years, a second electrical desk calculator was obtained with the aid of a Royal Society grant (£450) and an assistant was appointed to carry out the structure factor and Fourier calculations. That arrangement continued until such work could be transferred to the university's main-frame computer.

Around 1965, **Trevor King**, who had hitherto identified organic structures by the standard organic chemical methods of decomposition and synthesis, decided that crystallography would provide a quicker method of characterisation. So he learned crystallographic techniques from Stephen and soon became expert in applying them. He had a particular flair for computing and became the Chemistry Department's main advisor and representative on that topic, as well as helping staff and research students with one-off structure determinations. A Hilger and Watts linear diffractometer had been obtained in 1963 and this was superseded after about ten years by the first of a series of computer-controlled four-circle diffractometers. This was made possible because the organic chemists' use of crystallography had increased significantly when Leslie Crombie became Professor of Organic Chemistry in 1969 and subsequently he appointed Dr **Mike Begley** in 1970 to carry out structure determinations for him. One of Stephen's specialist areas was that of coordination compounds containing nitrate groups. His seminal paper published with Professor **David Garner** *et al* [*Quart Rev* **25**, 289, (1971)] has attracted over 630 citations and pointed the direction for future research. His second area of specialisation was that of the structures of organic compounds, particularly aromatic systems and charged bipyridylium salts, a topic that he pursued until the end of his career. His seminal work on hydrogen-bond radii [(*Acta Cryst* **15**, 758 (1962)], has attracted over 200 citations.

Stephen took early retirement in 1982, having published nearly 100 papers on the structures of important organic and inorganic compounds. Formal retirement did not reduce his enthusiasm for crystallography and he continued to teach part time and to publish until the late 1990s. I still have his book on 'X-ray Crystallography' published in 1989 with its accompanying cassette tape, designed to allow individual students to study at their own pace. Stephen's career spanned five decades and his contribution to the development of modern crystallography has been enormous. Stephen also continued to study beyond crystallography and graduated in 1985 with an MA in *'Local and Regional History'* from Nottingham University, leading to a further part time position in the Department of History. Professor Trevor King died in 1983 and Mike Begley died at a very early age in 1994. Many BCA chemists will remember Mike and his contributions to our meetings. Dr **Andrei Batsanov** (by then at Durham University) spent some months in Nottingham after Mike had died, to help fill the gap, fix the old diffractometer and determine crystal structures for the Department. By this time, the inorganic chemist **Brian Sowerby** had become a chemical crystallographer and was helping other research workers in the department with their structure determinations.

Stephen was truly a real chemical crystallographer. Through his graduate training at the University of Oxford, under the supervision of **Herbert "Tiny" Powell** he learnt all the skills, patience and rigour to undertake the full three dimensional structure of a crystalline compound, to determine the positions of the atoms and to make an assessment of the nature of the bonding that held the atoms together. In the late 1940s carrying out a crystal structure determination was no mean feat. Going from crystal to a complete structure was a labour of love and it could take many months to obtain a single result. However, the information that the crystallographers provided has underpinned much of the cutting-edge chemistry that has been carried out over the last 60 years.

Not only was Stephen an outstanding crystallographer but he cared deeply about the growing crystallographic community in the UK and he was very closely involved with the creation of the BCA and much of the correspondence from that time (1980-2) remains. He was an active member of the CCG, which then belonged to the RSC and he did a great deal of the work required to bring the PCG from the IOP, together with the CCG and the 'new' sections coming from Biology and Industry. He was secretary to the working group which drew up the constitution and the by-laws of our Association and he became a Founder Member of the newly created BCA. Members may wish to read his Royal Society article written with David Blow on the 'Pre-History of the BCA'.

Notes.Rec.R.Soc.Lond **58** (2) 177-186 (2004)

Stephen continued to contribute to the BCA throughout his career and attended its meetings regularly until quite recently. This photograph was taken when he attended the BCA meeting in Nottingham in 2016. He will be remembered too for his sage advice to the younger members of the community and for his kindness and support to students in the development of their careers. Amongst Stephen's other hobbies are listed photography and water-colour painting and when I was appointed to the new Chair in Durham in 1991, he sent me a painting that he had made of the old Gateway to Cathedral close, copied from a photograph which he may well have taken when the Inaugural BCA was held in Durham in 1982. I was touched by this very personal gift and I continue to treasure this water-colour which hung in my office here for over 23 years; now it stays in my study at home.

Judith AK Howard (Durham) and contributions from **Paul Raithby** (Bath) and **Sandy Blake** (Nottingham/Edinburgh).

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, news@crystallography.org.uk . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

2-6 June 2019
14th International Symposium on Macrocyclic and Supramolecular Chemistry, Lecce, Italy.
https://ismsc2019.eu/

2-8 June 2019
4th International Summer School of Crystallography, Hamburg, Germany.
https://conferences.cfel.de/issc19/

3-7 June 2019
Summer School on Mathematical Crystallography, Nancy, France.
http://www.crystallography.fr/mathcryst/nancy2019.php

4-7 June 2019
MLZ Conference 2019: Neutrons for Information and Quantum Technologies, Lenggries, Munich, Germany.
https://indico.frm2.tum.de/event/157/

6-7 June 2019
S4SAS 2019, Didcot.
https://www.diamond.ac.uk/Home/Events/2019/S4SAS-Workshop-and-Conference.html

9-14 June 2019
33rd Annual ResMed Course: The Residential School on Medicinal Chemistry and Biology in Drug Discovery, Madison, NJ, USA.
http://www.drew.edu/science-research/about-us/resmed/

12 June 2019
BCA-IG XRF Meeting, Sheffield.
https://sites.google.com/site/bcaxrf/

16-27 June 2019
The Zurich School of Crystallography 2019: Bring Your Own Crystals, Zurich, Switzerland.
http://www.chem.uzh.ch/linden/zsc/

17-19 June 2019
4th International Conference on Resonant Elastic X-ray Scattering (REXS 2019), Long Island, NY, USA.
https://www.bnl.gov/rexs2019/

17-24 June 2019
12th annual CCP4/APS school in macromolecular crystallography "From data collection to structure refinement and beyond", Argonne (near Chicago), USA.
https://www.ccp4.ac.uk/schools/APS-2019/application.php

22-23 June 2019
Crystal Growth and Assembly. GRS, Manchester, NH, USA.
https://www.grc.org/crystal-growth-and-assembly-grs-conference/2019/

23-28 June 2019
Crystal Growth and Assembly. GRC, Manchester, NH, USA.
https://www.grc.org/crystal-growth-and-assembly-conference/2019/

23-28 June 2019
11th International Conference on Inelastic X-ray Scattering (IXS2019), Stony Brook, NY, USA.
https://www.bnl.gov/ixs2019/

1-5 July 2019
10th Workshop – Combined Analysis in XRD by using MAUD software, Caen, France.
http://www.ecole.ensicaen.fr/~chateign/formation/agendas/2019agenda.pdf

1-5 July 2019
European Conference on Neutron Scattering, St Petersburg, Russia.
http://www.ecns2019.com/

1-5 July 2019
Mechanisms and Non-Linear Problems of Nucleation and Growth of Crystals and Thin Films, St Petersburg, Russia.
http://www.mgctf.ru/

1-5 July 2019
Intergranular and Interphase Boundaries in Materials, Paris, France.
http://iib2019.org/

2-5 July 2019
16th French Microscopy Society conference, Poitiers, France.
https://colloque.sfmu.fr/en/

2-5 July 2019
XIX International Meeting on Crystal Chemistry, X-ray Diffraction and Spectroscopy of Minerals, Apatity, Kola Peninsula, Russia.
https://www.ksc.ru/xrd2019/

4-5 July 2019
Macromolecules in Action, Grenoble, France.
http://www.esrf.eu/psbsymposium

8-10 July 2019
Workshop canSAS XI, Freising, Germany.
https://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/canSASXI/_node.html

8-11 July 2019
UCANS8: International Meeting of the Union for Compact Accelerator-Driven Neutron Sources, Paris, France.
https://ucans8.sciencesconf.org/

8-12 July 2019
DMI 2019. V International Workshop Dzyaloshinskii-Moriya Interaction and Exotic Spin Structures, Petrozavodsk, Russia.
https://oiks.pnpi.spb.ru/events/DMI-2019

9-11 July 2019
50th Annual Meeting of the British Association of Crystal Growth, Central London.
https://www.bacg.co.uk/bacg-50th-annual-conference/

14-17 July 2019
31st International Symposium on Chirality, Bordeaux, France.
https://chirality2019.sciencesconf.org/

17-19 July 2019
Advanced Correlative Light and Electron Microscopy (CLEM) Course 2019, London.
https://www.rms.org.uk/discover-engage/event-calendar/clem-course-2019.html

20-24 July 2019
American Crystallographic Association Annual Meeting, Covington, KY, USA.
http://www.amercrystalassn.org/content/pages/main-annual-meetings

21-26 July 2019
The 17th International Summer School on Crystal Growth (ISSCG-17), Granby, CO, USA.
https://www.iccge19.org/isscg-17

21-27 July 2019
The 17th International Summer School on Crystal Growth (ISSCG-17), Keystone, CO, USA.
http://www.crystalgrowth.org/ICCGE-19_-_ISSCG-17_Flyer_7-20-16.pdf

28 July – 2 August 2019
19th International Conference on Crystal Growth and Epitaxy (ICCGE-19) and 19th Biennial Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-19), Keystone, CO, USA.
https://www.iccge19.org/

4-8 August 2019
Microscopy & Microanalysis (M&M 2019), Portland, OR, USA.
https://www.microscopy.org/MandM/2019/

13-17 August 2019
High-Pressure Crystallography Workshop – Satellite meeting of the 32nd European Crystallographic Meeting, Vienna, Austria.
https://ecm2019.org/satellites/high-pressure-workshop/

16-18 August 2019
Mathematical and Theoretical Crystallographic Workshop – Satellite meeting of the 32nd European Crystallographic Meeting, Vienna, Austria.
http://www.crystallography.fr/mathcryst/wien2019.php

18-23 August 2019
32nd European Crystallographic Meeting, Vienna, Austria.
https://ecm2019.org/home/

1-4 September 2019
17th ECSSC European Conference on Solid State Chemistry, Lille, France.
https://ecssc17.com/

1-6 September 2019
57th European High Pressure Research Group Meeting on High Pressure Science and Technology, Prague, Czech Republic.
https://ehprg2019.org/

2-6 September 2019
1st International Conference on Non-Covalent Interactions, Lisbon, Portugal.
http://icni2019.eventos.chemistry.pt/#page-top

2-6 September 2019
Neutrons and Muons for Magnetism, Ispra (Varese), Italy.
http://www.sisn.it/nmm19/

2-13 September 2019
16th Oxford School on Neutron Scattering, Oxford.
https://www.oxfordneutronschool.org/

8-14 September 2019
Fourth International School on Aperiodic Crystals, Cabourg, Normandy, France.
https://isac4.sciencesconf.org/

12-14 September 2019
HEC22. 22nd Heart of Europe Bio-crystallography Meeting, Obergurgl, Austria.
https://hec22.i-med.ac.at/

16-18 September 2019
International Conference on Materials Science and Engineering, Melbourne, Australia.
https://www.materialsconferenceaustralia.com/

23-27 September 2019
EMBO Practical Course: Small Angle Neutron and X-ray Scattering from Biomacromolecules in Solution, Grenoble, France.
http://meetings.embo.org/event/19-small-angle-scattering

24-25 September 2019
International SAXS Symposium 2019: SAXS excites, Graz, Austria.
https://www.anton-paar.com/tu-graz/saxs-excites

30 September - 3 October 2019
EXPO&more International Workshop, Bari, Italy.
http://www.ba.ic.cnr.it/expo-more-workshop2019/

1-6 October 2019
Hot Topics in Contemporary Crystallography 4 Structural Biology, Mlini, Dubrovnik, Croatia.
http://htcc4.org/

7-9 October 2019
EMBO Workshop: Tools for Structural Biology of Membrane Proteins, Hamburg, Germany.
http://www.embl-hamburg.de/training/events/2019/TBP19-01/

7-10 October 2019
JCNS Workshop 2019 Trends and Perspectives in Neutron Instrumentation: Probing Structure and Dynamics in Soft Matter, Tutzing, Germany.
https://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2019Workshop/_node.html

7-11 October 2019
1st French Congress on Integrative Structural Biology, Toulouse, France.
http://bsi-2019.ipbs.fr/

15-30 October 2019
CSHL X-ray Methods in Structural Biology Course, Cold Spring Harbor, NY, USA.
https://meetings.cshl.edu/courses.aspx?course=C-CRYS&year=19

24-26 October 2019
The 77th Annual Pittsburgh Diffraction Conference, Oak Ridge, TN, USA.
https://conference.sns.gov/event/78/

3-9 November 2019
EMBO Course “Practical Integrative Structural Biology”, Hamburg, Germany.
http://meetings.embo.org/event/19-integrative-structural-biology.

4-5 November 2019
Engineering recombinant proteins for structural and functional studies, London.

20-22 November 2019
GISAXS 2019, Hamburg, Germany.
https://indico.desy.de/indico/event/22389/

1-6 December 2019
Advanced Materials Exploration with Neutrons, Boston, MA, USA.
https://mrs.org/fall2019/call-for-papers/call-for-papers-detail?code=MT04

9-13 December 2019
American Geophysical Union Fall Meeting, San Francisco, CA, USA.
https://www2.agu.org/fall-meeting

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