Crystallography News

British Crystallographic Association

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BCA-BACG Spring Meeting 2021

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

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Contents

Honorary Life Membership of the BCA

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

This month's cover:

BCA-BACG Spring Meeting 2021. Each line from left to right: Opening session (Simon Phillips, Nick Blagden); Named lecturers (Richard Henderson, William Jones, Lucy Clark, Elizabeth Driscoll); Young Scientist Prize lecturers (Veselina Marinove, Charlie McMonagle); Closing session (Nick Blagden, Ed Edwards).

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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by North Wolds, York. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews.
Please ensure that items for inclusion in the September 2021 issue are sent to the Editor to arrive before 25 July 2021.

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From the President

THIS is my first column since taking on the role of BCA President at the Spring Meeting this year. Thank you for your support; it is an amazing and slightly terrifying responsibility, and a great privilege to serve BCA members and the wider crystallographic community.

My background is in small molecule crystallography, with an interest in methods and software (particularly the refinement software CRYSTALS). I have remained a BCA member since I was a student through post-docs, industrial jobs, and back to a post in Chemistry at Oxford. I value being part of the BCA as it is a friendly and supportive community with regular opportunities to discuss research across a range of disciplines. I had my arm twisted to join the BCA's CCG committee at an early age and have been involved ever since in various different roles, organising and promoting meetings, and supporting BCA and group websites.

I referred to some archive copies of *Crystallography News* for ideas and inspiration for this column (available online at crystallography.org.uk). My immediate predecessor **Simon Phillips** closed his first column with the observation that "There are bound to be challenges". With hindsight, this may be something of an understatement. I am extremely grateful to Simon for leading the BCA to meet and overcome those challenges, particularly through the last year which nevertheless culminated in a well attended online version of our usual Spring Meeting. I am also extremely grateful for Simon's handover notes and advice, and pleased that he will remain on Council for the next year to ensure a smooth transfer of ongoing projects.

I would also like to thank BCA Council for its careful stewardship of the organisation over the thirty-nine years since its foundation, particularly, of course, the current members. At the AGM, we welcomed back **Cheryl Doherty** who was elected for a second term as Ordinary Member of Council, and welcomed for the first time **Christine Beavers** who takes over as Education and Outreach Coordinator from **Simon Coles** after he has served two terms in that role. Christine is planning to consolidate many of the resources that have been developed during and since IYCr 2014 and will join a review of the BCA communication strategy which includes thinking about how we can target our outreach and education activities for maximum engagement of members and our target audiences. Anyone who is keen to get involved is encouraged to contact Christine with ideas or promises of help.

The Spring Meeting programme was jointly organised by the BCA Programme Committee chaired by **'Ed' Tom Edwards** and the BACG committee chaired by **Nick Blagden**. While most will have missed the face-to-face socialising and catching up, not to mention the usual Ceilidh, we nevertheless enjoyed a splendid selection of scientific sessions with topics ranging from phase transitions and computational simulations to time-resolved macromolecular crystallography and electron crystallography. The overlap of BCA and BACG topics indicates that our subject areas are more interdependent than ever. In addition to the well-established common ground of crystal engineering, the interface between the field of crystal growth and nucleation and structure determination is essential to developments in both fields. Techniques such as electron diffraction, which featured in one of the meeting sessions, are providing structural information about crystals at early stages of crystal growth and nucleation. I encourage you to read the reports from the meeting which are available in this edition of *Crystallography News*.

Alongside the lectures was an online Q&A system and the panel discussions were possibly an improvement over the standard format of questions. I also particularly enjoyed watching the short summary videos from poster presenters which were available alongside each poster. It will be interesting to see how many of these innovations we can bring to future meetings, online or otherwise. It is also clear that we must commit to explore options to provide online access to future meetings both for members who cannot travel to a meeting, and to be able to attract and engage with researchers around the world without the financial and environmental travel costs associated with international travel.

I am delighted that **Iain Oswald** has agreed to chair for the 2022 Spring Meeting Programme Committee, and can report that early planning is already underway. Please contact your Group committee *as soon as possible* to feed in ideas for sessions or workshops, as the 2022 programme will start to crystallize within only a couple of weeks of this June edition of *CN* arriving on your doorstep or in your inbox.

At the time of writing, the exact format of the delayed IUCr Congress in Prague has not been announced. The decision to hold a hybrid or a fully remote meeting is expected in June. Those interested in attending either in person or virtually are encouraged to pre-register for free on the congress website iucr25.org. The BCA will be represented by a five-person delegation at the General Assembly during the Congress and any BCA member who wishes to see behind the curtain and contribute to the governance of our International Union at one – or more! – of this set of meetings please do drop me a line.

Looking much further ahead, the BCA Council is in favour of bidding to host a future IUCr meeting in the UK. This undertaking has commitments well beyond the elected terms – and possibly careers – of current Council members as such a meeting would be at least 15 – 20 years away. Therefore, we will bring a proposal on this to an AGM for discussion and approval.

Thank you once again for this opportunity to serve the BCA. During my term as President I will endeavour to represent all BCA members and work with the BCA Council on behalf of the entire UK crystallographic community. The long-term outlook for future meetings is brighter than it was 12 months ago, but we continue to plan cautiously. I welcome your thoughts on all and any aspects that can improve the running of the BCA. This includes boring stuff such as governance and finance, but also important and exciting stuff like promoting crystallographic science, improving accessibility of meetings, providing opportunities for education and outreach, and ensuring equality and diversity in representation in our organization.

Richard Cooper

BCA Council 2021

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Elections to BCA Council

There will be elections this year for:

- **BCA Vice President**
- **BCA Honorary Secretary**
- **Ordinary Member.**

Any two Members may make nominations, and such nominations should be accompanied by the written consent of the candidate to serve if elected. These must be received by the Secretary by 30th September 2021.

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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

AFTER a year off with different content from usual – thanks to the reason you will all know – your June issue is back to 'normal', focussing as it does every year on the BCA Spring Meeting which was this year run as a joint meeting with our colleagues in the British Association for Crystal Growth (BACG). In the last year, we have had the pleasure (?) of experiencing webinars, online seminars, and web-based scientific conferences of various lengths all over the world without leaving home. With our experience now of a major multi-day conference with the full gamut of plenaries, parallel oral sessions, poster and vendor sessions, perhaps we are in a good position now to evaluate their pros and cons to guide how we proceed once we again have the possibility of meeting in person.

So what do we now think about online conferences after this year's Spring Meeting? I think the platform chosen was the best one I have experienced in the last year, and congratulations are due to our friends at Hg3 who chose it. I have my own comments on both the things that worked well and not-so-well online, and I'm sure you do also. Looking at the reports of the bursary holders (see page 21), their comments were mostly positive. Taking a few of these:

- The talks being recorded made it possible to review some and check others that were missed through being in a clashing parallel session
- No more awkward exits half way through one session to get to a talk in a parallel session (and pre-preparation of the talks made it more likely the speakers would keep to time, making moves between sessions more practical)
- Posters accompanied by short, to the point, presentations
- Poster viewing and author engagement worked surprisingly well, and good to be able to look at them on the web after the event
- Vendor sessions were good opportunities for updates on equipment advances
- In the absence of the possibility to approach a speaker after a talk, speakers made the effort to share contact details for further enquiries

But...

- "I dearly missed in-person networking" (which the talk from down under by Chris Howard emphasised how this networking around the world "fosters and drives new discoveries, reminding us how important in-person meetings are to create collaborations").

Perhaps *my* main 'con' – apart from the inability to adjourn to the bar to 'foster further collaborations' – was that the pre-recording of talks, the inability to ask questions orally (at my age, typing in the Q&A box in mid-talk takes my mind off what the speaker is saying), and the lack of an opportunity for a questioner to respond immediately to a speaker's answer to a question, meant that the spontaneity that I value at conferences was somehow lacking. Though on the other hand, I and (at least one of the Bursary holders) was impressed by the efforts some chairs went to to stimulate discussion among the speaker panels to explore more deeply the implications of particular questions.

So what's the answer? With the experience of the use of the platform used for our Spring Meeting this year, there are so many positives that would be good to try to keep when we move towards in-person meetings. Hybrids? Possibly – but we would need to consider carefully if the hybridity might detract from some of the positives of both purely online and in-person ones.

What do you think? It would be good to have a discussion in these pages – email me at **john.finney@ucl.ac.uk** with your post-Spring Meeting views.

Coming back to what's in this issue, we sadly say goodbye to **Judith Milledge**. She has had a strong influence on many of today's crystallographers – including not only on our immediate Past President, who talked about her in his recent AGM presentation, but also on me in my early days (where did they all go?) at Birkbeck, where she took over from **Kathleen Lonsdale** (who died 50 years ago last April – see the item on page 7) in teaching on the Birkbeck M.Sc. Crystallography course.

Furthermore, earlier this year we heard of the passing of **John Sherwood** who spent most of his scientific career at the University of Strathclyde (formerly the Royal College of Science and Technology, Glasgow). John also had a strong influence on my early scientific activities, helping me and **Graham Bushnell-Wye** come to grips with the problems of taking X-ray topographs of very small crystals. It's particularly appropriate to remember him in this issue which reports on our joint meeting with the BACG, as not only was he a founder member of the that organisation, but he also served as its Chair and President. I urge you to look at the obituary written by **Kevin Roberts** of his 'friend and colleague' (a sentiment I would fully endorse) in The Guardian **https://www.theguardian.com/science/2021/jan/07/john-sherwood-obituary** and a longer one setting out more of his scientific work on the BACG website **https://www.bacg.co.uk/profsherwood/** . I'm personally indebted to them both and am saddened by their leaving us.

John Sherwood
Image courtesy of University of Strathclyde

John Finney

Puzzle Corner

THE picture *(right and the wallpaper on the front cover)*, shows a piece of bathroom wallpaper (courtesy of Sandy Blake) which has the all too familiar problem of two identical but symmetry-independent "molecules" in the unit cell. Select the unit cell and plane group. Assuming you could measure its diffraction pattern, would you expect any systematic variations in intensity for groups of reflections in hk, h0 or 0k? What shifts of one fish could give higher symmetry or a smaller cell?

Answer to March puzzle:

The only rotational symmetries possible are 2 and 4. Mirror lines are possible parallel to both pairs of edges and along both diagonals. This makes the point groups 2, m (4 settings), mm (2 settings), 4, and 4mm possible. In practice, symmetries higher than 2 or m are rare.

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:

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- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

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

BCA-BACG Spring Meeting 2021 Group Reports

THE meeting began, as usual, with the Young Crystallographers Satellite Meeting (including the Parkin Lecture) and continued with three days of four parallel sessions, interspersed with three named lectures and two young scientist prize lectures. In this write-up, the named and prize lectures follow the YCG report (which includes the Parkin Lecture), with the rest of the sessions arranged in random order by group.

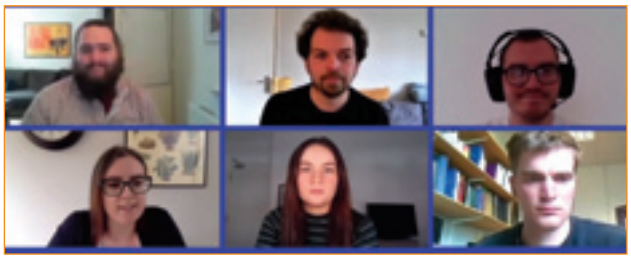
YCG-BACG Early Career Satellite Meeting

THE YCG satellite meeting was bound to be slightly different from the previous meeting in 2019. With the cancellation of the 2020 meeting due to the pandemic, the YCG committee were keen to adapt the 2021 meeting for a virtual platform. Although we will look forward to when we are all able to meet in-person again, the virtual format of this year's satellite meeting did not hamper participants' ability to communicate and discuss their recent work.

The day's sessions started with a plenary talk from **Cheryl Doherty** (GSK) with an industry perspective on identifying stable forms of Active Pharmaceutical Ingredients (API) through screening both computationally and synthetically. The plenary talk was followed by two talks from YCG members focusing on further understanding the properties of a couple of APIs. The first from **Reabetswe Zwane** (Dublin City University) focused on understanding the elastic properties of the crystalline state using computational modelling. This talk was directly followed by a presentation from **Eleanor Jones** (University of Strathclyde) exploring the phase transformation when pressure is applied to isonicotinamide. Eleanor was awarded a CCG-RSC poster prize for the poster presentation of this work. These talks were then followed by a live question and answer session allowing for speakers to further discuss computational methods and experimental techniques.

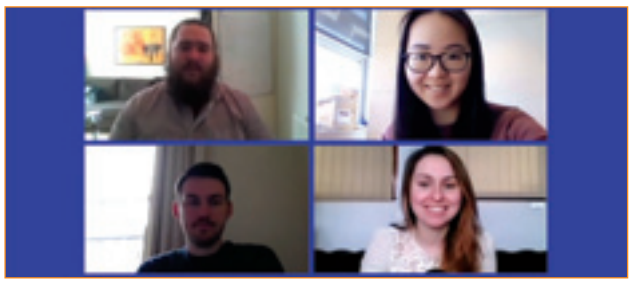
Session 1 Live Q&A. Clockwise from top left: ***Tom Roseveare*** *(Cochair),* ***Cheryl Doherty*** *(Speaker),* ***Eleanor Jones*** *(Speaker),* ***Reabetswe Zwane*** *(Speaker) and* ***Natalie Tatum*** *(Cochair)*

The second session of the day consisted of four early career speakers the first of which was **Adam Crawshaw** (Diamond Light Source), who focused on the challenges and recent developments of sample preparation on the VMxm beamline. The second speaker, **Lucy Hunter** (Newcastle University), spoke on recent synthesis of metal-organic framework materials using a *cis*-stilbenedicarboxylic acid. This work focused on how the *cis* isomer affected the dimensionality, topology and luminescent properties of the MOFs obtained. This was followed by a talk from **Lee Birchall** (University of Kent) reporting his finding on how the co-former present affected the spin crossover properties of an iron complex. Lee presented this as a poster, which was awarded, (jointly – see Entropy and Structure session below – with **Thomas Hitchings** (also University of Kent, but with a different supervisor)) an IUCr and ACA/AIPP poster prize (which carries IUCr Student Associateship, an IUCr book and a certificate). The fourth and final presentation in this session, by **Edward Broadhurst** (University of Edinburgh), discussed using 3D Electron Diffraction to explore the crystallisation of glycine. The session closed with a live question and answer session with the speakers discussing sample preparation for VMxm and 3D Electron Diffraction as well as crystal engineering employed in MOF and inorganic complex synthesis.



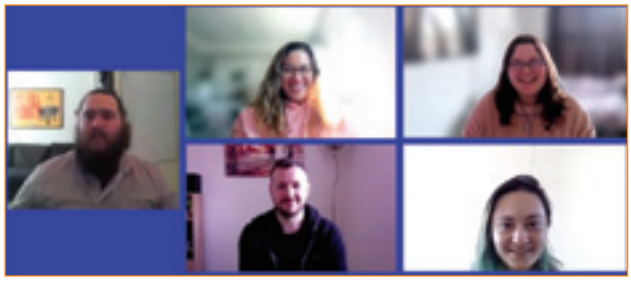
Session 2 Live Q&A. Top L-R then Bottom L-R: ***Tom Roseveare*** *(Cochair),* ***Adam Crawshaw*** *(Speaker),* ***Lee Birchall*** *(Speaker),* ***Natalie Tatum*** *(Cochair),* ***Lucy Hunter*** *(Speaker),* ***Edward Broadhurst*** *(Speaker)*

The third session started with the Parkin Prize Lecture, which was given by **Elizabeth Driscoll** (University of Birmingham). Elizabeth's lecture featured her experience developing public engagement resources both before and during the lockdown, as well as being mindful of ensuring that the resources are suitable for all. The second speaker was **Cameron Wilson** (University of Edinburgh) who talked about the development of software to monitor minor void space changes in crystals subjected to high pressures. The final speaker of the session was **Rachel Tang** (Diamond Light Source) and featured work monitoring the charge and discharge of sodium ion batteries using *in situ* diffraction at beamline I15-1. Rachel's poster presentation of this work was awarded a YCG MiTeGen poster prize. The session concluded with a live question and answer session.



Session 3 Live Q&A. Clockwise from top left: ***Tom Roseveare*** *(Chair),* ***Rachel Tang*** *(Speaker),* ***Elizabeth Driscoll*** *(Speaker) and* ***Cameron Wilson*** *(Speaker).*

The final oral presentation session of the YCG satellite meeting started with a presentation from **Anna Marini** (University of Southampton) who reported some recent *in situ* gas uptake studies of a porous molecular crystal as well the development of an *in situ* flow gas cell instrument. The second speaker, **Sara Morris** (Diamond Light Source), discussed variable temperature *in situ* powder X-ray diffraction as a means of testing a Martian surface simulant. Sara also presented this work as a poster, which was awarded a YCG MiTeGen poster prize. This was followed by a talk from **Ian Hope** (Newcastle University) about using FragLite, a fragment library, to screen active sites in Cyclin T. The final speaker of the meeting was **Rhona Lonergan** (University of Kent) who discussed a spin crossover complex, which can be produced by simple solid-state reactions, as well as how humidity affects these reactions. Rhona presented this work as a poster and was awarded a CCG-RSC Poster Prize. The session concluded with a live question and answer session.



Session 4 Live Q&A. Clockwise from far left: ***Tom Roseveare*** *(Chair),* ***Anna Marini*** *(Speaker),* ***Rhona Lonergan*** *(Speaker),* ***Sara Morris*** *(Speaker) and* ***Ian Hope*** *(Speaker)*

The final session of the YCG satellite meeting featured short presentations from early career researchers who were presenting posters throughout the main meeting. This was an interesting session demonstrating the true breadth of the research interests of YCG members as well as the variety of innovative ways to present their research projects in a short 3-minute presentation.

Thank you to all who presented, who attended, and all the people behind the scenes for making this year's YCG satellite meeting as informative and interesting as previous in-person meetings. The YCG committee looks forward to seeing everyone again next year.

Tom Roseveare
University of Sheffield

BCA-BACG 2021 Main Meeting Named Lectures

Lonsdale Lecture

THE Lonsdale lectures commemorate the work of the late Dame Kathleen Lonsdale. It is awarded by the BCA on the recommendation of the Young Crystallographers Group. The range of topics encompass all areas of crystallography and diffraction and the lectures tend to have an element of teaching.

An English Heritage Blue Plaque in Honour of Dame Kathleen Lonsdale

On the 50th anniversary of her death in 1st April 1971, English Heritage celebrated the achievements of Kathleen Lonsdale with a Blue Plaque on her childhood home at 19 Colenso Road in Seven Kings, London, where she lived from 1911 until 1927. Kathleen was known not only for her pioneering crystallographic work and her fundamental role in progressing X-ray crystallography, but also for her being a strong advocate for women in science as well as a passionate peace campaigner (the editor's wife has interesting tales of her granny working with Kathleen in the Women's International League for Peace and Freedom!). Kathleen was also the first female professor at UCL, and one of the first women to be appointed a member of the Royal Society.

It's good to see 'the system' recognise the achievements of one of the real scientific and humanitarian 'greats'.

Lucy Clark

This year's lecture, 'Quantum Magnetism and Crystallographic Complexity in Mineral Materials', was given by **Lucy Clark** (University of Liverpool) and addressed the issue of how magnetic function relates to the structure of crystalline materials. Lucy commenced her talk with an analogy between the structural (dis)order of gases, liquids and crystals and magnetic (dis)order in para-, ferro-and anti-ferromagnetic systems, and how cooling a magnetically disordered system led to strengthening interaction between the magnetic moments which facilitated a spin solid state in which the magnetic moments lined up in a ferro- or anti-ferromagnetic ordering. She took us back to the early neutron scattering work of Schull and Smart who used neutron diffraction to reveal for the first time the existence of the anti-ferromagnetic state through the appearance of magnetic Bragg peaks as the temperature was lowered through a transition temperature.

As Lucy explained with the example of the Kagomé lattice, which consists of corner-sharing triangles, such magnetic ordering can be frustrated by the structure of the crystal: there is no obvious way in which magnetic moments decorating such a lattice can order. So what is the arrangement of magnetic moments in such a system and how does it change as a function of temperature? Various proposals have been made as to how such a system behaves, and she explained the two possibilities of a gapped and a gapless quantum spin liquid.

An obvious way to find out what the magnetic state is is to perform experiments on a real system. Lucy explained the work on the mineral Herbertsmithite, which was considered to

be the first perfect realisation of an S=½ Kagomé lattice. Having being studied extensively using a range of experimental techniques, the conclusion that it's a *gapless* quantum spin liquid phase was considered to be an enormous advance in our understanding of such systems. However, there was a problem – theoretical work had concluded it should be a *fully gapped* spin liquid state! So the situation remained unclear, and the possibility was raised that Herbertsmithite was not after all a perfect realisation of the S=½ Kagomé lattice. Clearly, a close examination of the crystal structure, and any disorder present, was called for, and following the discovery of another candidate mineral Barlowite, there was a renaissance of work in the field.

The lecture continued to describe the work of Lucy's Ph.D. student Kate Tustin in tackling the problem. What's the structure of Barlowite and how does it relate to its properties? How and why do these properties change with temperature? Can the properties of Barlowite be tuned by varying its chemistry? Can it be doped towards a quantum spin liquid phase? And is this quantum spin liquid state universal to Barlowite and Herbertsmithite? Using neutron powder diffraction, the room temperature structure was determined. Cooling below T_S=250K resulted in structural distortions and the loss of the 3-fold symmetry of the Kagomé planes, while below T_N=15K the structure ordered magnetically and a space group could be identified that can describe both the nuclear and magnetic structures below this transition. Finally, some outstanding issues that are currently being tackled were described, such as what drives the structural distortion and its dynamics, and why are the energy scales of T_S and T_N so far removed? And why are the ordered moments so small (an issue further explored in the Q&A)?

The talk concluded with work on doping Barlowite to try to throw light on the origin of the structural transitions, and the use of muons as a local probe to map out the magnetic phase diagram.

In the following Q&A, the speaker was asked how optimistic she was that these complex issues would be finally resolved. She responded that they have the necessary tools at their disposal, but that what is challenging is to have the right materials on which to do the experiments, and the theoretical tools that match to the materials to hand. There was also discussion on the possibility of realising a 'structurally perfect' material that can manifest such a magnetic ground state and on the ability of DFT to identify the sites occupied in the muon experiments.

Bragg Lecture

Richard Henderson

THIS year's Bragg Lecture was a really stimulating talk by Richard Henderson (MRC Laboratory of Molecular Biology, Cambridge) on 'The Continuing CryoEM Revolution in Structural Biology'. He stressed at the start how the methodology had now come of age, and that it was now possible to solve atomic structures of all sorts of biological structures using single particle cryoEM spectroscopy.

Following a short explanation of how the technique works, Richard's talk fell into three parts – where we were 20 years ago, where we are now, and what the future might hold. After acknowledging the work of Dubochet in demonstrating rapid cooling to prepare samples embedded in amorphous ice, a procedure which underpins the whole technique, he used a number of examples – including the 70S ribosome subunit, hepatitis B cores and decorated actin, with respective resolutions of 11Å, 7Å,and 30Å – to illustrate the situation some 20 or so years ago. As techniques improved, he explained how the technique moved from 'blobology' to being able to see density in terms of atoms, resolve β-structure, and identify extended polypeptide chains and the odd sidechain. The technique made a further major step forward some 6-7 years ago with the development of direct electron detectors replacing film as the recording medium. This led to much better quality images through improved signal to noise ratios and, as the data were collected as movies, the ability to remove blurring resulting from drift or image motion. Emphasising also the extraordinary power of **Sjors Scheres**' RELION software, he showed a number of further examples of structures solved to resolutions down to around 3Å where sidechains are clearly resolved.

The reproducibility, quality and throughput of the technique has now developed to such a stage – it can reveal details of molecular interactions between fragments and a protein, and see how inhibitors or substrates bind – that 10-20 drug companies are using cryoEM in fragment-based drug discovery and design. Yet the specimens don't have to be crystallised, don't have to be pure, the molecules don't need to be in the same conformation and they can have disordered parts.

The progress of the technique was also illustrated by the rapid increase over the past 20 years in the number of structures solved by cryoEM. Compared to those solved by X-ray diffraction, 1 in ~1,000 were solved by cryoEM in 2000. With the improvement in electron microscopes, this had risen to 1 in ~100 by 2010, but with new detectors and more powerful software, this ratio currently stands at 1 in ~10 and falling, with many of the structures being those which just can't be solved by X-ray crystallography.

Looking to the future, Richard commented that the demand for cryoEM was now so great that it was difficult to get time on a machine and that manufacturers can barely keep up with the demand. He emphasised that what was critically needed was *affordable* cryoEM: not only do we need the microscopes for structure determination, but also – importantly – quick access for sample characterisation and preliminary evaluations. However, he emphasised that very high energy very costly microscopes were not necessarily the ones best to use for a particular problem: what was important was to optimise the ratio of elastic to inelastic scattering, which itself would depend not just on the energy of the microscope but also the sample thickness – so for a 300Å thick sample, a 100keV was the best bet, while a 1,000Å thick sample would justify using a more powerful (and expensive!) 300keV one. So his final conclusion was that we needed more detectors and more less expensive microscopes that a single group could afford.

The interesting Q&A session that followed discussed the need to optimise detectors for 100keV electrons, progress to higher resolutions than ~3Å, radiation damage and the problems and possibilities of seeing the hydrogens that are often relevant to function.

BACG Annual Lecture

William Jones

EACH year the BACG invites an individual who has made a significant contribution to crystal science to present the BACG Annual Lecture on a topic of interest to the community. This year, the Lecture was given by past President William Jones (University of Cambridge) with the title 'Exploring Form and Shape in Pharmaceutical Crystals'

Bill opened his talk by saying that it could equally have been entitled 'Making and Breaking Multicomponent Forms', as it was going to involve a lot of making and breaking! He addressed three topics: 'decomposing' cocrystals and solvates by thermal treatment; disappearing polymorphs as experienced in mechanochemistry; and the increasingly complex influence of the added liquid in liquid-assisted grinding (LAG) experiments.

The first topic addressed questions such as what the consequences are of drying a solvate. For example, amorphous regions might form on the surface which might affect particle-particle interactions. As an example of solvate formation, he described his work on a variety of carbamazepine (CBZ) cocrystals and solvates. Focussing on the CBZ.2H_20 hydrate, he looked at the variation of crystal morphology as a function of growth from different concentrations of water/ethanol mixtures. Although crystals grown from solutions containing 52% and 91% water looked the same, powder XRD showed strong preferred orientation effects, which indicated dominance of {0k0} faces in the crystals grown from the 91% solution compared to {h00} in those grown from the 52%. He explained these differences in terms of the different hydrophobicities/hydrophilicities of the two faces. He concluded this section with a study of multicomponent CBZ crystals with various coformers.

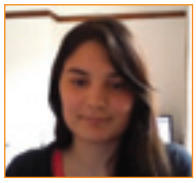
His second section discussed disappearing polymorphs as experienced in mechanochemistry. A quote he gave from one of his papers on caffeine-benzoic acid gave an idea of the kind of discussion that was to follow: "Once introduced, the designed heteronuclear seeds facilitated the formation of **1** and, significantly they (or seeds of the product cocrystal) continued to act as long-lasting 'contaminants', which encouraged cocrystal formation even when present at such low levels as to evade detection!". He followed up with a time sequence of experiments on caffeine-citric acid crystals formed by different researchers using a range of preparation methods, producing an amorphous form as well as three different polymorphs **I**, **II**, and **III**. The final message that came across is perhaps summarised by the statements: once form **I** emerged, **III** became unobtainable; once form **II** was made, **I** became unobtainable!

The final part of the talk can be perhaps summed up by the statement: depending on the liquid used in an LAG experiment, we can have normal 'catalytic and selective' reaction, but with some liquids reaction can be slow (inhibited) or even not occur (prohibitive). He illustrated this with experiments on the formation of vinpocetine hydrogenoxalate salt by the grinding of vinpocetine and hydrogenoxalate, where using different liquids led to the formation of different forms. He argued that these kinds of results confirmed the need to use a range of liquids in a screening protocol – failure to obtain a cocrystal or salt may say more about the liquid than the reactants.

He ended his fascinating talk with two final remarks. First, that 'seeding' may be an unknown underlying issue in any set of results. And finally, in a world of seeds, is any experiment or any conclusion really safe!?

Young Scientist Prize Lectures

BACG Young Scientist Medal



Veselina Marinove

THIS year the Medal was awarded to Veselina Marinove (University of Sheffield), whose Medal talk was entitled 'Dynamics and Thermodynamics of Ibuprofen Conformational Isomerism at the Crystal/Solution Interface'. She commenced by emphasising that crystal shape is the result of specific interfaces growing at different rates, and that contaminants and solvent can influence it. Moreover, for molecules with internal degrees of freedom, if we are to understand the solid/liquid interface during crystal growth, we need to understand the effect of that flexibility.

Using ibuprofen, which she described as having two internal degrees of freedom, Veselina performed MD simulations of four states along the path of incorporation of molecules into the bulk crystal: solution, adsorbed, surface and crystalline solid. The conformational landscapes emerging from the calculations showed six different conformers in solution. The landscape for the adsorbed state was similar to the solution one, that of the surface was significantly different, while the solid hosted only one conformer. From these landscapes, Veselina concluded that the equilibrium distribution depends on the relative position of the molecule with respect to the crystal, and that state to state transitions are limited by conformational rearrangement. Moving from the adsorbed to the surface state, the molecule has to make a conformational rearrangement that is likely to contribute to the kinetics of the process.

The main conclusions from this work were that the free energy landscape is environment dependent, and that state to state transitions may be limited by conformational rearrangement. Specific surface-solvent interactions alter the conformational population and conformational equilibrium time, and conformational rearrangement within the crystal surface affects growth and dissolution kinetics. Moreover, the conformational rearrangement mechanism changes in different environments relative to the crystal, and it is important to consider conformational flexibility individually in each state along the incorporation path.

CCDC/CCG Prize Lecture

Charlie McMonagle

THE CCDC/CCG Prize is awarded to a younger scientist who has made a significant contribution to the field. The winner this year was Charlie McMonagle (ESRF) for instrumentation development for single-crystal diffraction.

Charlie discussed two of his instrumentation developments. The first of these was a sapphire capillary pressure cell developed for I19 at Diamond. He set the scene by showing the rapid rise in high pressure crystallography since 2000, a rise made possible – and probably stimulated – by the increasing availability of pressure equipment. On synchrotrons, this is largely diamond anvil cells which make kbar pressures easily available; however, the high sealing pressure needed for these cells means that lowish pressures are difficult to obtain, so there's a 'gap' below the lowest available pressure. This is a problem for working on

structurally complex crystals which tend to have higher compressibilities and so may require lower pressures that are in the 'gap'. He described the design of his new cell which can go up to 1,500 bar, has very fine pressure control to *ca*. 1 bar, there is little reciprocal space restriction, and a phase separator allows many hydraulic mediums to be used. He illustrated the capability of the cell in a pressure dependence study of a metal-oxide framework crystal up to 1,200 bar using two different liquids.

His second challenge was to reduce the background in single crystal experiments at very low temperatures on a four circle diffractometer in Newcastle. He analysed the main sources of background in the modified displex cryostat with a ^{4}He ILL Joule-Thomson third stage which has a base temperature of 1.86K. The main source of background from the beamstop was much reduced by repositioning it inside the can. The radiation shield – Be or Al – was replaced by flexible graphite which gave a much smoother background. Finally, the background scattering from the point of entry of the beam into the cryostat was tackled by the insertion of a 3D-printed magnetically controlled rolling internal collimator with a 2mm pinhole. The end result was a reduction by a factor of 15 of the peak intensity of the background which was also much smoother and therefore easier to correct for. The whole development resulted in a step change in the quality of data that could be collected.

Charlie concluded by looking into the future of cryocrystallography, pointing out that older style CCRs are just not suited to modern facilities or the kind of experiments modern sources make possible. So his ongoing research continues to be involved in appropriate instrumentation developments that can meet current demands.

PCG Prize Lectures

Following Charlie's talk, Alex Gibbs, chair of the PCG, announced the joint winners of the 2020 PCG-SCMPG Physical Crystallography Prize: **Josie Auckett** (Durham University) and **Lucy Clark** (University of Birmingham). The lectures will be given at a meeting later in the year. Alex also announced **Richard Dixey** (Queen Mary University of London) as the winner of the 2020 Malvern Panalytical Thesis Prize. His lecture was scheduled to be given at a special prize seminar on April 26th 2020.

John Finney
UCL

BSG Report

The first BSG session, chaired by **Jane Endicott** (Newcastle University), was based around structure-based drug design and the keynote was given by **Puja Pathuri** (Astex) on the discovery of ASTX029, a novel ERK1/2 inhibitor. ERK2 has two distinct areas to target – the ATPase activity and the phosphorylation site of ERK itself. The phosphorylation was controlled by the position of Tyr36 which could be 'in' (no phosphorylation) or 'out'. The aim of the project was to create an inhibitor that could block both the ATP binding and the phosphorylation. An initial in-house fragment screen coupled with a mini-fragment screen (80 compounds) found several hits in the hinge region. The best was selected and elaborated to improve it. This first derivative acted as a selective ERK kinase inhibitor, but although Tyr36 was 'in' it did not stop phosphorylation. Further growing and refining resulted in ASTX029 which had all the correct attributes and is currently in Phase I/II trials. The next talk was by **Sabrina Mackinnon** (University of Oxford) who told us about their attempts to find an inhibitor for galactokinase 1, an enzyme involved in galactose metabolism, for which there are currently no useful drugs. After testing over 500K compounds without much success they turned to the XChem pipeline at Diamond to try and find some novel chemical space. After a full screen, 27 compounds were found over 3 main sites, most in a novel hydrophobic pocket. The fragments were merged and elaborated and a 100μM compound was created. The compound is not competitive with either substrate and is selective for GALK1 though the method of inhibition is still not understood. The third talk was given by **Filippo Prischi** (University of Essex) on targeting RSK4, which is involved in lung and bladder cancer. RSK proteins phosphorylate many transcription factors that contribute to the immediate-early gene response. After a screen with ~1600 known kinase inhibitors, moxifloxacin was found as a good inhibitor. Attempts to crystallise RSK4 with the compound failed though (either through soaking or co-crystallisation). Bioinformatics indicated that it may be binding at the back of the protein and this was confirmed by deuterium exchange mass spectrometry. The last talk was given by **Stephen Muench** (University of Leeds) who showed several projects where they were using Cryo-EM for drug discovery. Structures for IGPD, cytochrome bc1 and TrpC channels were shown at around 3Å resolution where the small molecule binding sites could be easily seen.

The BSG Plenary Lecture was given by **Gabriel Waksman** (UCL/Birkbeck, University of London) on the Bacterial Type IV Secretion System. This system is used by bacteria to transfer DNA from donor to recipient. It consists of at least 12 components – 3 ATPases, 5 channel-forming and 4 pilus components plus others. His cryo-EM study was able to image the pre-pilus stalk complex to atomic resolution, showing it had a lot of symmetry mismatch in the various subunits. The pilus structure was then solved independently to 3.6Å. This allowed the group to model how the pilus is formed and how the DNA could travel along the pilus.

The second session, chaired by **Briony Yorke** (University of Bradford), was entitled Time Resolved Crystallography. The plenary was given by **Jasper van Thor** (Imperial) on the optical control of structural dynamics by ultrafast time-resolved serial femtosecond crystallography (TR-SFX). Jasper explained that X-ray free electron lasers (XFELs) can be used for ultrafast data collection – femtosecond optical delays can get down to ~100fs, energy-chirped polychromatic X-rays from XFELs can get to ~200 attosecond resolutions. He then showed, using a fluorescent protein as a test case, isomerisation of the fluorophore at 1.3Å resolution and 500fs time resolution. The next talk was from **Elspeth Garman** (University of Oxford) who showed the extensions that are being added to the RADDOSE software tool for XFEL data. She explained the processes that cause radiation damage at synchrotrons, mostly due to Auger electrons. It was thought that for the very small crystals used at XFELs the photoelectrons can escape from the crystal before they cause any damage. However this seems not to be entirely true as radiation damage can still be seen in XFEL datasets. RADDOSE-XFEL is designed to predict when global and specific damage will occur and help to design experiments to avoid it. The second talk was from **Henrike Muller-Werkmeister** (University of Potsdam) who was using TR-SSX to study the enzyme fluoroacetate dehalogenase. He was using the fixed

target chips (25,000 sample funnels) to do 'hit-and-return experiments' (HARE), which allow the data to be collected at many different time delays. The model system used fluoroacetate dehydrogenase to break a C-F bond, after fast photo-decaging of the substrate. The experiment showed that four water molecules act as a wire connecting the two active sites of the dimer in an allosteric manner. The last talk for the session was from **Lauren Hatcher** (Cardiff University) who showed how they were using LED systems to photo-irradiate systems, rather than lasers, as these systems avoided problems of absorption effects, photobleaching, crystal heat load and laser damage. The system under study was a very temperature dependent isomerisation on NO_2 to ONO in ambidentate metal systems.

The third session was entitled Enzymes, and was chaired by **Wyatt Yue** (University of Oxford). **Peter Moody** (University of Leicester) gave the keynote on his research using neutron crystallography to study heme peroxidases. These enzymes use Fe centres to remove peroxides, which are created as by-products of the reduction of water. Peter was interested in what state the Fe centre was in: Fe=O or Fe-OH. This could normally be decided easily with crystallography by looking at the Fe-O bond length; however the act of measurement with X-rays causes redox reactions at the Fe centre which distort the result. Therefore, Peter was using neutrons to probe the metal site as these do not affect it and also have the benefit of showing any hydrogen atoms. Thus he was able to show that Compound I of the system was clearly Fe(IV)=O and Compound II was Fe(IV)-OH, and he could also show how the H gets from the ascorbate substrate to the ferryl centre by hopping through an uncharged Arginine.

The keynote lecture was followed by a talk given by **Mike Hough** (University of Essex) who showed how he used serial crystallography (SSX) to look at a different peroxidase system. The dye-decolourising peroxidases (DyPs) are industrially important enzymes that have a wide substrate specificity: most importantly they can break down lignin and also anthraquinone dyes. Mike was using SSX with the fixed target chips to allow him to capture data sets that ranged from 30kGy to 300kGy. This allowed him to calculate 'zero dose' bond lengths and show that the Fe-O bond length was 2.37Å in the Fe(III) water resting state and 1.65Å in the Fe(IV)=O state. **Stephen Marshall** (University of Manchester) gave the next talk on the UbiD-UbiX decarboxylase system. These enzymes can decarboxylate unsaturated carboxylic acids and may be useful to make feedstocks for natural energy sources. He was able to show that UbiD contains a modified Flavin mononucleotide that is made by the UbiX enzyme and then passed to UbiD, where it is further oxidised to be the active species. The group were able to get many high-resolution structures of the intermediates to study the mechanisms involved. The last talk on the DNA repair enzyme Artemis was given by **Yuliana Yosaatmadja** (University of Oxford). Artemis is a key enzyme in VDJ recombination (a site-specific recombination process) and non-homologous end joining (NHEJ) DNA repair and is part of the metal-β-lactamase family. The aim was to design inhibitors to help characterise and understand its mechanism of action. They managed to get one crystal, which gave the structure and showed a two-domain protein, similar to Apollo, but also that it had a Zn finger that was unique to Artemis. Mutations in the Zn binding residues result in severe combined immunodeficiency type diseases (SCIDs). The group are currently investigating small molecule inhibitors.

The fourth session, chaired by **Matteo Degiacomi** (University of Durham) was based around computational biophysics with the keynote given by **Franca Fraternali** (King's College London) on molecular mechanisms of disease. The aim was to understand the role of proteins in genetic variation. They analysed mis-sense variants in terms of how abundant and stable they were and found that the impact of the mutation was related to its position: interior, surface or interface. They showed that it was possible to calculate a 'variant enrichment score' to see if mutations were indicative of pathogenicity. They also analysed 6000 binary protein complexes from the Protein Data Bank to look at the interface itself or solvent accessible regions; they found they could help predict interfaces that would be targetable by small molecules and applied this to the SARS-Cov2 Ace2 structure. **Antonia May** (University of Edinburgh) then talked about the dynamics of proteins. She showed how proteins can be probed through molecular dynamics that allows testable predictions to be made about how the conformational changes in the protein help it to work. She showed how the molecular dynamics hinted that CypA catalysis was driven by the rotameric state of F113 and confirmed this with NMR and mutational studies. The next talk from **Deborah Harrus** (EMBL-EBI) showed us the new PDBe-KB (knowledge base) that helps to bring together all information that a structural biologist may require in one place. She also introduced a new viewer embedded in PDBe-KB called Molstar which can highlight all this useful information. The last talk by **Matthew Batchelor** (University of Leeds) showed us his work on Hsp72. He was interested in how the phosphorylation of Hsp72 by Nek6 affects its essential functions. The modelling showed that when Hsp72 was phosphorylated, there were new bridging interactions across the two domains of the protein which allow the nucleotide binding domain to talk to the substrate binding domain.

The fifth session on membrane proteins was chaired by **Bonnie Wallace** (Birkbeck, University of London). The keynote from **Amandine Maréchal** (University College London) was on the respiratory supercomplexes. Amandine was specifically interested in complex IV (cytochrome C oxidase) of the respiratory chain. The team worked on the yeast homologues as these were easier to produce and do site directed mutagenesis on. Crystals were obtained, but they didn't diffract, so they turned to cryo-EM, but again could get no better than ~7Å data. The structure was finally cracked when they isolated complex IV in the presence of complex III. These produce a 2:2 supercomplex that EM could resolve to ~3Å. In these maps an extra subunit was discovered and determined to be COX26 by mass spectrometry of the sample. The next talk, from **Altin Sula** (Birkbeck, University of London) was on drug interactions with the voltage-gated sodium channel, NavMs. All sodium channels are drug targets, but there are nine human isoforms – all of which are quite similar. Therefore, high resolution structures are required to guide drug discovery. To do this, they had to work on a prokaryote version (NavMS), which they could solve to 2.4Å. This allowed them to understand the mode of action of Cannabidiol (it enters through the fenestration site) and Tamoxifen (which enters through the intercellular gate region). The second talk by **Jannik Strauss** (University of Leeds) was on the membrane-bound pyrophosphatase (M-PPase) which is important for virulence and survival in pathogens. Using TR-SSX he was able to show that the two sites of the dimer were allosterically connected, so that only one channel at a time was occupied by Na^+. The last talk in this session was given by **Stephen Harborne** (Peak Proteins). The company specialises in producing membrane proteins and he introduced his program IMPROVER, that aims to make point mutants that stabilise the protein in a less

time-consuming method than alanine scanning. It uses structure-based models, deep sequencing and other bioinformatic tools to do this.

The final session on protein-protein interactions was chaired by **Richard Bayliss** (University of Leeds). The keynote was given by **Elton Zeqiraj** (also University of Leeds) on ubiquitin signalling complexes, in particular the BRCC36 DUB (part of the BRISC complex), which regulates inflammation. He could crystallise the inactive BRCC36 dimer, a highly active 2:2:2:2 complex of BRCC36, KIAA0157, BRCC45 and MERIT40, but could only get diffraction to ~6Å. Adding a further component (SHMT2) allowed the complex to be solved to 3.8Å by cryo-EM. This model was validated by site-directed mutants in the protein interfaces. The next talk by **Charlotte Scarff** (University of Leeds) was on the shutdown state of Myosin-2. For proper function, myosin has to be able to be turned on and off. In the turned-off state one of the heads is blocked and part of the tail covers it. Studying the structure by cryo-EM to 3.6Å showed that this shutdown state was stabilised by a latch mechanism that holds the tail in place. Using MD simulations they could show that phosphorylation of these latch residues would disrupt the latch and release the lockdown state. The next talk from **Martin Rennie** (University of Glasgow) was on the ubiquitation of the FANC1/FANCD2 complex. Cryo-EM was able to show that when the complex is ubiquitinated it encloses the DNA substrate via a clamping mechanism. To release the DNA, the ubiquitin has to be removed by a specific de-ubiquitinase (USP1). The last talk of the conference was given by **Selena Burgess** (University of Leeds) on using antibodies to inhibit kinases, specifically Aurora-A. It has proved difficult to generate specific inhibitors to Aurora-A as Aurora-B is 70% identical. It was known that Aurora-A was activated by small interacting partners, so was it possible to find others that would inhibit the protein? They turned to small, single domain antibodies (vNAR-D01 and Nb-1E04) that can bind to Aurora-A specifically and inactivate it, either by binding to the back of the hinge or by stopping the activation loop from ordering.

Mark Roe
University of Sussex

PCG Report

PCG Plenary

This year's PCG Plenary Lecture was delivered by **Václav Petříček** (Czech Academy of Sciences) and was entitled 'The Role of Crystal Structure Analysis in Investigation of Crystals with Important Physical Properties'. Václav is well known to many in the PCG community as the author of the Jana Rietveld refinement software, a program that, as session chair **Anthony Phillips** (Queen Mary University of London) put it, is well known for doing complicated things!

Václav's talk was a journey into the theory underpinning some of these 'complicated things', including an in depth discussion of different types of crystal twinning and the impact they have on structural analysis. It's possible that analysing a twinned diffraction pattern without knowing it will lead you to assign an incorrect translational symmetry to your structure – we now consider ourselves warned! The speaker went on to talk about modulated structures: the appearance of additional diffraction spots (or 'satellites') was first observed nearly 100 years ago but was long considered merely a curiosity. Its practical importance is now known, however, with many organic conductors and high-T_C superconductors having modulated structures. Václav touched upon superspace theory and the importance of charge flipping methods for the solution of modulated structures, before finishing with an overview of magnetic structures, including the impressive (if terrifying) statistic that there are more than 1000 Shubnikov groups used to describe magnetic structures.

The talk concluded with the message that besides all the fantastically clever software tricks we have available as crystallographers, the importance of "crystallographic intuition" and the ability to look a bit more closely when something just doesn't seem quite right, should not be underestimated.

Helen Playford
ISIS

Entropy and Structure

Chair and speakers in the Entropy and Structure session. Clockwise from far left: ***Anthony Phillips*** *(Chair),* ***Xavier Moya*** *(Speaker),* ***Jonathan Skelton*** *(Speaker),* ***Mario Falsaperna*** *(Speaker) and* ***Guanqun Cai*** *(Speaker)*

Increasingly, we are becoming aware of the importance of entropy not only with respect to relationships with physical properties and structural stability, but utilising it as a design concept in a host of different chemical and materials systems. This session, chaired by **Anthony Phillips** (Queen Mary University of London) was designed to look at entropy and its relation to structure in all aspects.

The plenary, delivered by **Xavier Moya** (University of Cambridge), provided an excellent introduction to caloric materials, ranging from magnetocaloric to elastocaloric materials, and the principles behind their functionality, including the relationship with entropy. Dr Moya went on to discuss in greater detail materials capable of demonstrating barocaloric effects, ranging from inorganic salts to organic materials. One of the barocaloric materials referenced in his talk, ammonium sulphate, was subsequently picked up in the second talk by **Guanqun Cai** (Queen Mary University of London) who discussed the origin of the high entropy of the material and the link to local structure. Using RMC modelling of neutron data, a higher level of tetrahedral distortion at higher temperature and dipole orientation disorder was noted that could be the origin of high entropy change exhibited by this material.

Mario Falsaperna (University of Kent) then proceeded to explore magnetocaloric materials. Introducing the concept of magnetic frustration in lattices, he explored the structure of and properties of materials in the family of $Ln(HCO_2)(C_2O_4)$ metal organic frameworks using a combination of techniques, including single crystal work, X-ray powder diffraction and magnetic susceptibility measurements. The work highlighted that the Gd(HCO2)(C2O4) material, in particular, demonstrated very promising magnetocaloric properties. Finally, **Jonathan Skelton** (University of Manchester) described a theoretical

approach to the prediction of the structural dynamics in a material. Using several different case example systems, he demonstrated how important the inclusion of entropy (particularly the vibrational entropy) in theoretical calculations is to accurately describe structural phase transitions and phase diagram prediction in many different chemical systems. The session concluded with a lively question and answer discussion with all of the speakers.

Finally, one of the IUCr poster prizes was won by a poster on the subject matter of this session, namely by **Thomas Hitchings** (University of Kent) on 'LnOHCO3 Magnetocaloric Frameworks: A Potential Sustainable Replacement for Liquid Helium Vapour Compression'.

Lewis Owen
University of Cambridge

<3D: Structure and Properties of Low-dimensional Materials

The second day of the Spring Meeting commenced with four parallel sessions highlighting the diversity of topics across the different fields of crystallography. Within the PCG, a session rich with a variety of topics, falling under the broad concept of low-dimensional materials and chaired by **Lucy Clark** (University of Birmingham), began with a plenary lecture from **Maria Grazia Francesconi** (University of Hull). In her insightful talk, Grazia introduced the concept of low dimensionality in the solid state, while focusing on ternary mixed metal non-oxide compounds, in which chemical bonding or interactions are effectively confined within one or two dimensions. Through a variety of innovative synthetic procedures, and a combination of diffraction and physical property measurements, Grazia illustrated the concept of anion-driven synthesis of new compounds. Furthermore, she gave an excellent illustration of successful anion-driven manipulation of the effective dimensionality of multiple materials, opening the door to new routes towards achieving designer structures.

Next, **Simon Cassidy** (University of Oxford) followed with a fascinating talk in which he introduced his multidisciplinary research group's work that mainly focuses on the structural determination of layered functional materials. By using a combination of *ab initio* techniques and neutron diffraction measurements, Simon was able to portray the difficulties pertaining to a successful meticulous structural-property relation determination. While the talk was mainly focused on the crystallography of the presented iron selenide intercalated materials, Simon gently explained the constraints and methods necessary through which one could carry out such analysis.

The following talk, given by **Aly Abdeldaim** (University of Birmingham), then switched the focus towards the low-temperature magnetic properties of low-dimensional materials and their intriguing phenomena. Aly began his talk by summarizing the design aspects necessary for the emergence of non-trivial magnetic ground states. Using as an example a coordination framework material, the interdisciplinary characterization methods – including diffraction, thermodynamic measurements, and *ab initio* techniques – that are necessary for an accurate determination of the ground state, were elucidated.

Finally, **Arianna Minelli** (University of Oxford) gave an exciting talk in which she highlighted the methods through which one might better understand the lattice dynamics of tungsten bronzes. For this purpose, Arianna successfully identified the theoretical framework through which the dynamical response of such systems can be understood by using a combination of diffuse and inelastic X-ray scattering techniques. The resulting conclusion, in which an interplay of the structural framework instability and electron-phonon-related instability generates this dynamical response, created an interesting discussion for the Q&A session.

Aly Abdeldaim
University of Birmingham

Structure Solution from Powders (joint with CCG)

The keynote speaker for this joint session was **Ken Shankland** (University of Reading) who wowed the audience with a talk about recent developments in the DASH program. The program had its first release back in April 2001 (when the BCA Spring Meeting was held, coincidentally, at the University of Reading) and found itself rather popular, benefiting from an efficient simulated annealing algorithm at its heart. Ken told us that this algorithm has hardly changed in the 20 years since its release, and yet the demands placed on it have increased massively, with structures getting larger and more complex. The process of optimising the algorithm involved a library of over 100 datasets and over 31,000 CPU hours, and it resulted in some new, rather different simulated annealing. The new values seemed counter-intuitive based on Ken's experience using the method, but in a head to head race the new version came out on top producing better results more quickly than the old! Ken's talk finished with a glimpse of the future – a new structure determination program aptly named GALLOP that can utilise the benefits of GPU processing. One impressive example was the molecule selexipag, which required 2 CPU *years* in DASH, and was solved in 41 minutes on a single GPU using GALLOP.

The next speaker was **Tony Bell** (Sheffield Hallam University) who described a series of detailed diffraction experiments which explored the high temperature phase transition in leucite analogues. The sheer number of structure types and analogues to explore in this family was impressive, and the talk finished with a bonus cat picture which I'm certain was appreciated by the audience! After Tony came **Chris Smalley** (Cardiff) whose talk focused on expanding the scope of structure determination, particularly in cases where things like impurities or preferred orientation make getting accurate intensities more challenging. Giving the example of β L-tyrosine, Chris showed that direct methods applied to electron diffraction could provide independent determination of the unit cell, and that NMR and DFT methods were able to validate the structure and explore its position amongst the landscape of predicted polymorphs. The final speaker in the session was **Tom Roseveare** (University of Sheffield) who talked about exploring the structures of small molecule solvates, in particular what happens when the solvent is removed. Tom presented some beautiful crystal structures with differences in their solvated structure and porosity after solvent removal.

Helen Playford
ISIS

>3D: Structure and Properties of Higher-dimensional Materials

*Chair and speakers in the Structure and Properties of Higher-dimensional Materials session. Clockwise from far left: **Phil Lightfoot** (Chair), **Fabio Orlandi** (Speaker), **John Claridge** (Speaker), **Kirsten Christensen** (Speaker) and **Chris Howard** (Speaker)*

The session on >3D structures was chaired by **Phil Lightfoot** (University of St Andrews) and featured all kinds of structures that don't fit into normal three-dimensional space; a journey into superspace was conducted.

Fabio Orlandi (ISIS) delivered the keynote talk on how to use superspace to characterise and investigate materials properties. His work on Type II multiferroics such as $TbMnO_3$ and $Gd_{0.5}Dy_{0.5}MnO_3$ showed how the mathematical formalism of superspace and the derived symmetry can be used to constrain material properties, i.e. analyse why polarisation is forbidden. He concluded his presentation with the electric dipole for helical magnetism found in Cu-doped $BiMn_7O_{12}$, where the doping allows the system to show this new exotic phase.

Kirsten Christensen (University of Oxford) took the audience through a broad range of samples that come through Oxford's Crystallography service. Quite often satellites and superstructures are observed, telling us there is more to the structure than we initially thought. We should not only pay attention to the high symmetry planes in the data reconstruction, but also the higher layers that will allow you to spot these features in the future! The aim of the talk was to eradicate the fear of modulated structures and to show that important information can be hidden in superspace.

A long journey with tungsten bronzes was presented by **Chris Howard** (Newcastle University, Australia), where he took the audience though the scientific process to algebraically understand the tilt modes in $Sr_3TiNb_4O_{15}$. The presentation nicely illustrated the value of networking at different conferences around the world and how this networking fosters and drives new discoveries, reminding us how important in-person meetings are to create collaborations. His journey started in 2014 when he was presenting the method he used on $SrZrO_3$ and they realized that a similar approach could be applied to structures like tungsten bronzes. Not only we can identify the tilt modes in the tungsten bronzes as they can be found in many minerals: we also have a general algebraic approach that can be used for cooperative rotations in networks of interconnected rigid units.

The session was concluded by **John Claridge** (University of Liverpool) and rounded the journey back to superspace with a nice introduction to aperiodic crystals and his thoughts on the definition of quasicrystals. Looking at $Ba_{10}Y_6Ti_4O_{27}$ presented a great challenge as not a single site in the average unit cell is fully occupied, but all can be described as modulated by crenel functions. The conclusion is: 'Doing it in superspace is worth the extra effort for the better $\chi 2$'.

At the end of the discussion a comment from Mike Glazer roused attention: the definition of a crystal in the IUCr dictionary is updated to include a real space description.

Arianna Minelli and **Ella Schmidt**
University of Oxford

Phase Transitions

This session was headed by **Joe Hriljac** (Diamond Light Source) whose talk explored the phase transition behaviour of the zeolites natrolite and clinoptilolite. The first section of the talk described some experiments carried out on natrolite in a diamond anvil cell (DAC) which revealed that the volume of the structure initially increases with pressure, something which seemed rather counter-intuitive until he was able to determine that it was due to the incorporation of water from the pressure transmitting medium into the structure! Joe then moved on to discuss ion exchange in clinoptilolite, which is of relevance to nuclear waste clean-up (and is in fact currently in use at Sellafield). *In situ* flow-cell apparatus was used to follow the structure of the zeolite during exchange of sodium for caesium and showed some preference for the caesium to enter the smaller of the two pore systems initially, followed by equilibration over a long time scale.

Joe was followed by **Julia Parker** (also Diamond Light Source) who introduced us to the hard X-ray nanoprobe beamline I14. This beamline is 185m long and boasts an impressively tiny 50 x 50 nm beam which can be used for a multitude of techniques including X-ray fluorescence, absorption spectroscopy, diffraction and imaging. Julia gave fascinating examples including compositional analysis of a section of meteorite and locating caesium in soil from close to the Fukushima nuclear power plant. The talk finished with the exciting news of the ongoing development of an *in situ* cell for use to assess the nanoscale structure and composition of, for example, battery materials. Next in the session was **Gwilherm Nénert** (Malvern Panalytical) whose talk about the polymorphism of $NaSrPO_4$ was an impressive example of a detailed XRD study of a challenging material (as the speaker pointed out, Na^+, $P5^+$ and O^{2-} all have the same X-ray form factor at q=0!) and revealed five new polymorphs with intriguing and complex structures. Finally in this session was **Toms Rekis** (University of Bayreuth) who demonstrated an application of superspace theory to aid the understanding of a high Z' polymorph of an amino acid compound Gly – L – Val. Superspace theory allowed the structure of the room temperature phase (Z'=7) to be understood in the context of the high temperature phase (Z'=1) using a commensurate modulated structure whose basic cell has excellent agreement with that high temperature phase.

Biominerals & Biomaterials (joint with BACG)

This session benefited from the digital platform allowing **Julia Parker** (Diamond Light Source) to chair this session while speaking in another parallel session!

The keynote lecture was given by **Melinda Duer** (University of Cambridge) and dived straight in to the immense challenge of developing an accurate and useful structural model for bone. Existing models consisting of carbonate-substituted hydroxyapatite are too simple to explain certain observations, for example the changes in bone properties with age. Melinda's work combines powder X-ray diffraction with NMR

'crystallography' to explore a new model candidate – octacalcium phosphate. In this fascinating lecture we learned about the importance of the inclusion of 'metabolic acids' like citrate and lactate in bone structure, and that an excellent model of bone can be formed by combining fingers of apatite-like material with hydrated octacalcium phosphate layers and highly disordered regions between the layers of fingers. The citrate and lactate inclusion provides flexibility and enhanced mechanical properties, and changes with age can be understood as changes in the incorporation of these metabolites. Melinda went on to talk about trying to understand how collagen fibres interface with the mineral crystals – this was a lengthy process that, among other things, involved feeding a mouse an isotopically enriched diet to allow for ^{13}C NMR to be carried out! Eventually the team discovered that the molecule poly(ADP ribose) bound to the collagen chains was responsible for controlling the nucleation and calcification of the mineral matrix. This was, according to Melinda, a "huge and wild surprise", but nevertheless evidence for it has been found in foetal bone growth plates.

The next speaker was **Emily Arnold** (Cranfield University) whose talk discussed hydroxyapatites in the context of carbonate impurities and their possible use as a biomarker for osteoporosis. Emily's work involved an array of biogenic and synthetic samples studied using X-ray pair distribution function analysis. She was able to find relationships between carbonate concentration and various structural parameters, suggesting that this technique is viable for the study of carbonate in hydroxyapatite. After Emily was **Jessica Walker** (Diamond Light Source) who talked about the use of a hard X-ray nanoprobe to study a mineral called celestite (strontium sulphate) produced by single-celled marine organisms called *Acantharia*. These tiny creatures produce sharp celestite 'spicules' which Jessica's work found had a barium-rich core and the inclusion of organic sulphur. Through these kinds of observations, it is hoped that an understanding of the way such biominerals are generated can be developed. The final speaker was **Alexander Korsunsky** (University of Oxford) whose studies on acid erosion of tooth enamel hope to provide means to strengthen teeth against decay. He showed that the structure of enamel, while consisting of 96% hydroxyapatite, is complex and hierarchical, with different elements of the structure having differing tolerance to acid erosion.

Helen Playford
ISIS

Industrial Group Report

This year the Industrial Group Plenary was given by **Marcus Neumann** (Avant Garde Materials Simulation) using Crystal Structure Prediction (CSP) to detect and avoid disappearing polymorph cases. Marcus's presentation showcased the advances of CSP methods and their wider applicability in drug development. He gave a quick overview of CSP theory and energy evaluation methods, before then covering three CSP applications: (i) phase transition as a function of temperature prediction, (ii) anhydrates and hydrates prediction as a function of relative humidity and temperature and (iii) high-throughput comparison of predicted structures with experimental powder diffraction patterns. Marcus finished up an exciting and engaging talk with the use of CSP solid form landscaping to inform crystallisation design and avoid disappearing polymorphs.

This year the Industrial Group organised two sessions at the meeting.

The first was a joint session with the BACG on Crystal Growth, Pitfalls and Challenges in Industrial Crystallisation. This was a popular session, with many audience questions. In this session we heard about crystallisation of agrochemicals from our keynote speaker **Adam Keates** from Syngenta. He was followed by **Anuradha Pallipurath** (University of Leeds) who talked about rational design and crystallisation control using X-ray PDF analysis. Next **Simon Coles** from the University of Southampton illustrated the development of the capability of the crystal sponge method and the last speaker of this session, **Michael Probert** (Newcastle University), presented the ENaCat Protocol and its applicability to small molecule crystallisation.

The second IG session was joint with the CCG and was on the topic of the Control and Prediction of Crystals, again another popular session with contributions from both industry and academia. The keynote was given by **Sten Nilsson-Lill** (AstraZeneca) telling us how computational techniques are used in AstraZeneca to inform about polymorphism risk during drug development. This was followed by **Graeme Day** (University of Southampton) who spoke about the importance of investigating high energy crystal structures in crystal structure prediction experiments. Next, **Mollie Trueman** (University of Manchester) described the CrystalGrower software, and how it can be applied to help us understand and control our crystal growth. Finally, **Cameron Brown** (University of Strathclyde) spoke about kinetic crystallisation and using a data mining approach to inform models for crystallisation processes.

This year's Industrial Group poster prize went to **Simon Coles** and colleagues (University of Southampton), who presented a fantastic poster on developing the capability of the Crystal Sponge method. The poster was selected for the IG prize due to the direct applicability of the research to industry.

BCA Industrial Group

CCG Report

CCG Plenary Lecture

This year's CCG Plenary lecture was given by **Franziska Emmerling** (Federal Institute for Materials Research and Testing, Germany), with the title 'Shaken Not Stirred: Enhancing the Flavour of Mechanochemistry'. Franziska gave a wonderful overview of the benefits and practicalities of mechanochemistry, illustrated by diverse examples from co-crystals, co-ordination polymers, metal-organic frameworks and even organic synthesis. She discussed how a range of *in situ* measurements have been developed to study mechanochemistry, as well as future challenges to understanding the molecular-level processes at work. The presentation prompted a fascinating discussion of *in situ* and *ex situ* methods and mechanisms with a wide variety of questions from several audience members. Clearly, mechanochemistry will continue to shake up the world of synthesis for years to come!

Hamish Yeung
University of Birmingham

Advances in Software for Crystallography

The CCG Advances in Software for Crystallography session took place on the first morning of the joint BCA-BACG Virtual

Spring Meeting. The aim of this session was to highlight the new methods being used in the community to address the latest chemical crystallography challenges.

The session opened with a keynote from **Florian Kleemiss** from the University of Regensburg with his talk entitled 'NoSpherA2: Non-Spherical Atom Refinements in Olex2 for General Application'. The talk described the NoSpherA2 method which implements non-spherical atoms, obtained from a Hirshfeld Stockholder partitioning of calculated electron density, in crystallographic refinement. Florian showed how an exciting feature of this method is the possibility to include atomic charge effects on the atomic scattering factor which has significant consequences for the modelling of hydrogen atoms in X-H covalent bonds.

The keynote was followed by a complementary talk from **Alexander Nazarenko** (SUNY College, Buffalo USA) entitled 'Seventy Years of Interatomic Scattering Study: Some notes from a user' including alternative methods to include models beyond the spherical atom in crystal structure refinements.

The session then switched gears to highlighting computational efforts in the area of electron diffraction. **Ella Schmidt** (University of Oxford) gave an excellent talk on '3D-ΔPDF from Electron Diffraction Data' describing a method to pull out the diffuse scattering from the intense electron diffraction Bragg peaks using an intensity 'punch, fill and interpolate' approach. This allows the complete diffuse scattering volume to be obtained which is then used to generate the 3D-ΔPDF in which the local order of atoms can be determined.

The final talk of the session was given by **Natalie Johnson** (CCDC) entitled 'Electron Diffraction Data in the CSD'. Natalie focused on the electron diffraction entries stored and maintained in the Cambridge Structural Database and explored ways to enrich the information of future entries.

The session was followed with a Q&A including some really great discussion points from the audience. It was a brilliant session to be involved in, covering both developing methods and techniques as well as ways in which reporting infrastructure is responding in order to keep up to date.

Lucy Saunders
Diamond Light Source

Electron Crystallography

Electron diffraction is one of the mostly rapidly developing and exciting areas of crystallography, generating enormous interest in the chemical crystallography community. The keynote lecture, 'Structure Refinement from 3D Electron Diffraction: Where are the Limits?', was delivered by **Lukáš Palatinus** (Czech Academy of Sciences, Prague). Interest in electron diffraction stems from the ability to collect single-crystal diffraction data using crystals with dimensions of tens of nanometres. Challenges, including instrument stability, radiation damage and treatment of dynamical effects, can now be addressed as the result of intense research in the field since Kolb's original work in 2007. A bewildering diversity of names for different techniques has developed, with the term '3-Dimensional Crystallography' or 3DED now recommended (Gemmi *et al. ACS Cent. Sci.* 2019, **5**, 1315–1329). To the end of 2020, 350 electron diffraction structures have been published, with data collection via the continuous rotation method gaining in popularity in recent years. Data can be treated in a variety of ways. One approach is to collect electron diffraction data to identify the unit cell and solve the structure, but to refine against X-ray powder data to avoid difficulties associated with dynamical scattering. A second approach involves refining the structure using a kinematical model; this yields low-accuracy structures with high figures of merit (R-factors of 20-30% are usual), which may nevertheless be fit for purpose. The most accurate models come from dynamical refinements. These are computationally more intensive than kinematical refinements and sensitive to data quality, but they have very recently been implemented in Jana2020 for data sets collected with the popular rotation method. Typical R-factors for dynamical refinements are 8-10%, but this figure should reduce with inclusion of inelastic scattering effects. Lukáš illustrated progress with crystal structures of CO_2-loaded chabazite and H-atom location in organic crystal structures, noting that bond distances involving H are typically slightly longer than determined by neutron diffraction. The last part of the lecture addressed limits, particularly the problem of beam damage in the determination of large structures. Fast data collection, more sensitive detectors and serial crystallography techniques should help address the problem. The prospects for electron diffraction stretch from structure determination to experimental charge density analysis, with the recent development of specialised electron diffractometers expected to help popularise the technique.

As crystals used for data collection become ever smaller, **Andy Stewart** (University of Limerick) addressed the question of at what point a particle becomes a crystal in his lecture 'Elucidating the Boundary between a Particle and a Nanocrystal in the Context of 3-dimensional Electron Crystallography'. Simulations were carried out using the structure of cubic $SrTiO_3$ as a model, in which scattering from crystallites consisting of $n \times n \times n$ blocks of unit cells was calculated with n starting at 2. The calculations took dynamical scattering into account by propagating scattering of the electron beam layer by layer in the models, with crystallinity being assessed by the 'essential sharpness' of the calculated diffraction pattern, a criterion based on the IUCr's (2014) definition of a crystal. Diffraction from a block of 2^3 unit cells was continuous, exhibiting fringes but no Bragg peaks. Bragg scattering began to emerge at only 4^3 unit cells, beginning to dominate over diffuse scattering at 7^3 unit cells, with the contribution levelling off at 18^3 unit cells. Andy concluded that a particle transforms into a crystal at between 7 and 18 unit cells in each dimension. Extensions of the theory, taking into account the effects of surface relaxation and beam damage, are expected to show an increase the number of cells corresponding to the crystal transition.

Fabio Nudelman (University of Edinburgh) discussed applications of electron diffraction in the study of biomineralisation in his lecture 'Solid-state Transformation and Polymorphism in Calcium Carbonate Crystallisation'. Calcite and aragonite are polymorphs of calcium carbonate which are found in the shells of organisms including coccolithophore algae, molluscs, sea urchins and corals. Corals initially form their shells in a structure consisting of amorphous $CaCO_3$, which then transforms to crystalline aragonite but without a change in morphology, implying that the transition is a solid state rearrangement. Crystallisation of $CaCO_3$ from water, with samples studied with SEM, showed initial formation of amorphous particles after one minute. The particles began to aggregate and grow by particle attachment into needle-like structures, developing into crystals with a granular morphology after 20 minutes, the sample consisting of needles of crystalline aragonite after one hour. The same process was studied by TEM, arresting crystallisation by plunging into ethane. The results paralleled those of the SEM study, with needle-like amorphous structures developing after

10 minutes. After one hour a needle-like structure exhibiting Bragg diffraction was observed. Dark field imaging, which enables a diffraction spot to be located and then the regions of the crystallite contributing to the spot to be imaged, showed that most of the crystallite was still amorphous at this stage, but with co-aligned crystalline regions of aragonite embedded within it. After being allowed to mature, the whole needle consisted of crystalline aragonite.

The final talk in the session was delivered by **Gustavo Santiso-Quiñones** (ELDICO Scientific AG) and entitled '3D-Electron Diffraction Continuous Rotation Method in Nanocrystallography: A Dedicated Device for Structural Elucidation of Nanocrystalline Particles'. Since 2007 there has been a resurgence of interest in electron diffraction. The ability to examine very small samples offers the promise of circumventing one of the great bottlenecks in structural chemistry: the need to grow large 'X-ray quality' crystals. Two papers, which appeared in 2018, highlighted the potential of electron diffraction to chemists, and led to nomination of the developments in the Science Breakthroughs of the Year listing. The field continues to develop rapidly, not only for structure determination, but also in applications such as pair distribution function analysis. Gustavo went on to emphasise the need, also highlighted in the first talk, for specialised electron diffraction instrumentation. At present, transmission electron microscopes need some adaptation for diffraction work, often at the detector or to stabilise the sample rotation axis. They also require expert technical support. Gustavo proceeded to describe an instrument which has been developed by Eldico designed to fulfil the need for dedicated diffraction instrumentation, with, for example a more stable sample rotation axis than is available on other instruments. The instrument has been developed with crystallography in mind and is interfaced with software for crystallographic data processing. The talk ended with the first, very recently collected, images and diffraction patterns obtained using the new instrument.

The organisers would like to thank Eldico for support of this session in the form of student bursaries and speaker support.

Simon Parsons
University of Edinburgh

Chemistry at Extreme Conditions

The CCG session on Chemistry at Extreme Conditions focussed on how crystallography can give insight into chemical processes that occur away from ambient conditions. The keynote lecture was given by **Colin Pulham** (University of Edinburgh), with the title 'Putting the Squeeze on Molecular Materials'. Colin showed how crystallographic studies at high pressure using X-rays and neutrons have revealed new phase behaviour in energetic materials and alkane mixtures – very useful information for new explosives and potential separation applications, but with caution advised!

Three fantastic back-to-back presentations followed from **Jake Musselle-Sexton** (Newcastle University), **Hanna Bostroem** (Max Planck Institute for Solid State Research, Germany) and **Lucy Saunders** (Diamond Light Source). Jake described an elegant synthetic strategy with which he had created a library of compounds to investigate temperature-induced spin crossover in iron II abpt analogues (abpt = 4-amino-3,5-di-2-pyridyl-4H-1,2,4-triazole). Hanna showed how Prussian Blue analogues undergo interesting and unusual phase transitions under high pressure that depend on defects, hydration and composition, of interest to Na-ion batteries and ferroelectric applications. Lucy described a new experimental cell that enables full structure determination under electric fields at Diamond beamline I19, and some interesting field-induced colour changes in the proton transfer material 4,4'-bipyridinium hydrogen squarate. The subsequent discussion around the audience's questions was lively and altogether showed that there is significant interest in extreme conditions crystallography in a wide variety of chemical contexts.

Structure Solution from Powders (joint with PCG)

As preludes to conference symposia go, this one was definitely the most unusual. A group Zoom call with the speakers and co-chair **Karen Johnston** (University of Durham), plus technical support from Hg3, shortly before the start of the session was used to check all microphones were working and to remind us of the format of the session. Then, a countdown just before 10 o'clock and Karen and I went 'live', side by side in Two Ronnies style, on the screens of everyone who had connected to the Structure Solution from Powders PCG/CCG session. Following our introduction, the simple session format consisted of four pre-recorded talks with all questions kept until the end of the fourth talk when they were discussed on a live video call. This worked really well for all concerned particularly as it allowed the speakers to prepare answers to the questions in advance.

Our keynote speaker was **Kenneth Shankland** (University of Reading) who spoke on major advances in structure solution methods in powder diffraction. In particular, large and complex structures can be handled by combining information from other methods (e.g. the Cambridge Structural Database) and possibly crystal structure prediction to set up a tunable, iterative algorithm to give the solution methods a helping hand. The success of this method, running on high performance computers, provides structure solutions in a matter of hours on large, flexible organic molecules which would have been unthinkable in 2003 when I first attended a powder diffraction solution session at the Spring Meeting in York, echoed by **Phil Lightfoot** (University of St Andrews) who commented "things have come on a lot!".

The next speaker was **Tony Bell** (Sheffield Hallam University) who spoke on a rather personal tale of chasing phase transitions in a variety of synthetic leucite analogues. The goal is to synthesise analogues which contain caesium rather than potassium such that the methods can be used to extract and safely store radioactive caesium and prevent pollution. Some of the transitions measured occur at very high temperatures and a full study of the effect of temperature on different materials can only be achieved by combining measurements made in home labs and at synchrotrons.

Following on was **Chris Smalley** (Cardiff University) who again touched on the importance of combining different methods to tackle the solution of structures from problem powders. He gave the example of using electron diffraction and X-ray powder diffraction together in the case of L-tyrosine where impurities in the powder pattern made indexing almost impossible. Other examples included the use of, for example, DFT in conjunction with powder diffraction to eliminate particular polymorph possibilities from consideration because they were deemed to be unstable, less stable or highly unlikely to form experimentally.

Our final speaker was **Tom Roseveare** (University of Sheffield) who spoke on applying powder diffraction to a range of

halogen-bonded solvated systems. Here, the systems provide a porous framework where the pores were filled with solvent, prepared by liquid-assisted grinding. Variable temperature X-ray powder diffractions, using a capillary setup with a modified Cryostream, were used to monitor changes as the compounds were systematically desolvated in a controlled way and ultimately identify those materials suitable for further gas sorption studies.

Gary S. Nichol
University of Edinburgh

Hot structures session

The hot structures session was chaired by **Charlie McMonagle** (ESRF/SNBL) and looked to take a deep dive into the world between the Bragg reflections and how the analysis of incommensurate diffraction and diffuse scattering can enhance our understanding of complex structures. Here, the most was made of this year's Spring Meeting taking place online with contributions from across Europe.

The session was opened by **Sven Lidin** (Lund University, Sweden) on incommensurate intermetallics. Sven introduced several examples of incommensurate structures of intermetallics along with some of the techniques employed to make sense of their structures, including, in the case of $LaRu_x$, indexing these complex diffraction patterns by hand. The final example of ht-Sn_3Sb_2 in this tour de force showed how a full range of tools is needed for these complex structures. *In situ* synthesis, coupled with measurements at the synchrotron where the energy was tuned for extra contrast between the Sn and Sb alongside developments in software, revealed a remarkably complex solution of a 7x7x7 super structure of 7x7x7 NaCl-type cubes terminated by Sn layers.

Arkadiy Simonov (ETH Zürich) moved the session from incommensurate patterns into the realm of diffuse scattering. Arkadiy presented the remarkable chemical control of local structure in the Prussian Blue analogue Mn[Co(CN)6]0.67*xH2O. A large number of environmental variables were shown to affect the local structure during crystallisation, and particularly thought provoking was how the depth of crystallisation in a gel matrix changes the level of disorder present.

Following on, **Emily Meekel** (University of Oxford) introduced correlated orientation disorder in MOFs. Changing from a tricarboxylate linker in the highly symmetric ZnO4(BTC) to a dicarboxylate linker to give ZnO4(1,3-BDC) forced local disorder that can be seen through the diffuse scattering. A model describing the local structure was derived from Monte Carlo simulations with the simulated diffraction patterns comparing favourably with experimentally collected patterns. Finally, control of the local structure was teased through the inclusion of iodine as a guest in the pores directing and blocking local distortions. This project is definitely one to follow and I look forward to hearing more from Emily in the future.

The final speaker of the session was **Stefano Canossa** (University of Antwerp) presenting on correlated disorder in MOFs and in particular correlated disorder in ZIF-90. Stefano found that while ZIF-90 is an extensively studied system, there is compelling evidence that the structural determination in the literature is deficient. Rather than a high symmetry I-43 structure reported, the presence of diffuse scattering due to correlated disorder of the unsymmetric imidazole-2-carboxaldehyde linker points to a merohedrally twined I23 structure. Monte Carlo simulations and simulated diffraction patterns showed the length scale on which these gradual distortions take place. This is not only an important observation for ZIF-90 but also for many other similar systems that could well have unrecognised local disorder that would enhance our understating of these materials.

This fascinating session shows us that we should not just ignore everything in between the Bragg reflections and highlights the importance of looking carefully at diffraction images. Through careful experimentation and data analysis, complex crystallographic problems like these can be solved, and with recent advances in software and documentation, working on incommensurate structures and 3D-ΔPDF is more accessible than ever. Thank you to all the speakers of this session and thank you to the audience for the participating in the lively discussion that followed.

Charlie McMonagle
ESRF/SNBL

BACG Sessions

In situ Monitoring of Crystallisation

The keynote talk by **Zoltan Nagy** (Purdue and Loughborough Universities) discussed 'Process Analytical Tools for Monitoring Design and Model-free Control of Crystallisation Systems'. He addressed a range of procedures including monitoring crystallisation through sensor integration, in-line monitoring of crystal purity, controlling polymorphs through semi-batch supersaturation control, batch to continuous process development and process intensification via online image analysis. Zoltan's talk was followed by **Gunjan Das** (University of Leeds and Diamond Light Source) who discussed 'Time Resolved X-Ray Phase Contrast Imaging of Continuous Antisolvent Crystallisation', and why this was a useful technique and the challenges it posed. **Nathan De Bruyn**'s (University of Manchester) presentation was an impressive pre-prepared video showing the power of ultra high speed *in situ* atomic force microscopy in following the crystal growth of paracetamol. He could observe directly and in real time phenomena that had never before been seen. Examples included concentration fluctuations showing both dissolution and growth, high index faceting as well as dissolution pinning of growth ledges. Other features observed included the shape of the dissolution (concave) and growth (convex) spirals and the development of a Frank-Read source. He concluded that we are now able to see and take measurements on complex phenomena that hadn't been previously possible. The final talk by **Qi Li** (University of Cambridge) explored the use of terahertz time domain spectroscopy to observe the whole crystallisation process. Using the example of magnesium sulphate solutions, she showed how the technique can investigate the behaviour of both the crystal and the solvent, and can provide information even before crystallisation occurs.

Crystal Growth – Theory to Practice

Karen Robertson (University of Nottingham) gave the keynote talk on using flow technologies to control and understand crystallisation. She looked at the different kinds of mixing control, encrustation mitigation and *in situ* crystal monitoring in relation to controlling different kinds of crystalline products, including crystal size and shape and uncovering polymorphic transitions of pharmaceutical compounds. She concluded her

talk by asking for systems to test out the system being developed that enables crystal structure analysis in flow using simultaneous Raman and XRD. In the second talk, **Caroline Offiler** (University of Manchester) described a new flow cell that, together with automated image analysis, enables the measurement of facet-specific crystal growth rates. Showing results on glycine for different supersaturations, she illustrated some of the advantages of the new cell, including the ability to make multiple measurements on the same crystal by going through cycles of growth and dissolution. **Zulaika Alharthi**'s (also University of Manchester) talk focussed on the effects of screw stress and modifiers on the crystal growth and dissolution of L-cystine. Using *in situ* AFM, she concluded that stress favours dissolution and causes step bunching, and that the modifier changes crystal morphology through the breaking and reforming of new hydrogen bonding patterns. The final talk by **Andrew Cashmore** (University of Strathclyde) gave new insight into the secondary nucleation and crystal growth of α-glycine, concluding that there is a close relationship between crystal growth and secondary nucleation.

Nucleation – Theory to Practice

The keynote lecture by **Klaas Wynne** (University of Glasgow) I found particularly fascinating, having been involved for many years in arguments about the (non)existence of a liquid-liquid critical point in water. Klaas was following up a 1997 suggestion of Daan Frenkel that a liquid-liquid critical point might enhance fluctuations and enhance crystal nucleation, and he thought that he might be able to tie this up with laser-induced nucleation. Working initially on liquid-liquid demixing in the nitrobenzene-decane system, he showed it was possible for a laser to induce a phase separation, and summarised the theory of why this could happen. He showed some impressive video clips of laser induction of what he called 'weird' (possibly amorphous) particles which, when zapped with the laser beam transformed into an unstable crystal phase which then transformed into the stable crystal phase. Klaas concluded that laser-induced phase separation followed by nucleation had not yet been achieved but that work was continuing on ternary mixtures and on better understanding the metastable regime. The second lecture by **Bart Vorselaars** (University of Lincoln) aimed to simulate the nucleation and growth of a model system using seeded simulation. Using NaCl in water as his system (one in which nucleation is a rare event implying long simulation times that suggest computer simulation of nucleation might be infeasible), he described the methodology he developed and showed the quantitative comparison with experiments of his MD with seeding results. Bart was followed by **David McKechnie** (University of Strathclyde) who was interested in the effects of interfaces on heterogeneous nucleation, a point of importance as, because nucleation is a stochastic process, small scale nucleation experimentation is often used as it can generate large amounts of data quickly. Effects explored included those of 'inert' interfaces, wall strength and interface concentration, and it was concluded that understanding effects such as these will enable control over the interfacial concentration that can be used for nucleation enhancement or anti-fouling applications. The final talk by **Alexander Jackson** (University of Leeds) was directed at the problem of the cold temperature performance of diesel fuel, the increased viscosity of which relates to the crystallisation of the n-alkane fraction. He carried out a series of measurement on the solubility and nucleation kinetics of a series of single and mixed diesel n-alkanes in dodecane and toluene with interesting results, including explaining the difference in solubility of even and odd alkanes in terms of their different crystal structures.

Crystal Growth of Framework Materials (including MOFs) (joint with CCG)

The title of the keynote lecture – 'Why Crystals Will Save The World' – might at first sight sound overdramatic, but the talk by **Michael Zaworotko** (University of Limerick) was indeed inspiring. Not only did he assert that we are now at the stage where crystal engineering can have a major effect on our future, but he demonstrated this with two examples of types of engineered crystals that can efficiently separate mixed gases and abstract water from the atmosphere. He set out the key design principles, and showed impressive examples of one step separation of gases such as CO_2 from the air at ambient temperature and pressure (of more than obvious world-saving potential), and of a system to extract atmospheric water that is currently under trials and that could help solve the developing world's need for clean water. I look forward to hearing more! **Paul Saines** (University of Kent) followed with a talk focussing on 'hybrid' inorganic-organic perovskites. He explored how the physical properties of these materials are changed through combining monovalent and divalent ligands, with interesting results for, for example, rigidity and (negative) thermal expansivity, and a possible route to a ferroelectric if polar ordering patterns can be created. Also from the University of Kent, **Patrick Doheny** took us through the crystal structure and physical properties of a particular metal-organic framework material. Cofacial stacking of the basic chemical unit was observed in the crystal structure which he identified as a means to access novel mixed valence and and intervalence charge transfer properties in MOF materials. The session concluded with **Lorenzo Metilli** (University of Leeds) explaining the construction and testing of an in-line ultrasonic velocimetry system to measure solid fat content, as current methods are not suitable for such in-line use. The trend in solid fat content was observed to be consistent with crystallisation, and analysis of the frequency spectrum of the sample signal was found to provide information on the length scale of the crystalline fat network.

Crystallisation of Pharmaceuticals

In her keynote lecture, **Susan Reutzel-Edens** (CCDC; previously Eli Lilly) took us through some of her experiences in predicting the minimum energy crystal structures of pharmaceuticals. Not only was it important to know which solid forms are wanted, but also which ones need to be prevented from forming. Commenting positively on the great progress that has been made in crystal structure prediction, she used two drug examples to illustrate particular issues, including the need to take disorder into account (vibrational and configurational free energy contributions can be critical) as well as strain energy, and the complexities introduced where solvates are involved. The next talk by **Wenqing Tian** (Loughborough University) described his work on Protein Crystallisation with Gas Bubbles generated by a microfluidic device. Amongst other results, he found that the protein acts as a surfactant, with the bubble surface providing a heterogeneous site with a lower nucleation free energy, which was useful for separation, and that crystals tend to form more on gas bubble surfaces. The third talk by **Martin Ward** (University of Strathclyde) described some of the insights gained into the role of impurities on polymorphism through spray-drying of chlorpropamide, a molecule which can exist in a number of different conformations, so facilitating a

diverse set of polymorphs. A new phase of this well studied active pharmaceutical ingredient was obtained by spray drying, and he found that structurally similar impurities were able to direct crystallisation of metastable phases. His main take home message was that to efficiently screen the solid form landscape a diverse range of experimental methods should be considered. Focussing on fluticasone propionate, a metered dose inhalant, **Vivian Walter Barron** (University of Leeds) set out to understand from first principles all the intermolecular interactions in such four component suspension preparations, with an emphasis on the solid state crystalline active API. He concluded that his range of approaches could be incorporated into alternative models to describe colloidal particle interactions in non-polar solutions and help with designing new formulations.

Crystal Engineering (joint with BCA)

Immediately after giving the title of his keynote lecture: 'Current Challenges in the Design and Preparation of Molecular Crystals', **Dejan-Kresimir Bucar** (UCL) said that he wasn't going to be able to say that these challenges had been met. Rather, he wanted to use his talk as an opportunity to trigger interest in the community to tackle some of the problems that have followed him from his time in Zagreb some 20 years ago. He argued that we have significant weaknesses in our abilities to *design*, *build*, and *use* crystals to their full potential – in one case he gave concerning the predictability of supramolecular interactions in a molecular co-crystal, he got different synthons in London from those he got in Cambridge, as well as when he used different solvents. After discussing a number of different systems, he concluding by listing about a dozen reasons why he was a 'cynical (but happy) crystal engineer' in relation to designing, making and using crystals – a list that could perhaps form a road map of where to go next to meet the challenges he set out.

The following talk by **Panayiotis Klitou** (University of Leeds) focussed on the relationship between the crystal structure of different solid forms of the flavonoid quercetin and their surface properties. Through molecular modelling, he examined the structures and explored the surface extrinsic synthons which can form on the different solid forms, and calculated the morphology, surface chemistry and polarity of the different facets of the different forms. In the third talk, **Petra Bombicz** (Research Centre for Natural Sciences, Hungary) described her work on a series of Labjack-like crystal structures of halogenated 2-phenylbenzimidazoles. Aiming to understand the roles of molecular conformation, supramolecular interactions and symmetries in order to be able to perform directed manipulation of molecular packing, she concluded with recommendations on how to recognise and numerically describe isostructurality. The final presentation of the session was a talk by **Toms Rekis** (University of Bayreuth) on molecular solid solutions and how we can use them to tune some luminescence properties. After summarising the ways in which luminescent properties of crystals can be varied (e.g. chemical substitutions, polymorphs, co-crystals), using the chloro- and iodo- derivatives of thioxanthone, he demonstrated how the luminescence colour can indeed be varied continuously in co-crystals of these two forms. He concluded by suggesting how this proof of concept work could be extended to technologically relevant systems such as nonlinear optical materials, semiconductors and actuators.

John Finney
UCL

NICOLA Hardaker and her staff at Hg3 were key to the Spring Meeting going so well. Not only did they choose what turned out to be an excellent platform, but they also worked tirelessly, not only to ensure that it all went smoothly during the conference, but also made sure that the pre-preparation was ready for lift-off on the day, and that everything was available online after the meeting. Thank you Nicola, Anna, Charlotte, Ellie, Moira and Rob!






Top row left to right: ***Nicola Hardaker, Anna Whitelaw, Charlotte Turpin.*** *Bottom row left to right:* ***Ellie Taylor, Moira Dopson, Rob Glynn Jones.***

BCA-BACG Spring Meeting 2021 Bursary Reports

This year the BCA has been able to support 6 students with bursaries for the 2021 Spring Meeting. This is thanks to the Arnold Beevers Bursary Fund and our kind sponsors Rigaku, ELDICO and the Royal Society of Chemistry journal *CrystEngComm.*

If you are interested in applying for one of our bursaries please apply at **https://crystallography.org.uk/prizes/bursaries** and if you would like to sponsor a future bursary please contact the bursary officer – **cheryl.x.Doherty@gsk.com**.

Lorella Spiteri

BEING that the last time that I attended the BCA Spring meeting was in 2018, I was very excited to be able to join again this year, especially due to the great list of speakers. Moreover, this conference offered a great ensemble of exciting current research work concerning all possible façades of crystallography. Apart from the exposure to beautiful scientific work, I was looking forward to be in virtual presence of people who like myself are fascinated by this field.

On the first day, the conference served as a platform for young researchers to share their research work, covering topics from *in silico* design of crystal forms to elastic properties of pharmaceuticals and intermolecular network volume calculations. I also enjoyed particularly the Parkin Lecture delivered by **Elizabeth Driscoll**, who shared innovative ways to explain scientific concepts while engaging with the general public, with infectious motivation.

The next days were filled with interesting talks, balancing between innovative approaches carried out through experimental work and computational work. An example of such parallelism can be illustrated through the issue of 'disappearing' or maybe 'elusive' polymorphs. This topic was discussed by **Dr Marcus Neumann** (prediction point of view) and **Professor William Jones** (experimental point of view), via different case studies including the infamous caffeine-citric acid co-crystal polymorphs. Another great highlight was the introduction of the novel philosophy of focusing on high crystal structures during structure prediction by **Professor Graeme Day**. The Medal talk delivered by **Dr Veselina Marinove** was also a remarkable insight on how to investigate crystal growth at the crystal/solution interface on a molecular level using dynamics and thermodynamics.

From this experience I got the opportunity to widen my horizons on familiar topics, and be introduced to new ideas and areas, while appreciating the beauty of this field even further. Despite being held remotely due to the current pandemic, the progression of the conference was very smooth and the delivery of information was conducted excellently, especially through the use of high quality graphical illustrations in certain presentations, which made it easier to follow and grasp concepts.

It was inevitable to miss dearly in-person networking, but I did appreciate the possibility of asking questions, as well as the effort made by speakers to share their contact details in case someone had further enquiries. Even though the past poster sessions were a great way to network, I loved the fact that each poster was accompanied by a short, to the point presentation, enabling all participants to maximise the intake of information. Furthermore, the fact that all talks were recorded and will remain temporarily available after the conference, made it possible for me to review some, while checking others that I missed during parallel sessions. I do hope that such initiative can still be retained in future meetings. Once again, I am very grateful to have attended and definitely feel inspired to continue to do more science!

Lorella Spiteri
University of Malta

WITH Covid forcing the rearrangement of the BCA Spring Meeting from 2020 to on-line in 2021, I was excited at being given the opportunity to attend and hear the fantastic range of speakers and talks that had been assembled.

The traditional YCG satellite meeting, this year joint with BACG, preceded the main conference with a series of talks involving presentations from early career researchers in the field of crystallography. These talks covered wide-ranging and diverse research areas and they were delivered very smoothly. Credit to the chairs **Tom Roseveare** and **Natalie Tatum** for fielding questions from the panel so effortlessly.

The next day began the main conference and the session I attended involved talks from **Florian Kleemis** and the impressive work on the NoSpherA2 software, **Alexander Nazarenko** showed us how to model interatomic scattering in SHELX, **Ella Schmidt** presented her work on diffuse scattering modelling using 3D-ΔPDF from electron data and **Natalie Johnson** rounded these off with best practices for depositing electron data in the CSD, important with ever-increasing

popularity of the technique. The afternoon session started with an excellent plenary talk from **Franziska Emmerling** on the use of mechanochemistry techniques. This led on to the Electron Crystallography session with **Lukáš Palatinus** giving us a 'where are we now' overview talk and his progress with dynamical refinement of continuous rotation data. **Andy Stewart** reconsidered the question of when is a crystal a crystal; **Fabio Nudelman** showed the use of dark-field TEM to probe the solid-state transformation of $CaCO_3$ and **Gustavo Santiso-Quiñones** alerted us to the fact that the reality of a dedicated electron diffractometer is nearly upon us.

Day 3 began with a session on the challenges of crystallisation in an industrial setting and some of the pitfalls that can occur. **Adam Keates** considered crystallisation in an agro-chemical setting while **Anuradha Pallipurath** showed her rationale for designing and controlling crystallisation using XRPD. **Simon Coles** updated us on the crystal sponge method and **Mike Probert** displayed his ENaCt protocol for tricky samples. The vendor session allowed opportunities for updates on the technical advancements in equipment. The afternoon's Bragg lecture by Nobel Prize winner **Richard Henderson** led us through his work on CryoEM and how structures of proteins can be obtained to high resolution with the developments of modern instrumentation. The following session on the crystallisation of pharmaceuticals was a great experience with **Susan Reutzel-Edens** explaining how to increase the speed of a potential API being brought to market through CSP; **Wenqing Tian** showed us how proteins can be crystallised through the use of bubbles; **Martin Ward** explored the polymorphism in chlorpropamide using additives through spray-drying and **Vivian Walter Barron** explored modelling of crystal surfaces in the context of nebulizer formulations.

The fourth and final day started with a keynote from **Colin Pulham** investigating the response of explosive materials to high pressures. **Jake Musselle-Sexton** went on to display the differing synthetic routes to complexes with spin crossover; **Hanna Bostroem** probed the response to pressure of analogues of Prussian Blue with differing composition and **Lucy Saunders** showed her work on the setup used to apply an electric field to samples for crystallographic measurements. The Lonsdale lecture given by **Lucy Clark** exploring the magnetic and crystallographic complexity of mineral materials was well-received. The day ended with a session on protein-protein interactions, beginning with ubiqutin signalling complexes structure and function by **Elton Zeqiraj**. **Charlotte Scarff** delved into the structure of Myosin-2 in the shutdown state, **Martin Rennie** showed the many facets of the process of ubiquitation and **Selena Burgess** finished off by looking at allosteric kinase inhibition using the example Aurora-A.

The lunch breaks across the days allowed participants to view the posters and engage with authors, which worked surprisingly well in a virtual environment. I have enjoyed browsing them as the conference page is still live with both posters and talks 24/7 until 12th May. Credit must go to all the chairs across the days for providing stimulating and insightful questions. Thanks also to the organisers within the BCA and Hg3. It was very nice to be back to some form of conference platform after the lack of opportunities for anything similar in 2020.

Edward Broadhurst (sponsored by EDICO Scientific)
University of Edinburgh

Ignas Pakamorė

THE joint BCA and BACG Spring Meeting was the first crystallography conference that I have attended during my Ph.D. Because of the current pandemic situation the meeting was held online. I could not imagine such a great online platform which enabled participants to switch between sections, ask speakers questions and have a live poster session! The outstanding advantage of this platform is that participants can access talks even after the conference is finished.

The conference started with the YCG/BCAG early career satellite meeting. This day is specially designated for early career researchers to present and discuss their research in a friendly environment. It was a great chance to hear talks in various fields ranging from crystal growth, material science to science communication. In this session, a great talk by **Edward Broadhurst** from the University of Edinburgh on application of 3D electron diffraction to study polymorph evolution during crystallisation dragged my attention. In this study, a prospect of using 3D electron diffraction to determine crystal structures much faster and using much smaller crystals compared to x-ray diffraction methods was exhibited, unveiling great future applications.

Furthermore, the amazing talk (Parkin lecture) by **Elizabeth Driscoll** from the University of Birmingham about battery technology and science communication exposed the essence of good science communication skills and tools for presenting research to various groups of people. I have been inspired by this talk and discussion afterwards; hence I started thinking of participating in outreach groups and volunteering in science events. Overall, I have greatly enjoyed attending this session and would highly recommend future conference attendees to join it for great presentations, poster sessions and inspiring discussions.

The following three days of the main conference focused on talks in various fields of crystallography ranging from software development to applications. I was very interested in latest development in new structure refinement method using the NoSpherA2 algorithm, which affords significantly more accurate structure modelling. I am very keen to learn more about this algorithm and apply it in my own research!

The biggest highlight of this conference for me were the talks in the section on electron crystallography. The keynote lecture by **Lukáš Palatinus** from the Czech Academy of Sciences gave a remarkable overview of the current status, progress and challenges in the field. I am personally very interested in this technique which enables data collection on relatively small crystals. That would enable structure solution for materials that cannot produce large enough crystals for x-ray diffraction data collection (like metal – organic frameworks).

Overall, this meeting was an incredible opportunity for me to virtually meet the members of the British crystallography community and learn about current research activities. I have been inspired by various talks and gained a lot of new ideas that I would like to implement in my research. Furthermore, attending this conference has aided my decision on my future career path choice for a post-doctoral position after I graduate.

Ignas Pakamorė
University of Glasgow

THIS was the first conference outside of Cardiff during my Ph.D., and luckily I was able to attend from the comfort of my own flat in Cardiff! Even so, I managed to have some great discussions with some more experienced crystallographers which are already having a great influence on my Ph.D. research.

The conference was so simple to access and navigate around: no more awkward exits halfway through one session to get to the next! The first session I attended was a BACG session on crystal growth, which provided some insight into more practical applications of crystallography. Following this, I attended what ended up being my favourite talk of the conference in **Marcus Neumann**'s presentation on crystal structure prediction as part of the Industrial Group plenary lecture. I think this conference did a great job of showcasing crystal structure prediction, but the work done by Avant Garde Materials Simulation is pushing boundaries that I imagine some of us didn't even know existed.

It was also a pleasure to attend the Bragg Lecture by **Richard Henderson**. I've seen him talk in other lectures and he never fails to impress even to a more physical crystallographer like myself. His contributions to science are huge and it's great that he is involved in the BCA and BACG meetings.

On the third day of the full meeting I was privileged to attend the Structure Solution from Powders session as a speaker to showcase the research I've been working on for my Ph.D. We had some great speakers, in particular the talk by **Kenneth Shankland** about structure solution in depth, as well as applied work by **Anthony Bell** and **Tom Roseveare**. This session was chaired by **Karen Johnston** and **Gary Nichol** who both did a fantastic job of facilitating the discussion. I was happy to answer many questions about my work and I learned a lot from the experience, especially as to how welcoming the crystallographic community are!

Given the turbulent times it has to be mentioned that the organising committee as well as Hg3 Conferences did an immaculate job in ensuring the conference ran well, was accessible and facilitated discussion. Although I would have loved to visit Leeds to meet the community in person it was a great opportunity, and I hope to present again sometime. I was very lucky to be awarded a bursary by the BCA which was sponsored by Rigaku and allowed me to attend.

Chris Smalley
Cardiff University

THIS year's meeting started under unique circumstances with the cancellation of the meeting last year and the virtual attendance this year due to COVID-19.

The meeting kicked off with the Young Crystallographers event on Monday, starting with an interesting talk by **Cheryl Doherty** on using digital methods for the design of solid form pharmaceuticals and providing insight to how crystallography is applied in an industrial setting. The Parkin Lecture by **Elizabeth Driscoll** focused on outreach and teaching children about science with various activities while talking about her research into battery technology. The day also included series of talks from young crystallographers displaying different parts of the work they have been doing during their Ph.Ds including such subjects as MOFs and spin crossover.

Over the next three days talks covering a wide range of subjects such as electron diffraction by **Lukáš Palatinus**, **Colin Pulham** showing explosive samples under extreme conditions, and talks on crystal structure predictions and new techniques for crystal structure determination. This wide range of talks allows for insight into the future of the field we work in, showing what is possible and what we can aim for in the near future.

During the final day there were presentations such as the Lonsdale Lecture given by **Lucy Clark** and from award winners such as **Charlie McMonagle** for his outstanding work during the early part of his career and **William Jones** for his contributions to crystallography.

We could not see one another in person this year due to external circumstances but the ability to speak to others who we would normally look forward to seeing at these conferences and discuss the work of others was refreshing nonetheless. Hopefully we can all look forward to being back in person next time.

Jake Musselle-Sexton
Newcastle University

Julia Gasol Cardona

AFTER a short trip from my bed to the desk, I turned my laptop on and logged into the 2021 BCA/BACG Online Joint Spring Meeting between the mornings of Monday 29 March and Thursday 1 April. Whilst the idea of an online event might not appeal to everybody, this meeting most certainly did not disappoint. From a fantastic programme and list of speakers to a straightforward and glossy platform that held the event, this meeting had a lot to offer.

The official event was preceded on Monday by the YCG/BACG Early Career Satellite Meeting. This meeting offers a great opportunity for early career researchers to present their work in a friendly and supportive environment. The quality and science behind the talks was remarkable, and it was encouraging to see so many familiar faces. I personally found the event to be an excellent chance for pinpointing which students were carrying research similar or linked to mine, with whom it would be incredibly interesting to discuss results and collaborate in the future.

The three day long Joint Spring Meeting officially opened on the Tuesday morning with a warm welcome from the event organisers. The event programme was jam-packed with talks and Q&A sessions, which left little to no time for social activities.

Two sets of four themed sessions ran every day. These featured a talk from a keynote speaker, followed by three further talks and a dynamic half-an-hour Q&A session to conclude. A balanced group of speakers was selected, which ranged from Ph.D. students to postdoctoral researchers, academics, synchrotron workers and industrial employees.

The four sessions ran parallel to one another and allowed for a wide range of science to be covered in a short period of time. It was fantastic to learn about such a variety of topics – from chemical to pharmaceutical and biological research, theoretical and practical studies, and both lab.-based and computational work. A particular highlight for me was **Dr Susan Reutzel-Edens**' excellent talk on the work carried out at Eli Lilly and Company on digital solid form design.

On top of the exceptional talks, the programme celebrated extraordinary work carried out in the fields of crystallography

and crystal growth by inviting individuals who had made significant contributions to give a lecture. These included **Elizabeth Driscoll** (Parkin Lecture), **Richard Henderson** (Bragg Lecture), **Lucy Clark** (Lonsdale Lecture), **Charlie McMonagle** (CCDC/CCG Prize Lecture), **William Jones** (BACG Annual Lecture) and **Veselina Marinove** (BACG Medal Talk).

For the remainder of the event, plenty of time was given to network with companies and colleagues through scheduled networking events, such as poster and vendor sessions, as well as to attend plenaries and AGMs.

The Joint Spring Meeting drew to a close with poster prizes granted to students and some final words from the event organisers. As a first year Ph.D. student, this highly enjoyable and stimulating event opened my eyes to the breadth of topics crystallography and crystal growth cover, and the endless directions in which I can take my project. I would like to thank Rigaku for sponsoring my attendance.

Julia Gasol Cardona
University of Strathclyde

Obituary – Judith Milledge 1927-2021

Judith at Atlantic College, Vale of Glamorgan, UK, in 2011.

OLDER members of the crystallographic and mineralogical communities will remember Dr H. Judith Milledge (née Grenville-Wells) who died in London on 23rd January 2021 aged 94.

Her parents having moved from England in 1923, Judith was born in 1927 in Kokstad, South Africa (a farming community in Kwa-Zulu, Natal, about 300 miles from Kimberley, where diamonds are famously mined) and she attended Rhodes University in the Eastern Cape Province just after the end of World War II. Judith's mother was determined that she should study a science, despite the fact that she had been to a school with no science in the curriculum. Judith said that she took Physics at Rhodes because, when she was discussing the merits of taking either Physics or Chemistry, the professor of Chemistry (probably unwilling to take on a total beginner) was very quick off the mark in assuring her that Physics would be the best for her! It must have been a strange experience, as in those days very few women were admitted to university to study science. Also, the majority of Judith's fellow students were men who had just returned from active war service and who found great amusement in livening up dull classes by discovering ever more spectacular ways of destroying parts of the teaching laboratory. After taking a B.Sc. and an M.Sc. from Rhodes, Judith went straight to work in the new De Beers Diamond Research Laboratory in Johannesburg, but she soon realised that she needed to take a PhD in crystallography. Initially, she approached R. W. James, Chair of Physics in the University of Cape Town, but he was too unwell to take her as a student and so he suggested that she contact Kathleen Lonsdale in London instead.

Judith in the De Beers laboratory, South Africa, ca 1948. Photo credit: Robert Caveney, De Beers.

In 1949, Judith left South Africa and moved to London to begin her Ph.D., working on diamonds at University College with Kathleen Lonsdale, and for some time she lodged with the Lonsdales in return for secretarial help in the preparation of the *International Tables for X-ray Crystallography*. After completion of her Ph.D., Judith moved to a post-doctoral position at MIT, working with Sidney Abrahams. On her return to UCL, she re-joined Lonsdale's research group in the Department of Chemistry, eventually achieving the position of Reader in Crystallography in the University of London, by which time the University had also awarded her a D.Sc. Kathleen was one of the most important influences on Judith's life and they became close collaborators. In later years, Judith was very proud of her association with Kathleen, who she clearly held in the highest regard, and she took her role as the executor of Kathleen's literary estate extremely seriously. By the late 1970s, after Kathleen's retirement, the Chemistry Department was going through a protracted phase of transferring to a new building, which did not suit Judith, and so, as her Readership was tenable in any department of the University, she moved to UCL's Department of Geology (now Earth Sciences), which enabled her laboratory to remain in the same location, and where she spent the rest of her career. This proved to be a wise decision, both for Judith and for the Geology Department, as it laid the foundation for the excellence in mineral physics at UCL that continues to this day. Judith continued to work until well after the normal age of retirement; she was still active scientifically until well into her eighties, and co-authored her last paper aged 87.

Judith published well over 100 scientific papers, covering an extremely wide range of topics in crystallography and mineralogy. This tendency to cast her net wide probably resulted in her being somewhat less well-known than if she had focused her work more narrowly. Also, although a very intelligent and clever person, she suffered from the problem that once she had an answer to a scientific question she always felt that further work needed to be done before it was ready for publication. On one occasion, relatively recently, an editor of Nature was heard to remark to Judith along the lines that "your work on these diamonds looks very interesting, I'm pretty sure that we would like to publish it" only to be told that "well – maybe – but I don't think it's quite finished enough to send to you yet" – a response that was greeted with incredulity by at least one younger colleague. Judith was very aware of Kathleen's frustration with her; reminiscing after her retirement, she remarked that "Kathleen was always saying to me 'Judy, you must publish these things' - but of course I never took a blind bit of notice".

Crystallographically, Judith had little interest in 'routine' structure determination, preferring instead to concentrate on crystals that showed disorder, phase transitions, or solid-state reactions. The advent of computers in the 1950s was of great interest to crystallographers and Kathleen Lonsdale observed to Judith that "one of us is going to learn to use a computer and I do not think it is going to be me". In the earlier part of her career, therefore, Judith became one of the pioneers in crystallographic computing. She was assisted in developing relevant programs, on a Ferranti Pegasus computer, by Derek Milledge from Ferranti, whom she married in 1958. Early in 1964, Kathleen and Judith acquired a Pegasus (now in the Science Museum) for their research group. Judith continued to use Pegasus until 1980 – it had the advantage of giving her full access to what was still a relatively powerful machine (for a single user), but the disadvantage that her codes, written in a very low-level language, could not easily be adopted by others. She did, though, retain an interest in the methods of structure determination, collaborating with colleagues in the Statistics Department at UCL in the use of Bayesian methods in structure refinement. Judith's interests in crystallographic techniques covered a very wide range, extending from apparatus for calculating Fourier transforms (pre electronic digital computers) to ingenious devices to improve the methods for collecting data from single crystals. During her time in the Chemistry Department, for single-crystal work, she greatly preferred to use photographic methods, rather than the more fashionable approach that was then extant using 4-circle goniometers with single-point counters, arguing that one should always look at the whole of the diffraction pattern, rather than just at the positions where the Bragg reflections were expected, as otherwise X-ray intensity from non-Bragg reflections, such as diffuse scattering, would be missed. She would have been very pleased to see the modern generation of instruments using area detectors.

Like Kathleen Lonsdale, Judith took the teaching of crystallography very seriously, considering that it was important to introduce students of many disciplines to crystallographic methods and also that the subject should be taught primarily by means of practical work. For the UCL Chemistry Department, they devised a week-long course during which students mounted and set a single crystal of either urea or hexamine on an oscillation camera, determined its cell parameters, measured set of intensities, and then 'solved' the structure (assuming the phase angles were known) by producing an electron density map using a von Eller 'Photosommateur'. After she moved to the Geology Department at UCL, Judith devised a similar set of practical exercises based around mineral samples, where students learned about such things as the determination of crystal morphology, cell parameters, orientation distributions, and phase identification from powder data. Sadly, the time taken, level of demonstrating required, and expense of running such courses means that they are probably now no longer practicable at universities in the U.K.; the students are much the poorer for their loss.

After joining the Geology Department at UCL, although Judith continued to collaborate with colleagues in other departments, principally in Engineering, she switched the main focus of her research back to the study of diamonds, the material which, in truth, was her dominant interest throughout all of her career. In collaboration with Monica Mendelssohn at UCL and with colleagues in other universities, she co-authored some highly regarded papers on the formation of diamonds, their isotopic compositions, their micro and macro inclusions, and their defects. An obvious necessity for diamond research is that the researcher should have access to diamonds for which the source is accurately recorded, information which, with modern mining practices, can now often be very difficult, or impossible, to obtain. It is probably in this area that Judith's work will have its most long-lasting legacy as she had very diligently, over many years, accumulated and characterised a very large collection of well-provenanced samples. After Judith retired, she arranged for her collection to be divided between South Africa and the U.K. where it will provide an invaluable resource for mineralogists for many years to come.

On a personal level, Judith was essentially a rather shy person and quite reluctant to talk about herself too much. She could, though, be an excellent companion over a convivial dinner and she was a loyal friend, adviser and helper to those she enjoyed working with, especially to her former Ph.D. students, several of whom have gone on to distinguished careers as scientists. One of her former students, Josh Thomas (Professor Emeritus at Uppsala University) has written of her "She was a unique person – and it was a privilege to have had her 'pushing me' as my supervisor. However excited I was to show her some new result – she would always (not listen!) and respond: 'Now what you should REALLY do is .... '! I learnt a lot from that – to never be satisfied with my latest result – it's upset a few of my own students over the years, but it made them, like me, better (true) scientists. I have never forgotten the genius of her studying garnet and olivine inclusions in a diamond – mounted on a thermocouple. A truly inventive 'poor man's HT/HP anvil for single-crystal XRD'!!! I'll miss her – but she's always there 'in my head'!"

Ian Wood, Monica Mendelssohn and **Mike Glazer**

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Judith at the 8th IUCr Congress in Stony Brook, NY, USA, in 1969. Photo contributed to the IUCr gallery by Sidney C. Abrahams, and published with permission. Judith served on the IUCr Commissions on Crystallographic Teaching (1954–1957) and Crystallographic Studies at Controlled Pressures and Temperatures (1968–1969; Chair 1969–1972).

Meetings of interest

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

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

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

14th Jun 2021 - 25th Jun 2021
Annual CCP4/APS Crystallographic School
Online.
https://www.ccp4.ac.uk/schools/APS-2021/application.php

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

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

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

5th Jul 2021 - 9th Jul 2021
Advanced School in Soft Condensed Matter 'Solutions in the Summer'
Online.
http://ascm2021.iopconfs.org/home

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

12th Jul 2021 - 15th Jul 2021
15th International conference on materials chemistry (MC15)
Online.
https://www.rsc.org/events/detail/43710/

12th Jul 2021 - 30th Jul 2021
23rd National School on Neutron and X-Ray Scattering
Online.
https://neutrons.ornl.gov/nxs

18th Jul 2021 - 23rd Jul 2021
11th Liquid Matter Conference
Online.
http://www.lmc2020.cz/

24th Jul - 28th July 2021
13th European Biophysics Conference
Vienna, Austria (hybrid conference).
https://www.ebsa2021.org

30th Jul 2021 - 5th Aug 2021
71st ACA Annual Meeting
Online.
https://www.acameeting.com

1st Aug 2021 - 3rd Aug 2021
IUCr2020 Computing School
Online.
https://www.xray.cz/iucr/workshops/nh/default.htm

9th Aug 2021 - 12th Aug 2021
SHUG (SNS/HFIR and Center for Nanophase Materials Sciences User Groups)
Online.
https://neutrons.ornl.gov/shug

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

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

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

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

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

8th Sep 2021 - 10th Sep 2021
Peptide-Membrane Interactions: Faraday Discussion
Online.
https://www.rsc.org/events/detail/37143/peptide-membrane-interactions-faraday-discussion

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

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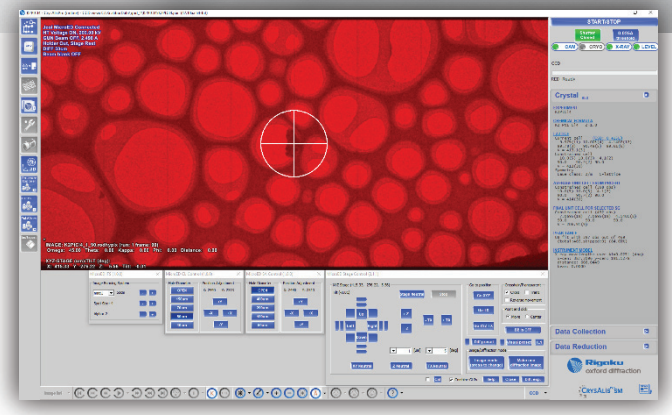

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