Crystallography News

British Crystallographic Association

Issue No. 169 June 2024
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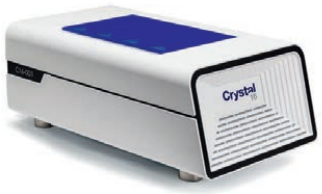

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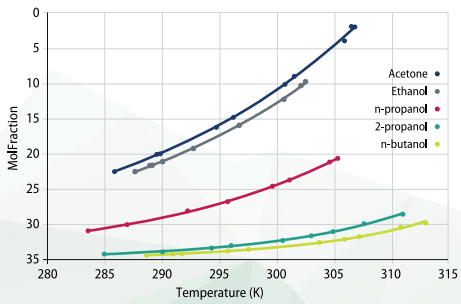

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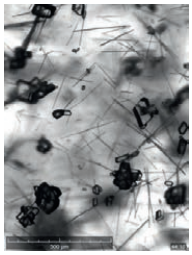

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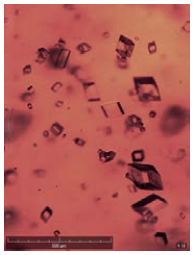

Coloured compounds

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British Crystallographic Association

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BCAIG

Contents

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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 2024 issue are sent to the Editor to arrive before 25 July 2024.

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This month's cover:

Scenes from the Spring Meeting in Leeds (left and right) with the late Prof P. McArdle and Dr S. Tarling above and below the new IUCr logo.

From the President

HAVING been given the great honour of becoming BCA President, one of my first tasks is to compose this column. Thankfully I have the treasure trove of past Presidents' work available to help me, although I must admit it is still a daunting prospect.

However, I take heart from the fact that the crystallographic community has always been a very welcoming one for me. I have been a member since my PhD student times, but it was a return between periods of postdoctoral work abroad in Japan and Germany that demonstrated the special nature of the BCA membership to me. Having attended (and enjoyed) meetings of other learned societies while I was away, I thought I knew what I was expecting when I returned to the familiarity of the BCA Spring Meeting after a few years' absence. But I was taken aback at the friendliness, openness and variety of scientific interests of the participants of that Spring Meeting. Any hesitation I might have had about coming back to the UK, and strengthening my focus on crystallography was gone. Having the joy of working in the Crystallography Group at the ISIS Neutron and Muon Source under the leadership of **Steve Hull** only reinforced this over the next few years, while **Kevin Knight** and **Dominic Fortes**, my colleagues on HRPD, transformed my understanding of the power of crystallography. Although I now lead my own research group at the University of St Andrews, working in the field of structure-property relationships in quantum and functional materials, my formal and informal links to ISIS remain precious. I look forward to enjoying the privilege over the next three years as BCA President of interacting with the many facets of the UK crystallographic community with which I am currently less familiar. I welcome communication from all areas of the membership on aspects which are important to them, and therefore the BCA.

I have consulted the trusty *Crystallography News* records and the fateful Spring Meeting I mentioned earlier was 10 years ago, in 2014. By coincidence, the Programme Chair of that meeting was **Lee Brammer** who went on to hold the President role himself, and who, during a visit of mine to Sheffield, was providing support and encouragement to me just the day before I sat down to write this column. With the danger of stretching this thread of coincidences too thin, during my visit **Phil Lightfoot**, now happily retired, came up in shared memories of both St Andrews and BCA activities. It was Phil, of course, who first got me involved in the wonderful business of crystallography, with the BCA and with the PCG Committee.

This week I have been at ISIS for experiments and had the pleasure to see the students on this year's ISIS Neutron Training Course getting their own start in one of the many forms of crystallography. I suspect this is another factor in my nostalgic reminiscences in this column. I attended the same course in 2009, and many of those I met there are now members of the BCA, along with many other colleagues I have formed links with over the years, across a whole range of techniques, scientific areas and job types. Whatever our favourite probe of crystal structure, dynamics or properties is, we are all united by the BCA, and that diversity and openness is something I have no doubt will continue. This year marks the 40th birthday of ISIS and the hugely important role it still plays in our community at all levels is vital. As is the contribution of the other national and local facilities and centres of excellence and learning at companies and universities across the UK.

On that note, it was good to hear that the newly renamed ESCG, which goes from strength to strength, started this year's Spring Meeting off with a very successful satellite event. I was unfortunate not to be able to attend the whole Spring Meeting, even missing the legendary ceilidh! I look forward to catching up through the reports which appear later in this issue.

We shall be returning to Leeds next year, to experiment with some stability in location, and this column provides a convenient opportunity to remind readers that any suggestions for sessions are very welcome and should be kept at the ready for the shortly forthcoming requests from the Groups. To this I will add a reminder of the Fellow category for membership, which provides a way to give additional support to the BCA. This category is open to those with an established career in crystallographic teaching or research, who normally should have been a BCA member for at least five years, and I encourage you to consider applying.

It is my pleasure to have the opportunity to thank the Programme Co-chairs of this year's Spring Meeting **Peter Moody** and **Hanna Kwon**, along with **Suzanna Ward**, the session chairs and HG3 for the outstanding programme and event they organised. Aside from myself we have a few other new members of Council and I note our thanks to the nominating committee for their work in filling these vacancies. We welcome **Jere Tidey** as an Ordinary Member and, following a year as co-opted Education and Outreach Coordinator, **Ilaria Gimondi** is officially elected to this position. Many thanks are due to **Cheryl Doherty** for her sterling work as Bursary Officer and also Ordinary Member for two terms. Current Council member **Lucy Saunders** will be taking up the Bursary Officer post. Finally, I thank **Richard Cooper** (who will remain on Council as a Co-opted Member) for his dedicated service as President, steering the BCA through a particularly challenging time, and for the kindness he has shown in supporting and patiently shepherding me in the right direction during this transition.

Alex Gibbs
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BCA Council 2024

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

From the Editor

I must take this opportunity to welcome the new BCA President Alex Gibbs (St Andrews) with whom I look forward to working, at least for the foreseeable future. It is also a great pleasure to bring you the June 2024 issue of *Crystallography News* which features reports on the many excellent sessions at the BCA Spring Meeting organised by Early Career Stage Crystallographers Group and the Physical Crystallography Group. We also have a large and fascinating collection of bursary awardee reports for the same meeting. I am very grateful to the awardees and to the Arnold Beevers bursary coordinator Cheryl Doherty (GSK) for their tireless efforts in getting the reports to me so promptly. These reports are followed by News from the CCDC and an article from the IUCr unveiling their new logo as well as their updated purpose, vision and value statements. This is followed, very sadly, by obituaries for Patrick McArdle (Galway) and Stephen Tarling (Birkbeck) before we end this issue with some forthcoming meetings which are hopefully of interest to members. Reporting on the Spring Meeting will continue in the next issue, when I hope that Down Memory Lane will return.

I am thrilled by the chance to resume, as promised, my semi-regular feature on *Crystallographic Forteana*. In one issue last year we discussed the interest shown by the US Department of Defence and NASA in anomalous phenomena, although not exactly the same anomalous phenomena which crystallographers are versed in. I am referring, of course, to unidentified anomalous phenomena or UAP's for short – better known as UFO's. Anyway, the long awaited report from the enquiry held by the above two organisations offers no conclusive evidence that aliens exist or are behind UAP's[1]. However, NASA have promised to investigate reports with improved technology and artificial intelligence, as well as to share the data with greater transparency, and have appointed a new director of research in this area. It struck me that one hears similar phraseology being used across the entire scientific spectrum these days.

Changing the subject slightly, we have all heard of cryptography, cryptocurrency, etc, and indeed the *Fortean Times* has regular features on such things including cryptozoology – the study of species identified in fossil records, thought to have long been extinct, some even before the dinosaurs evolved, which are found alive, well and thriving in some far flung corner of the planet or in the depths of the ocean. Whilst biology never ceases to amaze and many of these discoveries are published in refereed journals, Wikipedia refers to the discipline as a pseudoscience, steeped in studies of legendary creatures the popular media love so much. This got me thinking as to whether there might be scope for *cryptocrystallography* as a subject. Part of my thinking is the importance of symmetry (and asymmetry) in cryptography – indeed the vulnerability of the German Enigma machine to decryption by the allies in WW2 stemmed partly from the machine's use of symmetric encryption. But this is more mathematics than crystallography, so let's investigate a little bit.

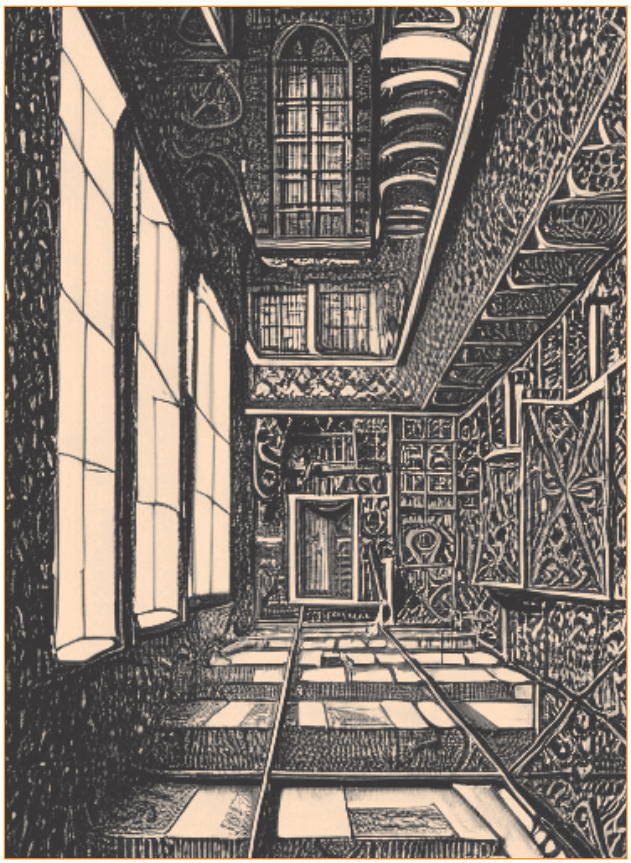
A few web searches revealed indeed that polycrystalline substances used to be classified as being either microcrystalline or, wait for it, *cryptocrystalline*. Microcrystalline substances are made up of crystallites which are visible in the microscope whereas in cryptocrystalline substances, the crystallites are too small to be seen microscopically. However, the many revolutions in microscopic techniques in recent decades mean that there really can be no crystal which is too small to be seen by one or other method! Thus the term has indeed been dropped and it seems that cryptocrystallography is itself now extinct! Do correct me if I am wrong.

Finally, I must thank the BCA membership for supplying the material that we publish in *Crystallography News*. Please do keep sending articles, meeting reports and photographs.

Jon Cooper
UCL

References:

1. https://www.bbc.co.uk/news/world-us-canada-66812332

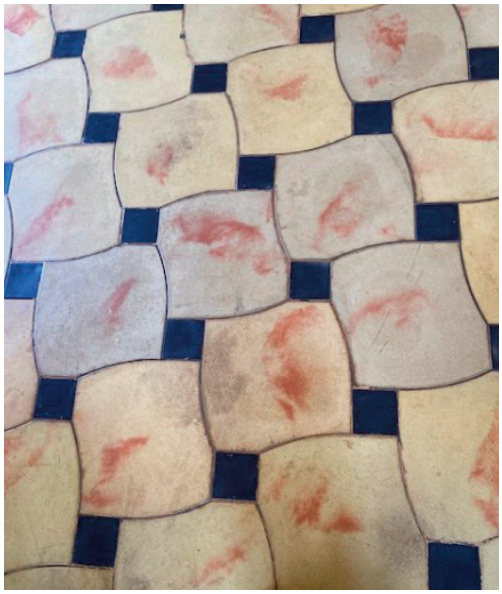


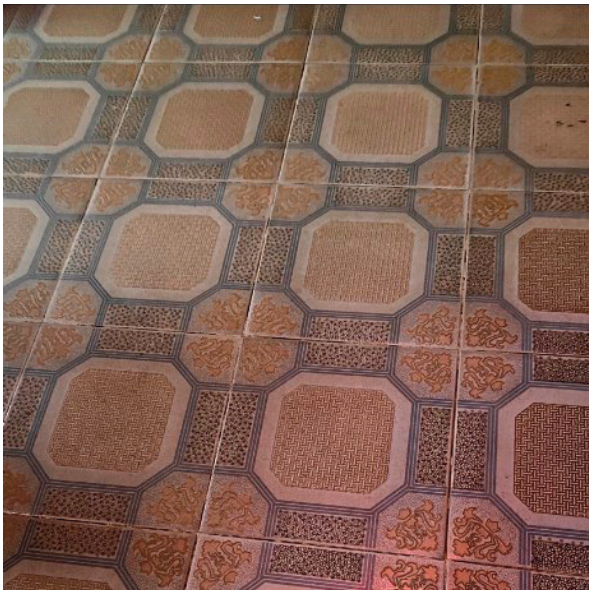
Erratum

Unfortunately, in the March 2024 issue *Crystallographic News* (No. 168) on pages 14 and 15 the affiliation of **Beijia Wang** (Imperial), a speaker and poster presenter at the BSG Winter Meeting, was incorrectly given as KCL. We apologise for this mistake.

Puzzle

THE challenge is to identify the plane groups of each of the following floor tile patterns which were photographed in Nairobi bars by **John Lisgarten** (London). Readers have the additional challenge of compensating for perspective in the photographs which John has very kindly sent.





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

Reports on the BCA Spring Meeting, Leeds 2024

Early Stage Crystallographers Group (ESCG)

The ESCG satellite meeting is an opportunity for all early stage researchers in crystallography from the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment, which is run by fellow early stage scientists.

The first ESCG satellite meeting (following a change in name from Young Crystallographers Group in 2023), kicked off with the opening plenary chaired by **Rebecca Clulow** (Uppsala). The lecture was given by **Lukáš Palatinus** (Czech Academy of Sciences) and was on the topic of "Small crystals, big results: the limits and prospects of electron crystallography." Electron diffraction methods are already growing in popularity and becoming more widely accessible hence the talk served as a great introduction for the members of the ESCG. The presentation focused on 3D electron diffraction and highlighted the many benefits but also some key limitations of the method which will be helpful to our future research. The speaker emphasised the challenges of dealing with the limited rotation range possible and the dynamical diffraction effects, both of which can be partially offset by averaging over a large number of crystals. The speaker described some of the problems with radiation damage and how the use of low temperatures can mitigate this effect. Dynamical refinement of 3DED structures is possible with specialised software.

Jumping straight into the following session of contributed talks, which was chaired by **Joshua Morris** (Cardiff), **Cecilia Hong** (Edinburgh) gave a presentation entitled "Insight into the correlated disorder of fumarate-based MIL-53 frameworks: a computational study of free-energy landscape." Cecilia told us about some breathing MOFs, their potential use as refrigerants through their barocaloric effect and how the correlated disorder in them can lead to improved efficiency. The speaker covered the classification and molecular dynamics studies of these frameworks. The next lecture was entitled "Structure guided drug design of novel antibiotics targeting DNA gyrase" and was given by **Harry Morgan** (DLS/Cardiff). The speaker described structural studies of the DNA gyrase inhibitor zoliflodacin bound to the *S. aureus* enzyme. The crystals suffer from variable twinning in $P6_1$ although the nano-focus beamline VMXm at DLS has allowed multiple small wedges of data to be collected and combined for structure analysis at high resolution. Studies to identify bound metal ions using the long-wavelength beamline I23 at DLS have been undertaken and time-resolved experiments are planned. We also heard from **Sam Thompson** (Durham), who spoke on "Symmetry searching for new molecular ferroelectrics." Since these materials traditionally contain heavy metals such as lead, there is interest in finding greener molecular alternatives. Interestingly the polarisation of these materials can be reversed with an external electric field. The speaker explained his work on symmetry searching of the CSD with FINDSYM to discover new potentially ferroelectric crystals. Only crystals in polar space groups can be ferroelectric and a large number of compounds of interest have been identified for further study. This involves testing for symmetry-increasing phase transitions and by measuring hysteresis loops. Last but not least, "Investigating the surface properties of pharmaceuticals" was the title of the lecture given by **Dave Collins** (Leeds). The speaker described powder X-ray and angle resolved polarised Raman spectroscopic (ARPRS) studies of the crystal facets of paracetamol as well as *ab initio* density functional theory (DFT) calculations. This session concluded with a coffee break, providing a first chance to glance at posters and speak to exhibitors.

ESCG Opening Plenary and Session 1. ***Dave Collins*** *(Leeds),* ***Sam Thompson*** *(Durham),* ***Cecilia Hong*** *(Edinburgh),* ***Harry Morgan*** *(Cardiff),* ***Lukáš Palatinus*** *(Prague) and session chair:* ***Rebecca Clulow*** *(Uppsala).*

Session two, which was chaired by **Olivia Breen** (Dublin) began with an excellent talk by **Aidan Meekings** (Essex) who spoke on the subject of "Structural studies on lytic polysaccharide monooxygenases from *Streptomyces lividans*." Aidan described the very interesting insights that atomic resolution X-ray crystallography of the catalytic domain and small angle X-ray solution scattering of the complete enzyme provided on the structure and function of these proteins. Seven of these copper-dependent enzymes are encoded by the *S. lividans* genome. AI modelling of the carbohydrate-binding domain allowed the full length structure to be fitted to the envelope derived from the SAXS data. **Bhaskar Tiwari** (Edinburgh) concluded the session with a very interesting talk entitled "Polymorphism of ribavirin at high pressure." Ribavirin is a nucleoside analogue which inhibits RNA synthesis and is used as a broad-spectrum antiviral. Bhaskar's talk looked at two different ambient condition polymorphs and their response under pressure and the phase transitions that one of the polymorphs undergoes. A diamond anvil cell was used for these experiments at the extreme conditions beamline at DESY which demonstrated that the sugar unit of this drug exhibits considerable flexibility under pressure. Both talks were well received, and the speakers very knowledgeably answered questions from the audience.

*ESCG Session 2. **Aiden Meekings** (Essex), **Olivia Breen** (Dublin, Chair) and **Bhaskar Tiwari** (Edinburgh).*

The next session was comprised of three very engaging talks spanning a range of applications of crystallography across both biological and chemical fields. **Audrey-Rose Skinner** (Leeds) got things started off with a lecture entitled "Investigating protein photostability using X-ray crystallography" describing how the photostability of one of the major constituent proteins of the eye lens (human γD crystallin) can be investigated using serial X-ray crystallography and also detailed her group's recent venture to SwissFEL to study these systems. The photostability of this protein is thought to stem from a UV rescue mechanism involving Trp and Cys residues. Following on, **Alice McNelly** (Oxford) gave a talk entitled "Furthering our understanding of modulation in silver analogues of Barluenga's reagent." Alice outlined their extensive work into understanding crystals with long range order but no translational symmetry (modulation) by studying silver analogues of Barluenga's reagent, alongside interesting properties such as their diffuse scattering and phase transitions. Finally, to end the session **Lewis Williams** (Essex/DLS) gave a lecture entitled "Visualising the peroxidase catalytic cycle: spectroscopically verified structures of heme intermediates from a dye-decolorizing peroxidase catalytic cycle obtained using synchronous time-resolved crystallography and X-ray emission spectroscopy." Lewis spoke about visualising the peroxidase catalytic cycle and the synergistic effects of combining X-ray emission spectroscopy with time-resolved serial femtosecond X-ray crystallography at the LCLS alongside the use of a fascinating tape drive mixing system to add hydrogen peroxide to the crystals. Narrowing of the Kα1 line in X-ray emission spectra is used to monitor oxidation of the ferric Fe(III) to the Fe(IV)=O ferryl intermediate of this *S. lividans* enzyme.

*ESCG Session 3. **Sam Lewis** (Cardiff/DLS, Chair), **Audrey-Rose Skinner** (Leeds), **Lewis Williams** (Essex/DLS) and **Alice McNelly** (Oxford).*

The talks for the day concluded with the flash presentation session, where those presenting posters each had 30 seconds to advertise their work. The quality of the presentations this year was high, each member prepared a slide in advance and all talks were within the time limit. The poster session then ensued with engaging discussions of delegates recent work extending into the evening.

Speakers with 30 seconds each queuing up in the ESCG Flash Presentations session.

Day two commenced with the 2024 Parkin Prize Lecture which was awarded by the ESCG to **Alex Browne** (St Andrews) following a compelling nomination from his current supervisor, **Alex Gibbs**. The Parkin Prize Lecture is awarded to an early-stage crystallographer for contributions to science beyond the purely academic, including outreach, science communication and volunteering – particularly in the field of crystallography. This session was chaired by **Thomas Hitchings** (Kent). Alex's talk entitled "How (not) to be a Scientist" captured the diverse range of experiences in an academic career with an emphasis on "separating the science from the scientist." Alex's scientific interests and career in the electronic structures of materials were covered. The ups, downs, to's and fro's of Alex's career were poignantly presented, with many in the room able to empathise with some of the shared experiences. The ESCG want to thank Alex for an exceptionally honest and personal talk filled with context and perspective. Highlights included the observation that "Scientists have a tendency to make exciting things sound boring" and how getting involved with science communication and outreach can help make science exciting and engaging for all involved. Alex explored how we measure success not just as academic output but also as the influence of wider engagement and building communities within which we can grow. This message of self reflection was also built

upon by the encouragement to "conduct our own peer review" to really understand what brings us joy and fulfilment. The book *Designing Your Life: How to Build a Well-Lived, Joyful Life* by Bill Burnett and Dave Evans (Knopf Doubleday, New York, 2016) was recommended for such a purpose. Although Alex may now be leaving academia, we wish him all the best in his future endeavours.

The final session of the ESCG Satellite Meeting was chaied by **Anna Herlihy** (ISIS/DLS) and began with a lecture by **Sam Lewis** (Cardiff / DLS) entitled "Diffract and destroy: the development and application of small molecule serial photocrystallography." The speaker outlined the development of fixed-target serial synchrotron crystallography (FT-SSX) at DLS. In contrast to macromolecular studies where stationary shots are obtained, for small molecule work, rotation of the sample during exposure will be required. Sam presented work on an archetypal photoswitch system, sodium nitroprusside dihydrate, used to demonstrate novel serial crystallography methodologies to account for beam damage which are likely to occur as a result of the increased brilliance stemming from the upcoming Diamond-II upgrade. The speaker emphasised that a great deal of crystallisation optimisation was required to achieve a suitable crystal morphology for these time-resolved experiments. **Evie Ladbrook** (Warwick) then gave a lecture entitled "Going head-to-head with domains: 3DXRD for discovering domain structure in hybrid improper ferroelectrics." Evie presented an impressive number of tomographic 3DXRD datasets, looking at domain structure in $(Ca,Sr)_3Ti_2O_7$, using symmetry mode analysis to investigate strain and atomic displacements. Data were collected at ESRF beamline ID11 using a 200 nm beamsize. Domain structure is fundamental to polarisation switching and devices that utilise domain walls as a key component have potential to meet the demands for fast high-density data storage. Following on from this **Lorella Spiteri** (Malta) gave a talk entitled "A quantitative investigation of molecular flexibility – an alternative method beyond the number of rotatable bonds." The speaker described efforts to predict the molecular flexibility of four antiviral molecules by mapping their accessible conformational space and Hirschfeld surface analysis. Closing the session, **Daniel Rainer** (Southampton) spoke on the subject of "The National Electron Diffraction Facility – what, where and how for 3DED". The speaker summarised the advantages of 3D electron diffraction techniques, introduced the newly established National Electron Diffraction Facility based at Southampton and Warwick and the access routes available to potential users with sub-micron sized crystals and samples with multiple crystalline phases!

Parkin prize lecture and ESCG session 4. ***Anna Herlihy*** *(ISIS/DLS, chair),* ***Daniel Rainer*** *(Southampton),* ***Evie Ladbrook*** *(Warwick),* ***Sam Lewis*** *(Cardiff/DLS),* ***Alex Browne*** *(St Andrews),* ***Lorella Spiteri*** *(Malta) and* ***Thomas Hitchings*** *(Kent, chair).*

The ESCG closing plenary lecture on "Teasing out the secrets of subtle protein dynamics" was given by **Helen Ginn** (Hamburg) in a session chaired by **Jake Hill** (Bradford). Helen gave an excellent talk explaining how best to extract small changes and subtle movements in protein structures using her software RoPE. We have a tendency as experimentalists to hoard piles of data and do "just one more experiment" to find the narrative we need to publish our data (something I am very guilty of!) but here Helen hopes that we can use RoPE to mine more from our existing data using SVD/PCA and new torsional interpolation methods to extract even the subtlest of both local and global protein movements. Helen gave a compelling talk with an excellent example of a subtle breathing motion in response to ligand binding, oxidation and UV irradiation, which I hope will inspire us to all start looking through our data piles for new insights!

ESCG closing plenary. ***Jake Hill*** *(Bradford, chair) and* ***Helen Ginn*** *(Hamburg).*

Lonsdale prize lecturer ***Helena Shepherd*** *(Kent) with chair* ***Anthony Carter*** *(Pharmaron).*

For the first ESCG satellite, the broad range of science and high-quality research presented throughout has highlighted what a diverse and active community of early stage researchers we have. We look forward to seeing everybody back in Leeds for the next satellite meeting in 2025!

By the 2023/2024 ESCG committee members: Thomas Hitchings (Kent), **Rebecca Clulow**, (Uppsala), **Olivia Breen** (Dublin), **Sam Lewis** (Cardiff/DLS), **Anna Herlihy** (ISIS/DLS) and **Jake Hill** (Bradford).

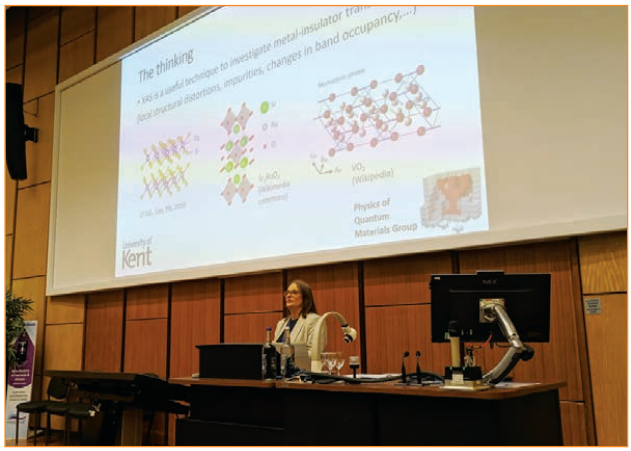
Main Meeting

Physical Crystallography Group (PCG)

This year we had a broad and exciting programme of sessions in the PCG section of the BCA. Although not strictly part of the PCG collection of talks, it is worth highlighting the award of the Parkin Prize Lecture to PCG Secretary **Alex Browne** (St Andrews). Alex gave an honest and heartfelt talk about his experience in science, which was incredibly inspirational to hear.

We kicked off with a joint session, in partnership with the ESCG, looking at "Recent Developments in Software" which ranged from individual experimental tools to new assessments of crystallographic databases. This was followed by a regular favourite of the PCG - a session on "Phase Transitions." On Wednesday, following the IG plenary from **Simon Coles** (Southampton), we had a fascinating session on "Electron Crystallography", including its benefits and drawbacks. In the afternoon we saw the PCG Prize talks, awarded on a biennial basis, as part of the BCA early career prize session. This year the prize was awarded to two PCG recipients. I was incredibly honoured to receive the award and delighted that **Hanna Boström** (Stockholm) was also an awardee. Following this, we had a brilliant session on "Analysis of local structure" covering a range of different techniques and possibilities.

A particular highlight of the BCA, was the PCG Plenary which was chaired by **Alex Gibbs** (St Andrews) and we were delighted that **Silvia Ramos** (Kent) was able to deliver the plenary lecture entitled "Structural signatures of metal-insulator transitions as seen by polarisation dependent X-ray absorption spectroscopy." Dr Ramos described her fascinating work exploring single crystals using XAS. She demonstrated how making measurements at different angles (which had different interactions with the polarised synchrotron source) enabled greater insight into subtle local structural effects within materials systems. After the plenary we had our second joint group session, in this instance with the IG – exploring the subject of "Energy and Sustainability". Finally, we closed the meeting with an Open Session, covering a range of topics.



Silvia Ramos (Kent) delivering the PCG Plenary Lecture.

Many thanks to all of our excellent chairs, keynotes and speakers from across the meeting. I would particularly like to extend my gratitude to **Glen Hebberd** (Durham), who served as one of the PCG reps (alongside myself) for the 2024 Spring Meeting. Glen worked incredibly hard throughout the year to bring together the meeting, and much of the success of the PCG sessions is down to his excellent work. Overall, it was an incredibly enjoyable BCA Spring meeting and we look forward to the meeting next year.

Recent Developments in Software (joint with ESCG)

The session, which was chaired by **Dan Porter** (DLS) and **Ben Tragheim** (Warwick), began with an invited talk entitled "Advanced tools for three-dimensional imaging of nanocrystals with coherent X-rays" given by **Marcus Newton** (Southampton). Marcus presented recent developments in software to reconstruct phase information from nanocrystals using Bragg Coherent Diffraction Imaging (BCDI) – a technique that allows 3D imaging of tiny single crystals using synchrotron X-rays. By using the Bonsu software it has been possible to reconstruct phase maps within $BiFeO_3$ nanocrystals. Using information from multiple Bragg reflections has provided full directional information of the strains between crystalline domains. Applying the same techniques for another system, VO_2, had proved more difficult due to the complexity of obtained diffraction patterns. However, by utilising novel machine learning techniques a successful reconstruction of phase maps from nanocrystals of this material was achieved.

Next, we had two talks looking at the requirements for algorithms to distinguish similar crystal structures within structural databases or when generated by structure prediction algorithms. In a talk entitled "Ultra-fast detection of (near-)duplicate structures across major crystal databases" **Daniel Widdowson** (Liverpool) presented the pointwise distance distribution (PDD) algorithm for quickly finding duplicate structures in various structural databases. Using this algorithm, Daniel showed that the entire catalogue of structures in CSD, ISCD and COD could be compared in a matter of minutes, identifying duplicated structures between and within the databases. **Nicholas Francia** (CCDC) then gave a lecture entitled "Comparison of crystal structure similarity algorithms for large sets of theoretically predicted structures." Nicholas provided an overview of a recent blind test study on over 700,000 crystal structure prediction (CSP)-generated structures based on 6 distinct compositions. Nicholas highlighted the success of utilising crystal packing similarity tools and PDD methods to distinguish duplicate structures, including simulation of powder patterns and comparison of topological symmetries.

The final speaker in the session, **Paul Niklas-Ruth** (Durham) gave a lecture entitled: "Adding Software into the unified

*Speakers and chairs in the PCG session "Recent developments in software." **Paul Niklas-Ruth** (Durham), **Marcus Newton** (Southampton), **Daniel Widdowson** (Liverpool), **Dan Porter** (DLS), **Nicholas Francia** (CCDC) and **Ben Tragheim** (Warwick).*

QCrBox package: the example of an Eval15 container." Paul presented a new software toolbox, QCrBox, which provides links between common pieces of crystallographic software, allowing common workflows to be created that can be shared and the full process of data analysis to be described and reproduced succinctly. The software uses modern tools such as Docker, Python and FastAPI to allow web interfaces to the contained software, reducing the usage activation barrier for new users. The process of adding additional software to the package was described and future developments were discussed.

Phase Transitions

The session which was chaired by **Nilanthy Balakrishnan** (Keele) began with an invited talk entitled "Pressure driven phase transitions: a look to the future of refrigeration" which was given by **Claire Hobday** (Edinburgh) who spoke on the potential of organic ionic plastic crystals (OIPCs) in the design of future solid-state refrigerants. OIPCs provide a rich parameter space in which to explore the tunability of the barocaloric effect experimentally. By employing pressure- and temperature-dependent single crystal/powder diffraction and differential scanning calorimetry experiments, Claire showed structurally and thermally how $FeCl_4$ and $FeBr_4$ behave and demonstrated the ability to tune the transition temperature, isothermal entropy change, ΔS, and the barocaloric coefficient, dT/dP. Moreover, molecular dynamics simulations provided complementary information into the atomistic details of the complex landscape of the phase behaviour of these materials.

Next, **Thomas Hitchings** (Kent) presented a lecture on "Using neutrons to clarify the ferroelectric phases of coordination frameworks." Thomas has shown the use of single crystal neutron diffraction and quasi-elastic neutron spectroscopy to determine the contributions of the molecular A-site cation to the ferroelectric $[NH_4]Mn(HCO_2)_3$ and $[NH_4]Zn(HCO_2)_3$ phases. He also used the same techniques to establish the A-site ordering patterns in the ferroelectric phases and probe the dynamics of the A-site cations in both ferroelectric and paraelectric phases.

The third talk was given by **Lewis Clough** (Edinburgh) and was entitled "The high pressure behaviour of $Nd(XeF_2)_3(TaF_6)_3$." Lewis discussed the high-pressure behaviour of $Nd(XeF_2)_3(TaF_6)_3$ under inert gases and halocarbon oil. Compression in halocarbon oil led to a first-order phase transition at 2.7 GPa. On the other hand, compression in neon resulted in drastically different behaviour, with the phase change suppressed, and a reduction in compressibility of the structure.

The final talk of this session was given by **Hanna Boström** (Stockholm) and was entitled "Pressure-composition phase diagrams of Prussian blue analogues." Hanna showed the high-pressure behaviour of $M[Co(CN)_6]^{2/3}$, $MPt(CN)_6$ and $AMCo(CN)_6$ (A = Rb, Cs) where M is Mn^{II} or Cu^{II}. The porosity decreased considerably from the porous $M[Co(CN)_6]^{2/3}$ to the dense $AMCo(CN)_6$. She also showed that the pressure-induced amorphisation of $Cu[Co(CN)_6]_{2/3}$ at ca 0.5 GPa, which is contrasted by the Mn analogue, where the crystallinity is retained to considerably higher pressures. This suggested that the presence of Jahn-Teller distortions is favourable for the mechanochemical creation of glassy Prussian blue analogues. Another system, $AMnCo(CN)_6$ showed pressure-induced octahedral tilt transitions. This arose since Jahn-Teller distortions provide an additional volume-reducing mechanism, hence decreasing the need for phase transitions. Interestingly, $RbMnCo(CN)_6$ showed a transition to an improper polar phase (Pn) at 0.9 GPa.

*Presenters in the PCG session on phase transitions: **Claire Hobday** (Edinburgh), **Nilanthy Balakrishnan** (Keele, chair), **Hanna Boström** (Stockholm), **Thomas Hitchings** (Kent) and **Lewis Clough** (Edinburgh).*

Electron Crystallography

This session, chaired by **Jeremiah Tidey** (Warwick/NEDF), was led by **Sean Collins** and his visually striking talk, "Scanning nanobeam analysis of defect domains, dislocations, and disorder in metal-organic frameworks and molecular crystals." Sean set out by describing the nature of different beam configurations and how they might yield different information. Whereas the rapidly growing field of 3DED uses, in general, very broad and parallel electron beams to collect at once more traditional diffraction patterns from whole samples, Sean's work focussed on a form of scanning electron diffraction which utilises a similarly parallel but much smaller diameter beam to probe structural variation across samples. Known as 4D-STEM, collecting 2D diffraction slices as a function of two spatial dimensions, the technique allows virtual reconstruction of diffraction contrasted images in a relatively very low-dose manner, making it suitable for beam-sensitive small molecule systems. Sean displayed the power of the technique in probing defects in a number of materials, most strikingly by the bending of waxy crystals to highlight packing defects, and describing how to identify the planes in which they occur. Sean also ventured into the topic of electron-PDF, displaying how results comparable to X-ray studies may be obtained, even in spite of contributions from multiple diffraction.

James Orton (Southampton) followed with a clear and methodical talk, "Scaling crystal sponge with electron diffraction", that discussed the trials and tribulations of the crystalline sponge method. The method employs absorption and immobilisation of non-crystallising materials at the pores of an electron-deficient MOF to enable their structural characterisation. However, the very success of the technique was described as being its major problem, where the rapid absorption of materials often results in significant degradation of the MOF crystals themselves, largely on account of the readiness with which the cocrystals grow. Here, electron diffraction was shown as a potential solution to the problem, allowing structure solution of the resulting, sub-microscopic crystallites that may be broken free by sonication. James showed early results of this method, which gave reasonable statistics even without significant optimisation, plans for which he discussed in closing.

The third talk was provided by **Andrew Stewart** (UCL), purportedly the UK's longest serving electron crystallographer.

Andrew's talk held true to its title: “Myths, truths and electron crystallography”, highlighting misconceptions and oft-forgotten considerations from across the entire experiment. By reminding us that beam coherence needs to be considered in the choice of emission source and that much development is still needed on dynamical refinement, no aspect of the experiment was shown to be safe from oversight. Even the very definition of a crystal came under fire, which is important when we now consider the study of truly nano-scale particles. While it was evident from this and several other talks that electron diffraction has arrived, is ready and raring to take the stage, issues such as the relative impact of inelastic scattering on data quality mean that there indeed remains plenty of wrinkles to be ironed out.

The session was closed by **Fraser White** (Rigaku) waving the flag for their now-available dedicated electron diffraction system with his talk entitled: “XtaLAB Synergy-ED: a journey through the ‘highs’ and ‘lows’ of variable temperature diffraction.” Fraser kicked off by succinctly outlining how Rigaku had put together a 3DED system that takes components from electron microscopy and X-ray crystallography equipment. He then showed how, through the use of the Gatan Elsa cryo-holder or the Hummingbird heating/biasing system, the instrument may be used for more than just routine structure determination, something we at the NEDF very much have our eyes upon. Fraser finished by describing their ongoing development of an automated approach to data collection which will very much streamline the work of the ED-operative and, in doing so, no doubt result in a higher success rate with the often very hit-or-miss samples which call for 3DED.

*Speakers in the PCG session on electron crystallography: **Andrew Stewart** (UCL), **Sean Collins** (Leeds), **Fraser White** (Rigaku), **James Orton** (Southampton) and **Jeremiah Tidey** (Warwick, chair).*

Energy and Sustainability (joint with IG)

This joint PCG/IG session was chaired by **Glen Hebberd** (Durham) and **Tony Bell** (Sheffield Hallam) and featured a wide range of energy materials that have properties suitable for use in battery, ferroelectric and barocaloric applications.

The exciting keynote lecture entitled “Elucidation of the structure and local diffusion dynamics in nickel rich layered oxide cathodes for lithium-ion batteries” was given by **Beth Johnston** (Sheffield) who started by describing muon spin resonance (μSR) undertaken at the ISIS neutron source and how this is well suited to monitor lithium diffusion in next-generation cathode materials, such as the mixed-anion $LiFeSO_4F$, as lithium is a difficult element to study with X-rays. She also discussed the idea of stabilising promising cathode materials with a high Ni content, such as $LiNiO_2$ (LNO), and how this can be achieved with a dual-doping strategy to minimise the adverse impacts a single dopant typically has on capacity retention in the battery.

This was followed by a fascinating talk by **Struan Simpson** (Warwick) entitled “Resolving the emergence of ferroelectricity in hexagonal $BaTiO_3$” covering the phase transitions of hexagonal $BaTiO_3$ ($P6_3/mmc$). Analysis using neutron diffraction, synchrotron X-ray diffraction and the ISODISTORT software package showed the piezoelectric transition at 210-220K to an orthorhombic space group ($C222_1$) followed by a ferroelectric transition at 50-75K to a polar monoclinic space group ($P2_1$). Diffuse scattering was also identified within the data which was attributed to the local displacements of the heavier Ba/Ti atoms.

Transitioning away from typical inorganic materials, **Shivani Grover** (Edinburgh) gave a lecture entitled “Understanding the barocaloric effect in choline based plastic crystals from *ab initio* molecular dynamics.” Shivani discussed the use of computational modelling, more specifically the use of *ab initio* molecular dynamics (AIMD) to monitor the differences in dynamics between the higher and lower temperature phases of choline-MCl_4 (M = Co, Zn) crystals and how the hydrogen bonds shift due to increased rotation of the MCl_4 tetrahedra at higher temperatures. The compounds studied in this work could have applications in more sustainable refrigeration devices. This was one of three interesting talks at the conference on these materials from the Hobday group.

The session was rounded off by **Andrew Jones** (Anton Paar) whose lecture was entitled “X-ray diffraction for battery analysis: common challenges and solutions.” Andrew discussed the demand for more operando and *in situ* measurements to analyse battery cells. It was mentioned that higher energy X-ray sources (e.g. Mo, Ag) are required to penetrate the typical Al casing of a pouch or coin cell. It was also stated that, in the industry, quality control is typically undertaken by measuring the degree of graphitisation using the position of the [002] peak, and so the accuracy of this measurement is vital. It was subsequently highlighted that Bragg-Brentano geometry is not the most suitable for this measurement due to an intrinsic peak shift and so a parallel beam set up is more optimal. Addition of an internal standard is also sometimes done to calibrate the peak position.

*Speakers in the IG/PCG Energy and Sustainability session: **Shivani Grover** (Edinburgh), **Andrew Jones** (Anton Paar), **Glen Hebberd** (Durham), **Beth Johnston** (Sheffield), **Tony Bell** (Sheffield Hallam, chair) and **Struan Simpson** (Warwick).*

Analysis of Local Structure

This session, chaired by **Anna Herlihy** (DLS), focussed on local structure techniques including total scattering, diffuse scattering and solid-state NMR, highlighting their importance particularly in unravelling complex structure-property relationships in functional materials.

The keynote lecture was given by **Phoebe Allan** (Birmingham) and was entitled "*In situ* pair distribution function analysis of next-generation battery materials." As we search for new and Li-free batteries, we need to understand the ion (de)insertion mechanisms of the new materials. Phoebe discussed a range of potential new battery materials including Sb- and Sn-Na alloys. These were found to have impressively complex metastable reaction pathways with structural changes including nano-sized structure and varying degrees of disorder, thus requiring local structure techniques to probe the structure. *In situ* pair distribution function (PDF) and solid-state NMR studies provided insight into these subtle changes, showing that the structures were often locally similar to expected crystalline phases.

Our second contribution was from **Celia Castillo-Blas** (Cambridge) who gave a fascinating talk entitled "Interfacial bonding between a metal-organic framework and an inorganic glass." Celia highlighted the challenges and importance of understanding the interfaces between components of functional materials. In this case, a MOF-glass composite of ZIF-8 embedded with a phosphate-based glass matrix (after meticulous optimisation of synthesis conditions) was studied with total scattering methods and analytical approaches including differential PDF, principle component analysis (PCA) and multilinear regression. This, combined with NMR spectroscopy allowed Celia to identify potential glass-ZIF atom-atom correlations, highlighting new avenues for interfacial characterisation. Conclusions prompted interesting discussion on the use of approaches such as PCA and non-negative matrix factorisation and the importance of correcting total scattering data for non-sample scattering.

This was followed by a comprehensive talk entitled "Unravelling the components of diffuse scattering using deep learning" which was given by **Chloe Fuller** (ESRF). Local structure information contained within diffuse scattering can be difficult to untangle and relate to the structure, particularly for single crystals, so Chloe has developed a freely available deep learning method, DSFU-Net, to alleviate some of the difficulties. DSFU-Net, trained on 198,421 samples of simulated data, performed impressively against a real experimental sample (molecular crystal tris-tert-butyl-1,3,5-benzene tricarboxamide), successfully extracting form-factor and short-range-order components. This new technique is incredibly fast, identifying the form factor and SRO components in a matter of seconds. Subject to testing against a few more "real life" data sets, this approach could offer a streamlined way of analysing diffuse scattering data.

The session concluded with a lecture entitled "Local structure of an industrial catalyst probed by surface sensitive solid-state NMR spectroscopy" given by **Sonja Egert** (St Andrews). The particular material of interest – a silica-based catalyst with zirconium oxides and caesium hydroxide grafted onto the surface – was particularly well-suited to solid-state NMR studies. The complex and disordered nature of the surface necessitated a number of in-depth studies based on systematic surface loadings, solid-state NMR studies and *ab initio* calculations. Further investigations including dried and room humidity conditions provided information about surface hydration, where it was found that Cs locally rearranges on the removal of surface water.

Speakers in the Analysis of Local Structure session: ***Anna Herlihy*** *(DLS, chair),* ***Phoebe Allan*** *(Birmingham),* ***Chloe Fuller*** *(ESRF),* ***Celia Castillo-Blas*** *(Cambridge) and* ***Sonja Egert*** *(St Andrews).*

Open Session

The BCA Spring Meeting came to a close with an Open Session for each of the groups to allow people to present their work in if it does not fit into another session. This year the PCG session was initially proposed by **Holly McPhillips** (Kent) who was unfortunately unable to attend the meeting, so organisation and chairing responsibilities were handed over to **Lewis Owen** (Sheffield).

The session started with a talk from **Ben Tragheim** (Warwick) entitled "Searching for orbital order-charge disorder striping in manganite perovskites." Ben gave an incredibly interesting talk exploring the orbital charge disorder in perovskites. By tracking the symmetry modes in a suite of materials with tuned tolerance factor he was able to show, monitor and describe the phase transitions in the system. This was followed by a talk entitled "Phase stability and magnetic properties of compositionally complex n = 2 Ruddlesden-Popper perovskites" given by **Rebecca Clulow** (Uppsala). Rebecca considered compositional complexity as a design component for making Ruddlesden-Popper perovskites. Exploring a mixture of 4 and 5 component systems, Rebecca was interested in potential magnetic properties that could be produced in these structurally interesting materials.

Moving away from perovskites, **Eliza Dempsey** (Edinburgh) described her work on mixed anion niobium oxyfluorides. In her lecture entitled "Negative thermal expansion and phase transitions in metal oxyfluorides" Eliza showed that by varying the amount of fluorine in the system they were able to control the negative thermal expansion properties of the materials – even producing a material that had essentially zero thermal expansion as a function of temperature! Finally, **Harry Lloyd** (Birmingham/DLS) brought things to a close with a lecture entitled "Driving forces in the phase behaviour of MDABCO-based ferroelectric perovskites." Harry showed how, through an exploration of different parameters across a family of MDABCO-based potential ferroelectric perovskites, they could model and predict variations in the phase transition temperature. Using this they were able to predict and subsequently produce a material with the highest phase transition temperature of the family explored.

It was a great pleasure to chair this session and hear from some exceptionally talented early career researchers! An incredibly enjoyable end to the Spring Meeting 2024.

Speakers in the PCG Open Session: ***Lewis Owen*** *(Sheffield, chair),* ***Ben Tragheim*** *(Warwick),* ***Rebecca Clulow*** *(Uppsala),* ***Harry Lloyd*** *(Birmingham/DLS) and* ***Eliza Dempsey*** *(Edinburgh).*

Lewis Owen
Sheffield

Arnold Beevers Bursary Awardee Reports

The 2024 BCA Spring Meeting took place at the University of Leeds from the 25th to the 28th of March. The programme of presentations covered a broad range of topics including the PCG session on the analysis of local structure. The session was chaired by **Anna Herlihy** (DLS) and included an exciting line up of speakers. The keynote lecture was given by **Phoebe Allan** (Birmingham) who presented her work on *in situ* PDF measurements of next generation battery materials. Her talk outlined the importance of local structure on the characterisation of lithium/sodium (de)insertion mechanisms which is challenging using conventional crystallographic analysis. The first contributed talk was from **Celia Castillo-Blas** (Cambridge) who presented her work on the interfacial bonding between metal organic frameworks and an inorganic glass. The local structure of the material was analysed using PDF and NMR spectroscopy and the results open new routes to characterise these challenging systems. The talk was followed by a presentation from **Chloe Fuller** (ESRF) on diffuse scattering and the use of a deep learning method to separate the contributions from the form factor and the chemical short-range order. The approach should allow for easier analysis of diffuse scattering. The final talk of the session was given by **Sonja Egert** (St Andrews) and focussed on the use of solid-state NMR spectroscopy in the analysis of the local structure of the catalyst in the synthesis of polymethyl methacrylate during the Mitsubishi Chemical's alpha process.

Rebecca Clulow
Uppsala

This year, the BCA spring meeting took place at the University of Leeds, Leeds, which is a beautiful city in West Yorkshire, England and easy to get to by trains from Edinburgh. I am pursuing postdoctoral research in the group of **Claire Hobday** (Edinburgh). This year, I attended the BCA spring meeting for the second time where I had the opportunity to share my research in the form of an oral and a poster presentation on choline based plastic crystals as barocaloric materials with insights from *ab initio* molecular dynamics. The energy and sustainability session involved two talks on battery materials and started with the keynote lecture by **Beth Johnston** (Sheffield), who shared her research on layered oxide cathodes for lithium-ion batteries. Beth's lecture provided us with a detailed understanding on the working principles and techniques involved in carrying out batteries research, especially the *μSR* technique, which was quite useful to know. She shared some fascinating results on the local diffusion dynamics in some of the layered oxide cathodes, and how muons can be used to perform diffusion analysis. This was both interesting and useful to know, as my research involves understanding of the local structure and dynamics using computational techniques, where I compute diffusion coefficients from atomic trajectories to quantify the local disorder. Following this, **Struan Simpson** (Warwick) gave a really interesting talk on hexagonal barium titanate ($BaTiO_3$). He shared his results on unravelling the microscopic origin of ferroelectricity in the hexagonal phase of $BaTiO_3$. This is important for several device applications, i.e. optoelectronics, spintronics, etc. Following this, I utilised the opportunity to share my research on *ab initio* modelling of choline based plastic crystals. Here, I shared my results on order-disorder phase transitions in $(C_5H_{14}NO)_2CoCl_4$ and $(C_5H_{14}NO)_2ZnCl_4$ using AIMD tools. This was followed by the final talk of the session given by **Andrew Jones** (Anton Paar), who shared some solutions to challenges encountered while using X-ray diffraction for battery analysis.

The BCA meeting provided us a platform to interact, share our research, network with the chemistry community and experimental crystallographers, as well as having discussions during tea/coffee breaks, lunch hours and dinners. The plenary lectures by **Aurora Cruz-Cabeza** (Durham) and **Syma Khalid** (Oxford) and the lecture by **Alexander Browne** (St Andrews) on "How (not) to become a successful scientist" were some of my favourites. On the conference dinner eve, several poster prizes and awards were presented to the students, early career researchers and exhibitors, etc., followed by a celebratory cèilidh, providing us with a wholesome experience.

Shivani Grover
Edinburgh

As another year flew by, our much larger research group was ready to embark on another adventure to the BCA Spring Meeting which took place in Leeds this year. I was especially excited and, truth be told, a little nervous this year as I was due to present my first talk at this conference. That said, I cannot think of a better conference for this as the crystallography community is filled with friendly and lovely people who gave me their undivided attention and showed interest towards my work. Even though I am a computational chemist, I felt so welcome in this community.

Thinking back, I must sing praises for the Early Stage Crystallographer's Group (ESCG) for organising the satellite

meeting so well and allowing early stage researchers such as myself to meet others and share our respective research without feeling intimated. The main BCA meeting was filled with amazing talks such as a really well explained introduction to "Thermally responsive molecules and materials" by **Helena Shepherd** (Kent) as well as a super fun one on the "Dynamics and reactivity in solids" by **Hajime Ito** (Hokkaido). I believe I learnt a lot on how to deliver a good and engaging presentation from this conference.

Out of the many interesting sessions throughout the conference, the one that caught my interest the most was the Framework Materials session as it aligned with my own research the most and I had really wanted to learn about what others do in the field. **Ross Forgan** (Glasgow) began the session with a really interesting talk on high-pressure single crystal X-ray diffraction of metal organic frameworks (MOFs). It was cool to listen to what the synthetic side of MOF research is up to, ranging from using modulators to influence the different steps of the synthesis to post synthetic modulations of linkers that give rise to very specific isomers that would otherwise be difficult to form. This was followed by **Anna Warren** (DLS), **Marc Little** (Heriot-Watt) and **Patrick Doheny** (Birmingham) who introduced otherwise foreign concepts to the audience such as diffraction of micron sized crystals, flexible hydrogen-bonded organic frameworks (HOFs) and pH-dependant phase selection of zeolitic imidazole framework (ZIF) synthesis. I am super grateful for the opportunity to listen to these talks from such great researchers who have inspired me a lot, both in my research and how I choose to tackle problems going forward.

Overall, I think the conference was a great success and I cannot wait for next year's to come!

Cecilia Hong
Edinburgh

The BCA spring meeting held in Leeds this year was once again a well-rounded and thought-provoking conference to attend. The theme this year was 'Breaking barriers', which provided the speakers and poster presenters with the opportunity to promote exciting topics such as electron diffraction (ED), extreme conditions X-ray diffraction, crystal engineering and the study of a variety of structures by crystallographic means.

In particular, I found the ESCG satellite meeting to be especially interesting and varied this year. The satellite meeting was kicked off with a talk from **Lukáš Palatinus** (Prague) entitled "Small crystals, big results: the limits and prospects of electron crystallography." Lukáš provided an excellent overview of the uses and capabilities of electron diffraction and the variety of ways dynamical effects can be dealt with and corrected for. The differences between XRD and ED were also highlighted – although much smaller crystals can be analysed and their absolute configuration determined, suitable quality crystals are still essential to the technique. Additionally, radiation damage and data redundancy need to be considered, although radiation damage can be mitigated somewhat by cryocooling or the use of serial crystallography. Avenues to further protect the samples are also being explored, such as embedding them in graphene or liquid. Follow-up talks on the topic of ED were also provided by **Simon Coles** (Southampton) and **Daniel Rainer** (Southampton) later in the scientific programme from the UK National Crystallography Service and the National Electron Diffraction Facility.

Other highlights for me were the talks given by **Bhaskar Tiwari** (Edinburgh) and **Evie Ladbrook** (Warwick). Bhaskar provided an overview about polymorphism of ribavirin at high pressure – the study in question was conducted at DESY with pressures up to ~10 GPa and a phase transition from the ambient pressure $P2_12_12_1$ phase was observed at *ca.* 5.6 GPa. The programme this year in general had a great emphasis on the use of non-standard crystallographic experiments (including extreme conditions crystallography) to pursue exciting new avenues of research. Going forward I hope to see many more talks on extreme conditions crystallography as the technique becomes more and more accessible with technological advances. Evie's talk on hybrid improper ferroelectrics provided an effective overview on the use of 3DXRD to determine the domain structure of her hybrid perovskite – the 3DXRD experiment in question (which was performed as the ESRF) utilised an extremely narrow beam that was smaller than the domains being studied to essentially perform an experiment akin to tomography on the sample.

Alexandra Longcake
Newcastle

A quick train ride from Waverley station in Edinburgh, followed by a brisk walk, led me to the pretty campus of the University of Leeds. It was this year's host for the annual spring meeting of the British Crystallographic Association. Fittingly, the campus was littered with grazing rabbits, adding to the feeling of a blossoming spring. It was my second time attending the BCA spring meeting and it was excitingly the first time I had the honour of giving a talk during the main meeting.

Upon arrival, as I read through the pocket programme booklet, I was greeted by a full schedule of wonderful talks. Over the following days I witnessed many truly fascinating talks on all aspects of crystallography, from the beautiful systematic investigation by **Hanna Boström** (Stockholm) on the structure-property relationships in Prussian blue analogs, to the Lonsdale lecture delivered by **Helena Shepherd** (Kent) on thermally responsive materials, covering the properties of many fascinating spin-crossover compounds.

As a solid-state chemist, organic chemistry is not my expertise and mostly brings up memories of highly stressful periods from my time as a chemistry undergraduate student. Therefore I did not expect that a personal highlight of the conference for me would be the 'Dynamics and Reactivity in Solids' session hosted by the Chemical Crystallography Group, which contained a collection of talks focused on the intersection of organic and structural chemistry. The keynote talk, given by **Hajime Ito** (Hokkaido) focused on the use of mechanochemical synthetic methods in several key organic reactions and the mechanochromism of organometallic crystals. It was fascinating. It was eye-opening to see ball mills, a staple in many solid-state chemistry labs, used in the world of organic chemistry to achieve more favorable synthesis conditions for a myriad of organic compounds. In some cases, they even incorporated a humble heat gun for temperature control. Following that, **John Wallis** (Nottingham Trent) thoroughly explained the interesting subtleties of the interactions between electrophilic and nucleophilic functional groups in the solid

state and their impact on the crystal structure. **Petra Bombicz** (Hungarian Academy of Sciences) showed the structural variety found in tricyclic and bicyclic guanidinium-type carbocation cocrystals. The session concluded with an illuminating talk by **Ben Coulson** (Cardiff) who studied packing effects on linkage isomerism via photocrystallography.

The final evening of the conference was marked by a celebratory cèilidh after a very enjoyable conference dinner and enough courage was found to participate in it. All in all, the variety of research topics that were highlighted during the conference show the breadth of the field of crystallography and makes for an inspiring conference where you are taken out of your own little niche. I would like to thank the Arnold Beevers Bursary Fund for the opportunity to participate in the spring meeting of the BCA.

Joshua Levinsky
Edinburgh

This was my first time at the BCA conference and my second conference ever. It was a thoroughly enjoyable and memorable experience. I felt truly welcomed into a warm and wonderful community. To get a glimpse into the wide world of crystallography, seeing what so many incredible people can achieve, the vastly different areas all connected by a handful of techniques, was inspirational.

The most memorable session for me was entitled Framework Materials and occurred on Wednesday morning, starting with **Ross Forgan** (Glasgow). Ross covered the many difficulties faced when trying to crystallise MOFs, mainly their high valent hard cation, which helps the MOF remain stable against water but inhibits synthesis and crystallinity. He then covered the methods available to combat these issues: the addition of modulators to the synthesis, with the capability to inhibit or increase crystal growth. Ross showed his work with the MOF UiO-67 and how he had managed to get crystals that were large enough for SCXRD by adding L-proline. He then showed us his work on changing the chemical formulas of single crystals after synthesis. The first was a bromination of the alkene bond in UiO-66, resulting in only the trans isomer forming. Next, he showed how substituting the aromatic hydrogens on the organic linker of UiO-66 with fluorine changed the MOF's properties from hydrophilic to hydrophobic. Finally, he showed the pressure-induced anion substitution of the μ-OH on the scandium node of GUF-1 to μ-OCH_3 while in methanol. A fantastic demonstration of MOFs' modular nature. Ross's range of techniques and research is truly inspiring as an early-stage crystallographer, seeing first-hand the multiple fantastic uses of crystallography to obtain materials with an array of physical properties. The next speaker was **Anna Warren** (DLS) who gave an engaging talk on the tips and techniques you can employ to make the most out of your micron-sized crystals. It was a joy to learn about the VMXm technique. **Marc Little** (Heriot-Watt) then spoke about his work on Hydrogen based Organic Frameworks, with an exciting HOF showing the potential for memory. The session ended with a talk from **Patrick Doheny** (Birmingham) who spoke about ZIFs and the difficulties you can face producing crystals large enough for XRD. It's inspiring to see such wonderful results from great challenges.

I have to say that my first ever BCA conference was a truly wonderful experience. It was a pleasure to have the opportunity to join such a welcoming community and I thoroughly look forward to next year's meeting!

Kate Mitchell
Edinburgh

I arrived in Leeds on Monday the 25th of March excited for another BCA meeting. It was lovely to catch up with familiar faces as we all began to congregate before the start of the talks. The feeling of community is always one of my favourite aspects of the meetings.

I was particularly impressed with the PCG Phase Transitions session within the second set of parallel sessions on the Tuesday. Chaired by **Nilanthy Balakrishnan** (Keele), the set of talks began with the keynote speaker, **Claire Hobday** (Edinburgh). Being my PhD supervisor, I may be a little biased, but I thought this was a fantastic opening to the session. The talk itself centred around the need for solid-state refrigerants and the work being carried out within the speaker's research group in order to characterise these materials. Particularly showcased was the effect of pressure on a series of hybrid ionic plastic crystals inducing disorder-order phase transitions.

Following on, was a brilliant talk from **Thomas Hitchings** (Kent) on "Using neutrons to clarify the ferroelectric phases of coordination frameworks." I particularly loved that this talk showcased the power of neutrons in crystallography as X-ray diffraction is most prevalent within talks throughout the BCA. A particularly exciting talk from **Lewis Clough** (Edinburgh) was next. This presentation featured some recent work on I15 (DLS) on "The high pressure behaviour of $Nd(XeF_2)_3(TaF_6)_3$." This project is very unique, working with both elusive compounds and high pressures. I would highly recommend catching one of his future talks if you are able.

The session concluded with **Hanna Boström** (Stockholm) speaking on "Pressure-composition phase diagrams of Prussian blue analogues." This talk was a fantastic example of the scientific research process, showcasing phases of each system that are known and still yet to be discovered. It was refreshing to also have the incomplete aspects of the project presented, and the various techniques used in an attempt to fully characterise these phases.

The remainder of the meeting followed with many more fascinating talks, an evening poster session, and a cèilidh. The quality of posters this year was high and it was interesting to see how people's research projects have developed since last year's spring meeting. As the week progressed, the sun emerged along with the rabbits throughout the campus. The BCA was ideally organised at the beginning of spring, perfect timing for coffee breaks outside watching the freshly born bunnies hopping around between the daffodils.

After another successful spring meeting completed, we ended the conference with a trip to Lil Bao Boy near the train station before beginning our journeys home. I'd highly recommend the detour if the meeting is held in Leeds in the future!

Phillippa Partridge
Edinburgh

Following the brilliant ESCG satellite meeting, the main part of the conference began with a session from some of the MX beamline staff working at Diamond Light Source entitled: "Getting the most from your protein crystals at the synchrotron." **David Aragao** (DLS) kicked off the session with an excellent talk describing how beamline I04 users can match data collection parameters to samples in order to achieve the best results from protein crystals. This was followed by a talk from **Anna Warren** (DLS) on the current experiments being carried out at VMXm, where diffraction data are being collected in vacuum from very small crystals. **James Sandy** (DLS) gave an interesting talk on the VMXi beamline as he discussed the applications of *in situ* data collection for assisting aspects of crystallisation experiments such as condition screening, and the software improvements that have been made to facilitate the delivery of new science. The session was concluded with **Ramona Duman** (DLS) who spoke on the use of X-ray anomalous scattering at I23 to identify light ions in protein structures which has been applied to many exciting protein targets.

Overall, the session was highly informative, and I can safely say that learning about several of the MX beamlines through these exciting talks, in particular their capabilities and current progress, has greatly informed me on the best ways to achieve as much data from my protein crystals as possible. Attending the conference as an undergraduate student and being able to hear about all the research being undertaken in this field has been an amazing experience. It has certainly made me more passionate about my own future in scientific research which I am now even more excited for!

Cicely Tam
DLS

As the last stragglers filtered into the Rupert Beckett lecture theatre at 13:05 **Aurora Cruz-Cabeza** (Durham) began her CCG Plenary lecture. Any general lethargy that followed the lunch break was swiftly dispelled as the speaker's warmth and wit grabbed the audience's attention. We were treated to a three-quarter-of-an-hour discussion on polymorphism, a topic of great importance to the pharmaceutical industry, perhaps second only to drug discovery itself. Polymorph discovery is very valuable because it allows for patent extension and thus financial incentive. Different polymorphs also often have different physical properties, of special note is bioavailability, which can greatly affect the dose and thus efficacy of a given active ingredient.

Aurora's research has long-focussed on polymorph interconversion using ball-milling. The first example described was of an aromatic disulfide compound whose conversion from Form A to Form B required 30 mins of liquid-assisted-grinding (LAG) in MeCN, with the reverse process fully completed after 150 mins of neat grinding. Multiple other examples were provided to show generalisability. The rationale for this clever technique comes from the balance of lattice energies and surface effects. With the tiny particle sizes present in the ball mill (~10 nm), about 40% of molecules are sitting on the surface of the crystal rather than in the bulk. The surface stabilising effects of the right solvent can invert the thermodynamic stability of two crystalline polymorphs.

A famous example of the lack of knowledge with respect to polymorphism was the case of Ritonavir in the late 90s. Two years after it was first introduced to the market, a second polymorph completely displaced the original one resulting in a much-reduced solubility. Form-I was not recoverable and the laboratory that produced Ritonavir lost $250 million. Aurora set her student the task of applying the ball-milling technique to Ritonavir. Incredibly, just 150 mins of LAG with water was sufficient to recover a pure powder sample of Ritonavir Form I.

The first observation of polymorphism was that of benzamide in 1832. However, the structure of this second polymorph (Form III) remained elusive until 2009 (Form II was discovered in 2005 during an attempt to crystallise Form III). It was reported in ChemComm that seeding with a small amount of nicotinamide was able to easily select for the crystallisation of benzamide Form III. Aurora's group were also able to show a similar effect with 3-fluorobenzamide. Using an advanced computational technique, they were able to rationalise these observations with calculated free energy diagrams. Aurora has hypothesised that the common phenomenon of polymorphism appearing very late on in the drug discovery cycle is a result of this kind of impurity seeding. In the preliminary stages of drug development, benchtop syntheses result in slightly crude products selecting crystallisation of Form I. As the product is prepared for market, extremely high purities are required which then may select for Form II.

Thank you to Aurora for such an interesting talk and the BCA for organising the week. A report such as this cannot do justice to the humour and scientific intrigue of the delivery. I hope you catch a chance to listen to her yourself first-hand.

Sam Thompson
Durham

Speakers in the CCG Framework Materials session: ***Marc Little*** *(Heriot-Watt),* ***Patrick Doheny*** *(Birmingham),* ***Ross Forgan*** *(Glasgow),* ***Anna Warren*** *(DLS) and* ***Georgia Orton*** *(Birmingham, chair).*

Speakers in the BSG session entitled "Getting the most from your protein crystals at the synchrotron" ***Ramona Duman, Adam Crawshaw*** *(chair),* ***David Aragao, James Sandy, Anna Warren*** *and* ***Cicely Tam*** *(all DLS).*

News from CCDC

CoreTrustSeal Certification – the CSD as a Trustworthy Data Repository

We are delighted to announce that the CSD has now renewed its certification as a Trustworthy Data Repository by the CoreTrustSeal certification board by the revised and updated 2023-2025 certification standards. This certification provides our depositors and partner organizations with assurances of the reliability and quality of our data stewardship and the access to data extended to users of the database.

Blogs highlights

Remembering Professor Arnold Rheingold

We were saddened to learn of the passing of Professor Arnold Rheingold earlier in March. Arnold, known by many in the community as Arnie, was a predominant figure in crystallography and his prolific output of structural data meant he had a huge influence on the contents of the Cambridge Structural Database (CSD). In total Professor Arnold Rheingold authored 7,665 structures in the CSD. This is nearly 800 more structures than anyone else in the database, which is an outstanding achievement. Read more on the CCDC website.

Dr Patrick Doheny Wins the CCDC Chemical Crystallography Prize for Younger Scientists 2024

Congratulations to **Patrick Doheny** (Birmingham) for winning the CCDC Chemical Crystallography Prize for Younger Scientists 2024.

Patrick Doheny obtained his BSc (Hons. I) in 2015 followed by a PhD in Inorganic Chemistry in 2019 under the supervision of Professor Deanna D'Alessandro and Professor Cameron Kepert at the University of Sydney. His PhD focused on the fundamental characterization of electroactive metal-organic framework (MOF) materials, with a particular focus on frameworks exhibiting intervalence charge transfer and spin crossover properties. Dr Doheny presented his Prize lecture on Wednesday 27th March during the Chemical Crystallography Group (CCG) Early Career Prize Lectures session at the BCA Spring Meeting 2024.

More information can be found on the CCDC website.
All our blogs can be found on the CCDC website.

CCDC Online Events

User Webinar: Automated Design of Kinase Inhibitors Using AlphaFold 2 Models

Exscientia has developed an automated structure-based method for compound discovery, bypassing the need for manual design inspiration and 2D models. Leveraging AI, this approach is particularly useful for targets with limited data and offers novel starting points for well-studied targets. Utilizing AlphaFold2 models, they tested compounds against DYRK1B and PKD1, achieving a 44% hit rate with promising IC_{50} values. These results, even with lower quality protein models like PKD1, indicate the potential for kinome-wide design, revolutionizing target assessment and offering opportunities for novelty in drug discovery.

Join the webinar on the **25th of June at 3 p.m.** (BST) to learn more.

Registration is via the CCDC website.

In-Person Events

The CCDC-sponsored PhD students and their supervisors are coming to Cambridge on the 27th of June to present their cutting-edge research. This event promises to be a day filled with scientific presentations, interactive discussions, and valuable networking opportunities. If you want to attend, please email us at hello@ccdc.cam.ac.uk for further details.

For more information on how to register, visit our events page at the CCDC website.

Free self-guided workshop: Particle Shape Calculation Using CSD-Particle

This workshop will take approximately 25 minutes and will show you the morphology features included with Mercury under the CSD-Particle toolset, called BFDH Morphology and VisualHabit. By the end of the workshop you will be able to:

- Calculate the BFDH morphology for a crystal.
- Set up and run a VisualHabit calculation and interpret the resulting lattice energies.
- Visualize and analyse morphologies and surface energies.
- Visualize and interpret intermolecular interactions (synthons).

Download workshop
https://www.ccdc.cam.ac.uk/media/Particle-shape-calculation-using-CSD-particle.pdf

If you would like to suggest topics for our workshops, webinars and CSDU online training modules in 2024, please email us at hello@ccdc.cam.ac.uk.

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Introducing the new IUCr Logo

Announcing a new logo for the IUCr

HELLO, dear colleagues, friends and valued members of the IUCr community! First and foremost, we want to extend our heartfelt gratitude to each and every one of you for your unwavering support of the IUCr.

Today, we're thrilled to share some exciting news that's been going on behind the scenes. After taking on board feedback and several reviews, we would like to unveil our new logo and branding for the Union.

The IUCr was formed in 1947 and the first General Assembly was held in London, UK, in 1948 and has been successful at continuing its mission to advance crystallography worldwide. Some of our major milestones have included the launch of the *Acta Crystallographica* journal in 1948 and in 1952, the International Tables for X-ray Crystallography. In 1991 CIF was adopted and more recently, in 2014, the International Year of Crystallography was a huge success.

In 1988, a competition was announced in the IUCr Journals to create a logo for the Union. The winning entry was designed by Professor Giovanni Predieri and Mrs Susanna Ciribolla, both from the University of Parma, Italy.

After the celebrations of the 75th anniversary of the organisation in 2023, it was time to acknowledge our past, celebrate our achievements and plan for our future. As such, it was decided that the IUCr should re-visit not only our brand, but also our purpose, vision and value statements. Members across the world contributed to this exercise via two surveys and a well-attended workshop during the 2023 Congress, held in Melbourne, Australia.

The new purpose and vision statements have been formally adopted as follows:

Purpose Statement: Advancing Structural Science Globally

Vision Statement: Empower a Thriving Structural Science Community

And, in support of our vision and purpose statements, the IUCr values have been prioritized as follows:

IUCr Values

- We exemplify scientific excellence and rigour
- We operate responsibly, sustainably, ethically and with integrity
- We are diverse, inclusive and welcoming to all
- We are future-focused and innovative
- We collaborate widely and champion the next generation

These statements and values were developed to reflect the organisation's commitment to its members and its role in advancing crystallography and sharing knowledge globally. In practice, these aspects are delivered through our ethical publishing strategies, outreach commitments and the organisation and support of meetings, workshops and schools.

The new logo and branding

It is intended that this refreshed logo and branding reflect a modern-day scientific Union that has a wide appeal to a variety of audiences beyond the traditional idea of pure crystallography. The logo does not shy away from our name and incorporates facets of a crystal or polyhedral shapes observed in crystal packing. The strong connecting lines between these facets symbolise the strong network and community that has been the foundation of our union and is inherent in our vision and value statements.

The clean design and colour palette ensure its perception as a modern-day scientific union and increases the appeal to a wide audience.

This logo was designed by a professional graphic designer, with input and guidance from the IUCr Executive Committee, IUCr Chester staff and members of the Journals Management Board. After several iterations and reviews, we are proud to present this new logo in 2024, giving the IUCr an updated identity alongside the purpose, vision and value statements.

Over the coming weeks and months, we will be updating our online presence with this new logo, and we encourage you to support this by downloading the logo pack and updating on your own webpages where necessary.

As we embark on this exciting new chapter with our refreshed logo and branding, we remain steadfast in our dedication to serving you, our valued members, in every endeavour we undertake to advance the field of structural science. Your ongoing support and collaboration are the driving force behind our mission, and we look forward to continuing this journey together towards new discoveries and innovations in crystallography.

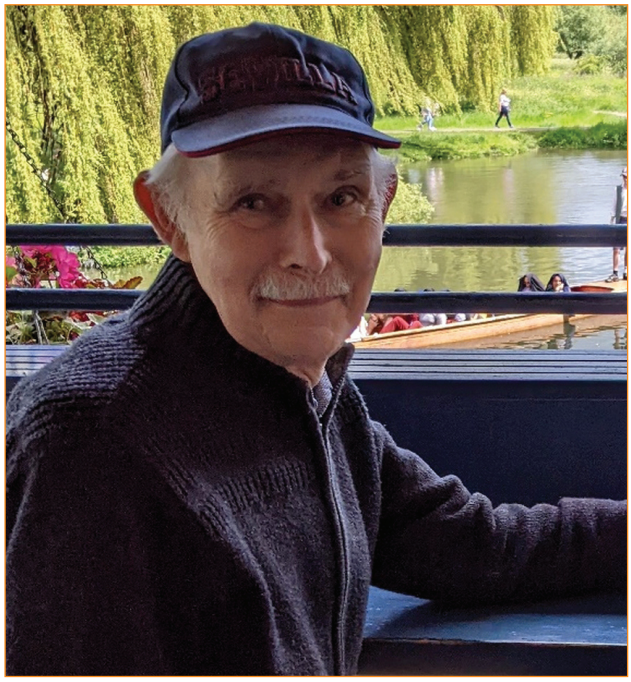
Warm regards,
Alex Stanley, IUCr CEO on behalf of **Prof. Santiago Garcia-Granda,** IUCr President

Please direct any questions or feedback to:
marketing@iucr.org

*The original IUCr logo from 1988 which was designed by **Giovanni Predieri** and **Susanna Ciribolla** both of Parma, Italy.*

Two variants of the new IUCr logo.

Obituaries



*The late **Prof Patrick J. McArdle**, Galway.*

Prof Patrick J. McArdle

Prof Patrick J. McArdle from the University of Galway passed away unexpectedly but peacefully, at home in Galway, surrounded by his family on the 2nd of January 2024, and was laid to rest in Rahoon cemetery, Galway on the 5th of January 2024.

Pat was a professor of inorganic chemistry with expertise in X-ray crystallography and nuclear magnetic resonance (NMR), who has published over 400 papers on a range of topics, from small-molecule pharmaceuticals, organometallics to carbohydrates. Born and raised in Drogheda, Co. Louth, Pat's first job was at his family hotel, The White Horse. He pursued his B.Sc and PhD (1962 – 1969) from University College Dublin (Tautomerism in Some Binuclear Metal Carbonyl Derivatives) and a D.Sc. (1989) from the National University of Ireland Galway (now University of Galway), where he worked until his passing. Pat was also the last academic staff member in Galway who gave chemistry lectures in Irish until he retired (as the Head of the School of Chemistry) from teaching in 2010. He was elected to the Royal Irish Academy on his first application in 1998.

Pat's research work initially concentrated on the organometallic chemistry of iron and later included the synthesis and reaction kinetics of quadruply-bonded metal complexes. He started working in crystallography in the early 1980s when the first four-circle diffractometer in Ireland was set up in Galway. He was one of the five founding PIs of the SFI- and industry-funded Synthesis and Solid State Pharmaceutical Centre (SSPC) in 2007. The setting up of this Research Centre, led by Kieran Hodnett at the University of Limerick, was very important for chemistry in Ireland as it was the first research centre funded by SFI which did research in chemistry. In the SSPC Pat's work concentrated on solid-state analysis of pharmaceutical solids, the use of sublimation for crystal growth and cocrystal synthesis, crystal growth mechanisms and theoretical analysis of solid-state interactions. Together with Pavel Karen (Oslo) and Josef Takats (Alberta), starting in 2009, he worked on an IUPAC project that examined the use of the oxidation state in chemistry. After 10 years of effort the first comprehensive definition of the oxidation state was produced together with an 86-page technical report. He was also a member of the IUCr commission that organised the meeting at Hyderabad, India in 2017.

Pat's passing is a great loss for the crystallography community as well as the University of Galway. Having trained under eminent scientists such as Jack Lewis at University College London and Massachusetts (1969 – 1972), Cambridge during his post-doctoral work, Frank Albert Cotton at Texas A&M (1978), Jack Norton at Princeton and Columbia USA and Guy Dodson at the University of York, UK (1991) on sabbatical, Pat developed a passion for crystallography and contributed novel computational methods for structural analysis. In 1996, he developed and published the ABSEN program to predict all possible space groups in different orientations from an HKL file. He also developed the ORTEX program to visualise ORTEP diagrams interactively. His interest in computing and crystallography led him to develop the OSCAIL software[1] that integrated several crystallographic tools and is widely used in Ireland to date.

Pat was a very hands-on researcher. Having sourced Ireland's first diffractometer in 1981 along with his colleague Desmond Cunningham, a second-hand Hilger & Watts Y290 4-circle diffractometer from Canada, he had the confidence to take it all apart and put it back together in a functioning form. He believed in innovation but also respected heritage. True to this, he never got rid of older goniometer set-ups when the diffractometers were upgraded and used them to train his students. These are still on display in the crystallography labs in Galway and are soon to be added to the National Museum of Ireland's National Scientific Instruments Collection. Pat sought to bring a modern influence on the direction of capital spending on facilities in the new Science building in Galway which opened in 1974. In collaboration with Prof. R.N. Butler, this effort also brought the first 100 MHz NMR spectrometer to Ireland which was followed by a ^{13}C spectrometer and the first high-field NMR spectrometer.

Pat was also an innovator who was not afraid of drilling a hole through a vacuum oven to modify it to control the temperature of his sample for the sublimation process to generate single crystals. He believed in sharing the knowledge he gathered. To that end, his YouTube channel has tutorial videos for the tools he has incorporated in OSCAIL, on how to set up a cyclone vacuum at home for cleaning, and as an avid cyclist, on how to prevent your cycle chain from falling out.

In his colleague Niall Geraghty's words, "Pat is a renaissance man", who could talk about any topic from molecular orbital theory, history, art, opera, film, theatre and politics. He was a man of outstanding intellect and someone who was interested in everything till the end. His very humble and gentle approach made him a great mentor and a great teacher. Reading through his condolences book reveals how many lives he touched and how many people owe their careers to his training.

His dedication was not just to science but also to his family. Pat is survived by his wife Aideen, children Orla, Eoin, Aideen Óg and their families, as well as his siblings and their respective families.

Anuradha Pallipurath
Leeds
Andrea Erxleben
Galway

References

1. McArdle, P. (2017). Oscail, a program package for small-molecule single-crystal crystallography with crystal morphology prediction and molecular modelling. *J. Appl. Crystallogr.* **50**, 320-326. https://doi.org/10.1107/S1600576716018446).

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As editor, I thought members would be interested in the following comments from the online book of condolences which are reproduced with permission of the authors.

"I had the pleasure of being trained by Pat in crystallography, having worked with him for my first post doctoral position from 2014 – 2017. Talking to him was like reading a textbook. He was so knowledgeable, but, so unassuming as well, which made him a great mentor. I owe my career in academia to his training and the conversations with him that sparked ideas that I am currently developing. Thinking of all his innovations like drilling through a sealed vacuum pump to precisely control temperature on the sample and the cyclone vacuum installation in his house that he told me about, makes me chuckle even now. I hope we all and most of all, his nearest and dearest find the strength to bear his loss. He shall live on in our fond memories."

Anu Pallipurath (Leeds)

"Very sorry to hear the news of Pat's passing. He is very fondly remembered by all who were lucky enough to meet him on his visit to York with colleagues to explore protein crystallography around 1990. He was great company and always full of entertaining anecdotes. Best wishes to all his family and friends."

Tony Wilkinson (York)

"My sincere condolences to the McArdle family. Pat was an extraordinary scientist, chemist, teacher and crystallographer. He had a wonderful way of putting chemistry into context and of course recounting his achievements and those of the many others he had met or worked with, was always riveting, mischievous and entertaining – many fond memories of the escapades we got up to during my PhD with him on trips to Daresbury and York. He will be sorely missed."

Martin Walsh (DLS)

"Pat's passing is a huge loss to Chemistry in Galway. Pat was a great person. He is most highly regarded by his students, to whom he was very helpful. He was also very helpful to his colleagues. He was a brilliant crystallographer and helped solve many structures for students and academic colleagues, which were included in numerous research publications and theses. He was passionate about Chemistry and all its developments and enthusiastic to discuss many topics. Pat was most helpful and supportive when I moved from Dublin to Galway in 2008 and in the following years, for which I am very grateful. May he rest in peace."

Paul Murphy (Galway)

***Dr Stephen Edward Tarling** (1960-2023). Photograph taken for Sway Council and used with permission.*

Stephen Edward Tarling (1960-2023)

Dr Stephen Tarling, who died suddenly from pancreatic cancer at the end of October 2023, was a larger than life figure. As an undergraduate he studied chemistry at the University of Surrey at Guildford, where he became interested in crystallography, no doubt as a result of the influence of Robin Shirley with whom he did his third year project. Robin started his PhD with Prof. Kathleen Lonsdale at UCL, so Stephen was following on in fine footsteps. Stephen then moved to the Department of Crystallography at Birkbeck College, where he studied for a PhD supervised by Prof. Paul Barnes and with co-supervision from Prof. Alan Mackay. For his thesis, he worked on the structure of pigments, and in particular ultramarine, as he had a case studentship sponsored by the Colours Division of Reckitt & Colman. I still recall a great talk he gave on the subject, probably at a BCA meeting, in which he discussed the importance of ultramarine in Renaissance paintings. At that time, ultramarine from *lapis lazuli* was a very valuable mineral pigment and would be used, for example, for the blue in the clothes worn by the Virgin Mary.

It was at around this point in time that I first encountered Stephen as a fellow PhD student. Paul Barnes had taken what appeared to be his whole research group, known as the Industrial Materials Group, to do an experiment at the Institut Laue Langevin, Grenoble. Working on D1A at that time, I regularly interacted with any British-based team visiting the ILL and I was immediately struck by this "cheeky chap" working on D1B on the other side of the guide tube to myself who was clearly enjoying his first visit to the ILL. I recall discussing powder diffraction with Stephen amongst other topics during his stay. I also learnt that the whole group had taken a ferry across the Channel to the Netherlands (which was perfect for Stephen as he was half Dutch) and had driven down to Grenoble, presumably as the Science Research Council in those days would only fund flights for 3 people.

Following that early meeting, I came across Stephen on several other occasions through BCA meetings. In particular, via Paul Barnes' contact with Mike Glazer in Oxford, Stephen started to use his expertise in PXRD to work in patent litigation. In particular, Stephen worked on many of the famous pharmaceutical patent cases from the late 80s to the early 90s and I can vividly recall him giving several enjoyable talks on this subject with Mike Glazer at BCA events. Stephen was clearly in his element in this field: he had a brain that was very quick on the uptake and he was well suited to answering the sort of questions that lawyers try to use to trip up unwary expert witnesses. In another career, he might well have become an excellent patent attorney.

Stephen was also a great teacher and, with Paul Barnes, taught crystallography in the Department of Archaeology at UCL in the late 1980s. Stephen's work on pigments led him to work with Anna Bennett, who worked at Birkbeck College and who researched objects for the British Museum, and in particular, whether the objects were genuine or fake. Stephen also examined historical material from Uppark House, a National Trust property in Hampshire, after it was ravaged by fire. Many years later following the restoration of the house, Stephen very kindly invited Martin Vickers and myself to view it at a special opening, even though I had had nothing to do with the analysis work. As I had no car at that time, Stephen even detoured on his trip from London in order to pick me up in his sports car. This was a typical example of Stephen's generosity.

On finishing his PhD, Stephen had a 5-year appointment with British Gas. Around that time, they consolidated their research facilities with their X-ray equipment being moved from London to Loughborough. When British Gas decided subsequently that they wanted to dispose of their Stoe transmission powder X-ray diffractometer, Stephen very generously tipped me off. The only condition: it was free for us to collect but it had to be collected by the end of the week! Needless to say, I leapt at the opportunity and I still recall dashing up the M1 with Martin Vickers in a small hire van to collect it, but unwittingly leaving behind around £10k of electronics, which were hidden out of sight behind an aluminium panel.

When Stephen's position at British Gas came to an end, he returned to a technical position he had held at the end of his PhD in the Department of Crystallography, for which he was well over qualified. Given that Martin Vickers, had by then been appointed to run the PXRD equipment within the Industrial Materials Group, Stephen was given the departmental role of interacting with the college Estates team. I am told that he ran rings around them: he was noted for his famous clipboard on which he noted everything down at meetings. At the following meetings when work had not been done as promised, he would then quote back to them all of their promises! In addition, Stephen became heavily involved in writing web pages to benefit the Department, a job he took on with gusto and especially to the benefit of those needing it most, for example, the facilities provided by the workshop technician Paul Stukas.

One of my final interactions with Stephen as a crystallographer was at a satellite meeting to the IUCr Beijing Congress in 1993. We both attended the Powder Diffraction meeting in Hangzhou, and we both met up with Robin Shirley. Stephen was an enthusiastic cyclist and so he persuaded us to rent bicycles so that we could get easily around the city, this being a time when bicycles were still the dominant form of transport within most Chinese cities. Stephen had always been keen on going to restaurants and so we ended up having some great meals out together as well.

The late 1990s saw a period of change in universities with lots of staff- and student-support roles being created. Stephen became a Scientific Staff Development Officer at Birkbeck College before moving down the road to UCL in the same role, oddly enough at about the same time the Industrial Materials Group at Birkbeck College moved to the Department of Chemistry at UCL, with the old Department of Crystallography becoming purely biological. Stephen subsequently moved to the University of Southampton in a similar role, an opportunity for him and his partner Anita to setup home in the village of Sway in the New Forest. At a celebration to mark Stephen's life last November, I heard from many local people about how Stephen had been the life and soul of the village. For a number of years, he had been an active local parish councillor as well as being a board member of the New Forest National Park Authority. As at Birkbeck College, he had brought his Internet skills to the fore again in creating local web pages for the benefit of others. At local fetes, he would interact with all of the stall holders, encouraging them when he could by buying local produce and, if not buying, encouraging them to sell their wares. Stephen's death came very suddenly: he had attended local meetings fortnightly as regular as clockwork, so it was notable when he missed one; by the next meeting he was sadly dead. Stephen will be missed by all of us who knew him well.

Jeremy Karl Cockcroft
UCL

As the editor, I can vouch for Stephen's tireless enthusiasm for the BCA, having seen him at many Spring meetings in the 1980's –1990's.

Meetings of interest

WHERE possible, information on the following meetings has been abstracted from the conference websites, where further details may be obtained.

Assistance from the IUCr website is also gratefully acknowledged.

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

British Association for Crystal Growth 2024 Annual Conference

Start Date: **Monday 1st July 2024**
End Date: **Wednesday 3rd July 2024**

We welcome abstract submissions for oral or poster presentations in the following categories: crystal features and engineering designs, molecular synthesis, crystal structure, molecular interaction, molecular simulation, computational modelling, thermodynamics, kinetics, process control, polymorph control and nanotechnology. The meeting will be held in Loughborough and more details may be found here: **https://www.bacg2024.co.uk/**

74th ACA Annual Meeting

Start Date: **Sunday 7th July 2024**
End Date: **Friday 12th July 2024**

The ACA Meeting is an annual event providing scientists from a wide variety of backgrounds the opportunity to exchange cutting-edge ideas and techniques in multiple areas of research. The meeting will highlight various aspects of crystallography and demonstrate their significance to the greater scientific community. Vendors display the latest technology at the exhibit show. More details of the meeting which will be held in Denver can be found here: **https://www.acameeting24.com/**

4th European School on Crystal Growth

Start Date: **Wednesday 17th July 2024**
End Date: **Saturday 20th July 2024**

European School on Crystal Growth (ESCG) has been an accompanying event to the European Conference on Crystal Growth since 2015. It is an opportunity to learn about basics and recent discoveries in the various research fields related to the growth of crystals during extended lectures given by scientists active in their research fields. We also foresee lectures on the growth of novel materials, various epitaxial growth techniques, methods of materials characterization and computer simulation of the growth processes. The meeting will be held in Jachranka near Warsaw, Poland. More details of the meeting can be found here: **https://eccg8.syskonf.pl/**

8th European Conference on Crystal Growth

Start Date: **Sunday 21st July 2024**
End Date: **Thursday 25th July 2024**

ECCG-8 will cover all topics related to bulk crystal growth, 2D-epitaxial growth, 3D-epitaxial growth, the relation between optical/electrical properties of crystals and their microstructure, crystallization in the semiconductor industry, crystallization in biology and medicine, crystal characterization methods. The meeting will be held in Warsaw, Poland and more details may be found here: **https://eccg8.syskonf.pl/**

Electron Crystallography School 2024 (ElCryS24)

The International Union of Crystallography (IUCr), IUCr Commission on Electron Crystallography, Special Interest Group for Electron Crystallography (SIG4) of the European Crystallographic Association (ECA) and Italian Crystallographic Association (ICA) are organizing the “Electron Crystallography School 2024" (ElCryS24) as a satellite event to the 34th European Crystallographic Meeting (ECM34), held in Padua, Italy. The school will take place right before ECM34, on 24 – 26 August 2024 in the Department of Geoscience in Padua. Details and further information can be found on the School website: **https://elcrys24.sciencesconf.org/**

ECM34

The European Crystallographic Association (ECA) and the Italian Association of Crystallography (AIC) are hosting the 34th European Crystallographic Meeting in Padova (Italy) 26 – 30 August 2024. The organisers of this event are **Gilberto Artioli** (Chair), **Giuseppe Zanotti** (Co-chair) and further details can be found here: **https://www.ecm34.org**

ILL and ESS European Users Meeting

Europe’s two multinational neutron facilities, warmly invite you to the ILL and ESS European Users Meeting. In 2018 the ESS and the ILL jointly inaugurated a collaborative European User Meeting, which has since been conducted biennially, alternating between each facility.

These meetings provide the opportunity to review the achievements of the user community, present the current status of ILL and ESS and, most importantly, to look forward to the scientific opportunities ahead for neutron science. In 2022 the meeting was held in Lund, Sweden. We are delighted to announce that this year’s event is scheduled for December 10–11 in Grenoble.

The event spans over two days, from noon to noon, featuring exclusively plenary sessions. Talks will outline the future landscape, and updates on the status of the ILL and ESS facilities will be presented, alongside scientific discussions on socially relevant topics. More details can be found here: **https://workshops.ill.fr/event/422/**

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