Crystallography News

British Crystallographic Association

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BCA Spring Meeting 15th-18th April 2019

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This month's cover:

Jubilee Campus invites us next spring; keen EPDIC-16 and SWSBC delegates

From the President

THIS is only my second column as President, and I already have to apologise for an error in my first. An eagle-eyed reader pointed out that John McGeehan is at Portsmouth, not Plymouth as I mistakenly typed last time. In fact, I knew this very well, but my fingers did not seem to agree, so my apologies are due to John, the team at Portsmouth and all my readers.

I am still finding my feet in this new job, but I have had the chance to meet my excellent team of Council Officers. Richard, Claire and Elizabeth are all impressively efficient, and I am looking forward to working with them, not least because it looks like my life will be easy with such strong support. Their hard work behind the scenes will not always have been evident to the members. I also attended a planning meeting for the 2019 Spring Meeting in Nottingham, and was impressed by the energy and enthusiasm of that team, with special thanks due to **Emma McCabe** as Programme Chair. I hope to see you all there next year.

I mentioned last time that we would soon be going to the Stanford Linear Coherent Light Source (LCLS) free-electron laser to try it out on our NiFe Hydrogenase crystals. As predicted, the weather outside was warm and sunny, but all the action takes place underground, with the end-stations at the end of a long sloping tunnel. We were part of a team of around twenty people, working on various metalloenzymes, with groups from the UK, Germany and the USA, using the the serial crystallography station MXI. When collecting our access badges, we were warned by the security officer to watch out for rattlesnakes, as it was apparently the season they like to be out and about. We were not sure how seriously to take this until several team members snapped pictures of rattlesnakes on their 'phones, not selfies I hasten to add, with one lounging across a footpath. This damped our enthusiasm for wandering around the site in the dark, although we suffered no casualties.

The LCLS was the first X-ray free-electron laser (XFEL), but there are now four others in operation, notably the more powerful European XFEL in Hamburg, to which the UK has recently signed up. XFELs use similar technology to synchrotrons, but employ long linear accelerators to generate much more intense, pulsed, coherent beams. The LCLS produces femtosecond pulses at up to 120 Hz, and each pulse results in 10^{12} photons arriving at the MXI station, orders of magnitude brighter than a synchrotron. The downside is that a single pulse instantly vaporises your precious crystal. The thermal explosion, however, happens on a much slower timescale than the diffraction event, so your data have been generated before the sample is destroyed (phew!). The result is one diffraction pattern collected per crystal, but each is a still, so large numbers of crystals are required, together with novel data processing techniques, to arrive at a full dataset of integrated intensities. Since only microcrystals are required, in large numbers, the crystallization experiment is changed from making a few good, large crystals to making millions of tiny ones, something of a culture shock to the hardened crystallographer.

In the first XFEL serial crystallography experiments, crystals were prepared as a slurry in buffer, and squirted in a liquid jet across the X-ray beam. This works, but is inefficient, with only a few percent of X-ray pulses striking a crystal in the liquid stream and generating an indexable diffraction pattern at the detector, leading to the consumption of large amounts of sample. The team we worked with use a tape, similar in size to an old-fashioned cassette tape, driven across the beam. Small droplets of crystal slurry are accurately spotted onto the tape by a piezoelectric device, synchronised to meet the X-ray pulses, giving a hit rate of over 90% with typically 10-50% pulses giving indexable diffraction patterns. In our particular case we had rather less than one ml of slurry with about $0.8x10^{7}$ hydrogenase microcrystals per ml. Running at 30Hz we collected 17,000 indexed diffraction patterns (i.e. crystals) leading to a complete high-resolution dataset. While this may not be the first choice of method for routine structure determination, it is invaluable for materials susceptible to radiation damage, such as metalloezymes where metal centres are rapidly reduced by X-ray exposure, and for dynamical studies of fast processes at room temperature. The tape transport system allows the crystals in the droplets to be exposed to specific stimuli, such as a laser flash or change of gases in the local environment at precisely timed moments before X-ray exposure, in experiments designed to capture reaction intermediates. XFELs are also useful in chemistry and materials science, such as studying fast chemical processes or electron-phonon coupling in crystals. The UK has an XFEL Hub at Diamond Light Source (DLS), funded by the Research Councils and Wellcome Trust, and any member of the UK scientific community can access advice and training on XFEL capability and use from them (see the DLS website).

I have been a crystallographer for 47 years, and a quick calculation shows that the 17,000 indexed diffraction patterns in that one, 10 minute experiment would correspond to collecting one pattern for every day of my crystallographic life, including holidays, and I would have had to prepare 600 crystals every day to generate the sample. Things have certainly changed since I started on a Weissenberg camera in 1971.

Congratulations are due BCA member **Richard Henderson**, who was made a Companion of Honour in the Queen's Birthday Honours List, a rare and prestigious award, and to **Elspeth Garman**, who has been awarded the 2018 Sosei Heptares Prize for Biophysics.

I should remind readers that nominations will be due for Council membership elections by September 30th, for Vice-President, Secretary and one Ordinary Member. **Richard Cooper** and **Claire Wilson** are not eligible for re-election, but **Anna Warren** has served one three-year term and would be eligible. Any two Members may make nominations for any vacancy. Such nominations should be accompanied by the written consent of the candidate to serve if elected, and must be received by the Secretary by the nomination deadline. I should also remind you that there some interesting meetings coming up, including the CCG and IG meetings on 31 October and 13-14 November, the BSG Winter Meeting at Imperial College on 17th December and, of course, the BCA 2019 Spring Meeting in Nottingham.

Simon Phillips

BCA Council 2018

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

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

From the Editor

I START with very sad news: my counterpart in the American Crystallographic Association, the Co-Editor of *ACA RefleXions*, Judith Flippen-Anderson, passed away on March 31, 2018. The staffing arrangement for this publication differs from ours: two Co-Editors as well as specialist editors for certain parts. Nevertheless, it was Judy, as a particularly long-serving Co-Editor, who enabled continuity and ensured that all parts fitted smoothly together. Judy was a generous person who was very helpful to me. When I wanted some information for *Crystallography News* about the workings of the ACA or new developments in crystallographic methodology originating in the USA and Canada or the development of North American facilities, Judy cheerfully provided it even though she was always very busy. When Joan and I came up to the registration desk at the start of an ACA meeting, we would usually find Judy there helping out the hard-working staff and welcoming old friends like us. This loyal support of the ACA came on top of a highly distinguished scientific career. She was a small-molecule crystallographer at the Laboratory for the Structure of Matter (Naval Research Laboratory) for 35 years. There she started out working with Isabella Karle using the Karles' direct methods, which many crystallographers at that time regarded as black magic, to solve important structures. I searched the Cambridge Structural Database for "Flippen" as author and came up with 519 hits! Until I got tired, I checked the author lists and verified that indeed they included "J. L. Flippen" or "J. L. Flippen-Anderson". She was elected to high office in the ACA and became President in 1991. She also made a major contribution to the successful launch of the journal *Structural Dynamics*. Judy will be much missed by her many friends on several continents.

The early summer is the time for several meetings covering specialised areas of crystallography. Because of their small size they may not get as much publicity as the ACA and European meetings, but their sharp focus endows them with great value to participants. I am grateful to the providers of reports on three such meetings which appear in this issue. **Pete Wood** reports on the annual CCDC Research Day, where the research students supported by this institution presented their research to an audience of fellow students, supervisors, CCDC staff and distinguished visiting scientists. **Tony Bell** has not only summarised the well-attended XRF meeting jointly sponsored by our Industrial Group and the Royal Society of Chemistry, but also encouraged / persuaded / arm-twisted five students into writing reports on this meeting. **Nic Harmer** and **Jenny Littlechild** describe the most recent meeting of the South West Structural Biology Consortium. This meeting, which migrates around various universities in the South West and took place at Exeter this year, provides a valuable opportunity for early career researchers to present their research, receive feedback on it and network with other researchers in the region. In addition, **Mark Senn** reports on the very successful inaugural Intensive School in Physical Crystallography offered by our Physical Crystallography Group.

One pan-European meeting recently took place in the UK. Dedicated to all aspects of the analysis of polycrystalline materials by diffraction methods, EPDIC16, the 16th European Powder Diffraction Conference was held in Edinburgh at the beginning of July. I thank **Tony Bell** once again for the write-up he has contributed on this important meeting.

As I write this column, the heat wave still dominates the news, and the disciplines of meteorology and climatology have attracted a great deal of public interest. Of course, these subjects have important implications for biology. As the climate warms, many life forms in the Northern Hemisphere adjust their range northwards. Crystallographers, being the highest form of life known to exist, appear to follow this trend. Our 2018 Spring Meeting was held at the University of Warwick. Next year's meeting will be in Nottingham, and it has recently been decided that the 2020 meeting will take place in Leeds. The distances between the respective venues are 90 km and 116 km in a generally northward direction. Long years of marking first-year practical reports have convinced me that three data points following a roughly similar trend are sufficient to support wild extrapolation. Given the average annual northward move of 103 km, I can confidently predict that the 2028 Spring Meeting will be held in Kirkwall, Orkney, which from Leeds is 811 km to the north.

But I have digressed from the main point of this discussion, which is to highlight the excellent programme that has been assembled for next year's Spring Meeting by the Programme Committee, chaired by **Emma McCabe**. This meeting will take place at the Jubilee Campus of the University of Nottingham from 15-18 April 2019. The details presented in this issue show that a distinguished panel of speakers for the named and plenary lectures has been assembled, and the session topics will both broaden and deepen your knowledge.

Of course, our Group Meetings will ensure that you don't need to wait until next spring for BCA stimulation. The Chemical Crystallography Group Autumn Meeting on October 31 at Queen's University Belfast will cover the topic of "Chemical Crystallography @ Central Facilities". The Physical Crystallography Group meeting held jointly with the ISIS Crystallography User Group, and for the first time this year also joined by the Diamond Crystallography Group, will be on 5th – 6th November 2018 at Milton Hill House near Didcot. The Industrial Group Autumn Meeting, which will take place on 13-14 November at Durham University on "Holistic approaches to structural characterisation", also specially welcomes Young Crystallographers. The Biological Structures Group Winter Meeting will be held on Monday 17th December 2018 at the Sir Alexander Fleming Building, Imperial College, London, and will end with a Christmas-themed reception.

Finally, I hope that all of you who teach at universities have had a relaxing summer and now can look forward to the influx of new students with happy anticipation rather than trepidation.

Carl Schwalbe

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Puzzle Corner

FUELS with oxygen in the molecular formula such as ethers tend to be easy to ignite. I propose the hypothesis that conference venues (cities) with a high content of O's in their name facilitate the ignition of productive discussion.

Of the venues for this year's ACA and ECA meetings as well as those listed in "Meetings of interest", which has the highest and which has the second highest percentage of O's in the name?

Answers to June Puzzle Corner

omercy… **cryo-EM**

openstart… **Patterson**

didectotherms… **direct methods**

ourfire… **Fourier**

flingapigperch… **charge flipping**

BCA Spring Meeting
15th – 18th April 2019, University of Nottingham

PLANNING is well underway for the 2019 BCA spring meeting to be held in Nottingham so please put the dates in your diaries! Details and titles for sessions are given below to give you time to think ahead to the abstract deadlines in January 2019.

Monday 15th April – Tuesday 16th April:
YCG Meeting

YCG Research
(Chairs: Natalie Tatum and Tom Roseveare)

The YCG satellite meeting is an opportunity for all early career researchers in the field of crystallography to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

YCG/CCG:
Galvanising science through outreach and social media
(Chairs: Elliot Carrington and Rachael Wilkinson)

The session will focus on how different methods of outreach can be used to teach and inspire the public about crystallography and its associated research.

Plenary: **Tim Easun**

Lonsdale Lecture:
Professor George Sheldrick (University of Göttingen)

SHELXT – dual space structure determination using the phases to determine the space group

Tuesday 16th April – Thursday 18th April:
Main Meeting

BSG:
Novel data collection strategies

Getting 'ideal crystals' for macromolecules has been the limiting factor for determining crystal structures. With the advent of novel diffraction techniques for micro/nano crystals, data collection strategies have accordingly evolved. This session will focus on novel data collection strategies such as 'Mesh and collect', line diffraction, *in situ* data collection, data collection of nano-crystals using micro/nanofocus instrument.

CCG:
I didn't know Mercury could do that!

PCG:
Local structure probes
(Chair: Helen Playford)

An understanding of local structure and disorder in crystalline materials is increasingly recognized as the key to understanding their functional properties. Negative thermal expansion, dielectric response, thermoelectric properties, ionic conductivity, the list goes on. In all cases, a clear picture of the local atomic arrangements is essential for understanding these physical phenomena and developing new materials for practical applications. This session invites contributions from a variety of fields, including total scattering/PDF analysis, X-ray absorption spectroscopy, NMR, and other techniques which aim to view structures from a local perspective.

BSG:
Complementary Structural Biology techniques

The session will focus on complementary structural biology techniques such as SAXS, NMR, Neutron diffraction, X-ray spectrometry that aid biological structure determination.

CCG:
Neat structures
(Chair: Lucy Saunders)

PCG/IG:
Surfaces of alloys and glass
(Chairs: Dr Tony Bell and TBC)

PCG Plenary: **Professor Igor Levin** (N.I.S.T.)
(Chair: Anthony Phillips)
Data fusion for determining atomic order on the nanoscale via the reverse Monte Carlo method

IG Plenary: **Professor Kevin Roberts** (University of Leeds)
(Chair: Helen Blade)
The Crystallisation Structural Pathway of Para amino Benzoic acid: From Solvated Molecule through Solute Clustering and Nucleation to the Growth of Facetted Crystals

BSG:
Alternative Crystallisation techniques

This session will focus on various crystallisation techniques for diffraction experiments using novel nucleants, novel buffer systems, membrane protein crystallisation techniques, crystallisation for serial crystallography etc.

PCG:
Energy materials
(Chairs: Tony West and Paz Vaqueiro)

IG:
Characterisation of surfaces
(Chair: Mat Bryant)

When manufacturing a crystalline product in industry, understanding the chemistry and structure present at the surfaces of crystals is every bit as important as understanding the bulk. In this session we will explore cutting edge techniques to characterise and study the surfaces of crystals.

Early Career Prize Lectures

BSG:
Computational structural biology

This session will focus on the synergy between simulation and crystallography to biological structure analysis and inform future functional studies. The session will include molecular dynamics, QM/MM simulations, fragment screening, molecular docking etc.

CCG:
Chemistry of voids
(Chair: Hamish Yeung)

IG:
Prediction and modelling of surfaces
(Chair: Helen Blade)

BCA Prize Lecture:
Professor Clare Grey (University of Cambridge)

BCA AGM and conference dinner followed by ceilidh.

BSG:
CryoEM and crystallography

This session will focus on Cryo-EM and crystallography as structural techniques and how both complement each other in determining large macromolecular structures.

CCG:
Crystallography in chemical research

PCG:
Magnetic structures
(Chair: John Claridge)

BSG:
Hot topics

PCG/YCG:
In-situ methods

PCG:
Topologically interesting materials
(Chair: Alex Gibbs)

BCA Industrial Group XRF Meeting

Sheffield Hallam University – 13th June 2018

THE annual X-Ray Fluorescence meeting took place at Sheffield Hallam University. The new venue helped to attract 90 delegates, almost twice the number who attended in 2017.

There was a change in the programme for this meeting compared to previous years. There were two parallel sessions in the morning, one for experienced users and one for beginners. The session for beginners was very well attended and provided a useful training opportunity for PhD students.

The meeting was well supported by representatives of 13 different companies. After the parallel sessions we then had the usual Sponsor Slot where these 13 companies were able to give short talks to publicise their latest developments.

After lunch everyone came together for the afternoon session. Of particular interest was a talk by Dr **Tom Knott** (University of Leicester) on how XRF was used to study the after effects of volcanic eruptions. The meeting was ended by a talk from Dr **Karen Vernon-Parry** (Sheffield Hallam University) describing her public outreach work using a hand-held XRF spectrometer for analysis of counterfeit coins.

Dr **David Beveridge** (Harmon Technology) came to the end of his term as chair of the BCA IG XRF committee so Dr **Tony Bell** (Sheffield Hallam University) was elected as the new chair.

Five student delegates have written meeting reports:-

Alex Borrill (Warwick University).

I attended the session for experienced XRF users, I found it to be informative and a good reminder of a lot of the theory and principles that are essential but that you don't consider on a daily basis. Several of the talks went through how particular parts of XRF have been developed or improved, such as detectors and methods to allow several labs to have comparable data. Although I do not consider myself to be a very advanced user of XRF I had already come across almost all of the concepts and points brought up during the morning session, I was expecting it to be a bit more advanced than it was. I particularly enjoyed the plenary session given by Dr **Tom Knott**, it demonstrated how both handheld and lab based XRF systems have their place in geological research as well as fascinating insights into his recent research in volcanoes. It was interesting to hear his account of his journey from a beginner to an experienced XRF user and some of the issues that can arise when comparing data taken in different places (other labs or in the field). Another interesting talk was presented by Dr **Karen Vernon-Parry** who uses handheld XRF for outreach projects, she talked about how it has enabled her to run successful sessions in identifying counterfeit coins, it's a great example of analytical science that has been made accessible and will hopefully spark interest in the fields of science and engineering.

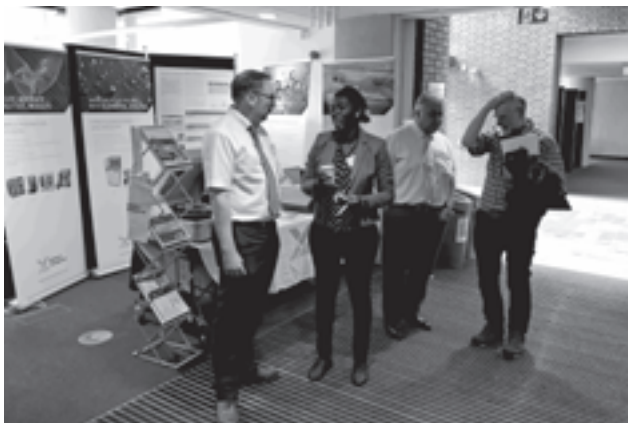
During the coffee and lunch breaks there were plenty of companies present to talk to, I learned about several new companies, suppliers and products that I was previously unaware of because of these breaks and the flash presentation session. I was able to make connections and discuss ideas and methods with more experienced people which was beneficial. Overall I found the conference to be a very useful experience.

Lygia Silva de Moraes (University of Strathclyde).

This X-Ray Fluorescence spectrometry meeting occurred on 13th June 2018 at Sheffield Hallam University. As a novice user I did not have a solid background in X-Ray Fluorescence, so I decided to attend in the morning Session 1, Introduction to XRF for Beginners. The session was chaired by Dr **David Beveridge** and started with a very enthusiastic introduction to X-Ray Fluorescence theory and use of statistics in XRF ministered by **Nick Marsh**. The presenter of the second talk in this session, **John Martin**, described the advantages and disadvantages between different techniques in XRF. It was interesting to observe those different techniques that can be chosen to optimize the experiment according to the target elements. The third talk of this session described the best techniques to prepare and mount the samples to make XRF spectrometry measurements were given by Dr **Rainer Schramm**. The last presentation in this session was a description of the applications using XRF in primary industries, manufacturing, regulatory, research and waste. The last presentation was delivered by **Phil Russell**.

There were very interesting talks in the Plenary Session. The first talk, by Dr **Tom Knott**, showed an overview about his research analysing composition of geological materials. Two of my favourite talks were in the end of the session, where **Christine Vanhoof** showed applications of Micro-X-ray fluorescence spectrometry (μ-XRF) in point analysis and imaging. The most interesting part of this talk was μ-XRF spectrometry being able to trace elements in the surface of the material, which can be useful in my research mapping the composition of the surface of crystal structures. Also, the last talk ministered by Dr **Karen Vernon-Parry** showed how XRF can be applied to analyse the high presence of Pb and Al in the composition of counterfeit old one-pound coins.

In summary, the conference was successful offering two parallel sessions in the morning for beginners and experienced XRF users. The talks in the Plenary Session showed XRF spectrometry as an important tool to analytical research and industry.



Nicole Reily (Warwick University).

The XRF users meeting was a very useful and interesting day. Despite using XRF the research group is not very familiar with the technique and it was a useful opportunity to talk to people who use and develop XRF technology regularly. The broad range of applications for XRF in industry, regulations, research and public engagement is extraordinary. Even within research the variation of samples, from bulk geological samples to mapping analysis of brain tissue, shows the diversity of the technique. The range of products at the conference shows the ongoing development of the technique and associated sample preparation. Often analytical techniques feel like mysterious boxes that output a number. The introduction to XRF for beginners provided a clear introduction as to how this technology works and how to ensure you utilise it effectively. Be this by trying different XRF devices or the importance of sample preparation to ensure efficient analysis. I particularly enjoyed the talk by Dr **Tom Knott** about the use of XRF in the geological laboratory. Having a fast and reliable method to confirm composition of strata as one super volcanic eruption on site saves a lot of sample processing and uncertainty before samples can be analysed.

Gloria Wie-Addo (Sheffield Hallam University).

This year's XRF meeting which was located at Sheffield Hallam University on the 13th of June 2018 was well planned out in my opinion especially for the beginner's sessions in which I enrolled.

As a user of the XRF at my department at SHU, I believe the selected modules: the theoretical introduction, different approaches to XRF, sample preparation and applications were very nicely arrayed for the novice. For example, the session held by **Nick Marsh** was so helpful but he had to rush through his presentation because of time constraints. These sessions gave me a great insight into the technique with its varying sample preparations and factors that affect the analysis which were related to my own studies.

The meeting also brought to our doorsteps the best companies whose products are constantly helping in the technique as well as having discussions and learning of their newest brands on the market.

Overall, the meeting was very satisfactory for both learners and companies who displayed their products to create awareness to XRF users.

My sincere thanks go to the organisers for this year's meeting and granting me the opportunity to be a part of the programme.

Prince Rautiyal (Sheffield Hallam University).

The meeting took place at Sheffield Hallam University this year and a huge number of delegates from academia and industry attended. The meeting was opened with a small plenary introduction about the agenda and the university by local host and organizer Dr **Tony Bell**. This was followed by two parallel sessions – one for the beginners and the other for the experienced XRF users.

The beginner's session was chaired by Dr **David Beveridge** from Harman Technology. **Nick Marsh** from University of Leicester talked about the "Theoretical introduction to XRF". I found this talk the most interesting talk from a beginner's point of view. The other interesting talk in the session was given by Dr **Rainer Schramm** from FLUXANA GmbH & Co. KG. He discussed the importance of sample preparation for the best results and for reducing the analytical errors. He also pointed out that considerations of sample depth and surface area are crucial while preparing sample and can have a greater impact on the results.

There was a sponsor slot kept for all the sponsor partners to pitch their innovative ideas and inventions of XRF analytical tools. This session was organized by **Nick Marsh** and assisted by Dr **Tom Knott** from University of Leicester. Each industrial sponsor partner was given three minutes to pitch their products and technology. It was a rigorous exercise but turned out to be a more fun and audience engaging activity.

After the lunch Dr **Tom Knott** gave a very interesting talk about the use of XRF in a geological laboratory. He discussed how XRF has been the first choice for years for geoscientists to analyse the chemical compositions of rocks which gave some very interesting geological research answers and is still helping the fraternity.

Finally, in the last session Dr **Karen Vernon-Parry** from Sheffield Hallam University delivered a talk about how hand-held XRF analysis can give on-site real time confirmation of counterfeit coins. Karen has been involved in this work for over five years.

AMT Bell (Sheffield Hallam University)

2018 CCDC Research Day

Introduction

THE Cambridge Crystallographic Data Centre (CCDC) hosts a research day each year when all the PhD students supported by the not-for-profit, charitable institution are invited to present their research to the organisation, their peers and a selection of high profile visiting scientists. This year we had eight students in attendance from the UK and USA, along with their supervisors, presenting an impressive breadth of research to the audience. We were lucky to have in the room such eminent visiting scientists as Jack Dunitz, Robin Taylor and Andrew Bond, as well as some of the CCDC Board of Trustees such as Judith Currano, Paul Raithby, Alessia Bacchi and Dave Martinsen.

Session 1

The 2018 CCDC Research Day was opened with welcoming remarks by **Pete Wood** (CCDC), who then introduced two impressive talks focussed on metal-organic research. **Matthew Reeves** (University of Edinburgh), took us on a tour of oxidation state assignment methods for transition metal complexes with one metal centre. The applicability of the Bond-Valence Sum (BVS) method can be increased by generating missing parameters used in the calculation with newly determined parameters from CSD data. The accuracy significantly improves when combined with the Lowest Energy Ligand Charge Method (MOPAC), which sums the individual ligand charges. The MLX method was then further introduced to address organometallic compounds. **Aurelia Li** (University of Cambridge), described the challenge of extracting useful information from a vast cloud of data. She discussed the creation of a subset of metal-organic frameworks (MOFs) from the Cambridge Structural Database (CSD). This subset was made simulation-ready for calculating properties relevant to gas adsorption applications. Aurelia analysed the adsorption properties for known MOF families and considered applying it to broader categories of porous materials.

Clare Tovee & Caroline Davies

Session 2

The second session was introduced by **Andy Maloney** (CCDC) and covered research focussed towards pharmaceutical solid form development. **Jakub Janowiak** (University of Leeds) began by outlining the value of the matched-molecular-pairs (MMPs) approach in molecular property prediction but pointed out that its application to the solid-state has so far been overlooked. He went on to describe his work in developing a large dataset of MMPs using the CSD, its subsequent application to solid state applications such as propensity of polymorphism, and finally some ideas for further work using graph neural networks. Next, **Bhupinder Sandhu** (Kansas State University) discussed the application of various stability assessment tools towards the understanding of complex solid-form landscapes, particularly polymorphs and co-crystals. Bhupinder described a systematic test set of compounds that were generated, computationally screened against a library of co-formers with multiple methods and then experimentally screened for co-crystal formation in the lab. It was determined that the CCDC's hydrogen bond propensity approach remains the most successful methodology for prediction of co-crystal formation. The session was rounded off with a fascinating talk by **Alexandru Moldovan** (University of Leeds) in which both the computational and experimental aspects of studying crystal-surface interactions were demonstrated. Alex began with a description of the computational modelling approach based on applying forcefield calculations to the interactions between two slabs of molecules. He then described the progress made in experimentally validating the approach, by functionalising an AFM tip with a single microcrystal to measure the adhesion to another crystal surface.

Mathew Bryant

Session 3

The last session, focussed on crystal and structure prediction of organic molecular crystals, was chaired by **Jason Cole** (CCDC). **Lucca Iuzzolino** (UCL) opened the session highlighting the concern of the pharmaceutical industry with polymorphism how computational techniques, such as crystal structure prediction (CSP), can help in this area. He outlined the challenges that CSP methods still face when dealing with very flexible, drug-like, molecules and how his research aims to reduce the computational cost and improve the CSP workflow. Luca showed very encouraging results with significant reductions on the computational cost of the CSP calculations of six drug-like molecules. The next presentation, by **Sarah Wright** (University of Manchester), also focussed on polymorphism. She explained how theoretical (knowledge-based and DFT calculations) and experimental approaches will be combined in her research looking at conformational molecular space and polymorphism risk assessment. She told us how computational techniques were applied to build a library of organic crystals with unusual molecular geometries, perhaps molecular conformations kinetically trapped in the solid form; and how this information will be used in crystallization screening. The last presentation, came from a very enthusiastic and recently started student, **Laura Straughair** (University of Strathclyde). She explained how theoretical and experimental approaches will be combined in her research with the final aim of developing new methods for predicting hydrate and solvate formation of small molecules. She outlined the progress of her project since she joined the PhD program in January; and how she has been familiarizing herself with the research and required techniques.

Angeles Pulido

Final comments

Overall the CCDC Research Day was an excellent reflection of the breadth of science taking place using, or connected to, the CSD. It was very noticeable also how important the **CSD Python API** has becoming in enabling most of these research projects. The quality of the presentations from this group of PhD students was very impressive and we look forward to hearing about the progress in each of these projects next year at the 2019 CCDC Research Day.

Pete Wood

16th European Powder Diffraction Conference (EPDIC-16) Report

THE EPDIC conference series started in 1991; I first attended EPDIC-2 in Enschede, Netherlands as a young scientist in 1992. 26 years later I went to Scotland to attend my 8th EPDIC at EPDIC-16 in Edinburgh. Even though this is the European Powder Diffraction Conference it is open to the world; I saw scientists from all 5 continents in Edinburgh.

As always the EPDIC conference was full of interesting scientific presentations. My personal highlights were:-

The conference opened with a fascinating plenary lecture; *New Opportunities at European XFEL* by **Robert Feidenhans'l**, the director of the European X-Ray Free Electron Laser (Schenefeld, Germany). I worked at the neighbouring DESY Laboratory in Hamburg 2009-2012 when XFEL was a tunnel digging project and construction site. It was good to see that XFEL is now an operational X-ray source which can give the opportunity to do ultrafast X-ray scattering experiments. The UK has now rejoined the XFEL consortium.

In-Situ Diffraction Studies of Uranium Oxides. How to safely reduce $SrUO_4$ at a beamline by **Brendan Kennedy** (University of Sydney) was also of interest to me as I started my career in the nuclear power industry before moving to work at a synchrotron. This work was done at the Australian synchrotron and neutron sources; this material is of interest as Sr fission products can react with UO_2 nuclear fuel.

There was an interesting session on new sources and instrumentation for powder diffraction. This included *DanMAX – The new materials science beamline at MAX IV* by **Mads Jørgensen** (Aarhus University / MAX IV Laboratory). This described the new Danish beamline under construction at the MAX-IV synchrotron in Sweden, expected to be available for users in 2020. This beamline will have two instruments, one for high resolution and the other with an area detector for large and bulky samples.

The winner of the Young Powder Diffractionist Award was **Stef Smeets** (Stockholm University) who gave a fascinating presentation entitled *Structure determination of polycrystalline materials using X-rays and electrons*. Electron diffraction measurements are made (in a TEM) on a moving sample to look at different parts of the sample; this can also give information on impurity phases. These results are combined with X-ray diffraction and ^{29}Si NMR to study the crystal structures of zeolites. I found this particularly interesting as I also study the crystal structures of silicate framework materials.

Pamela Whitfield (Excelsus, Switzerland) presented *Applications of PDF analysis to molecular organic compounds*. Pharmaceutical companies are interested in amorphous materials as they are more soluble. However, amorphous materials are a problem for powder diffractionists. Therefore PDF is used to get structural information but this work can be challenging as most pharmaceuticals consist of low Z materials and can have problems due to intermolecular distortion. This work is done by a spinoff company of the Swiss Light Source and it uses the SLS and other synchrotron sources for data collection. Radiation damage can be a problem although it is less of a problem with higher energy X-ray sources.

The co-chairman of the conference was Professor **Paul Attfield** (University of Edinburgh); I did my PhD with Paul at Cambridge in the 1990s where I studied Iron Oxides. Over 20 years later the Attfield group is still doing excellent work on Iron Oxides! *Unconventional magnetic order in $GeFe_2O_4$ and γ-$SiFe_2O_4$* by **Giuditta Perversi** (University of Edinburgh). These materials both have the spinel structure at ambient temperature but low temperature neutron powder diffraction shows both materials have low temperature incommensurate magnetically ordered structures.

High Pressure Synthesis and Characterisation of $MnFe_3O_5$ by **Ka Hou Hong** (University of Edinburgh).This material is isostructural with Fe_4O_5 and was prepared at high pressure. Synchrotron (ID22- ESRF) and neutron (WISH – ISIS) data show that this material also has a complicated low temperature structures. There are magnetic phase transitions and a Fe^{2+}/Fe^{3+} cation ordered structure below 60K.

Synthesis and characterization, by high pressure neutron powder diffraction, of the defect perovskite $He_{2-x}[CaZr]F_6$ by **Angus Wilkinson** (Georgia Institute of Technology). $CaZrF_6$ is a Negative Thermal Expansion material, the unit cell volume decreases and then increases with increasing pressure as He from the pressure cell medium is incorporated onto the perovskite A sites.

The conference ended with the EPDIC distinguished powder diffraction award lecture. *The power of powder diffraction* by **Bill David** (STFC, UK). Bill gave an entertaining talk on his illustrious forty year career in powder diffraction. Bill has worked on many different materials and has helped to produce some excellent crystallographic software.

EPDIC-17 will be held in Šibenik, Croatia 26th-30th May 2020.

Tony Bell, Sheffield Hallam University.

South West Structural Biology Consortium (SWSBC) Meeting

THE 17th annual meeting of the South West Structural Biology Consortium (SWSBC) was held in Exeter on 21st-22nd June. Researchers from across the south of England and Wales convened to discuss a broad range of topics in modern structural biology and related techniques. The meeting with over 100 delegates and exhibitors was hosted at the Living Systems Institute at the University of Exeter.

The SWSBC meetings offer the opportunity for early career researchers (PhD students, postdocs and junior group leaders) to present their research across a broad range of structural biology topics. The meeting includes plenty of time to allow researchers to network with others in similar fields across the region, and to discuss informally with more senior colleagues and exhibitors. The meeting included sixteen presentations from early career researchers, and nineteen poster presentations. The presentations covered a wide range of structural biology, including X-ray crystallography, electron microscopy, NMR, SAXS, molecular dynamics and other modelling techniques, enzymology and super-resolution microscopy. A common feature of the talks was the integration of multiple techniques to gain greater biological insight. The conference was treated to high quality presentations and posters. In particular, we were treated to an outstanding plenary lecture from **Helen Saibil** (Birkbeck) on cellular machinery for protein disaggregation. The prize for the best presentation was awarded to **Harry Austin** from the University of Portsmouth for his excellent presentation on the PETase plastic degrading enzyme. Poster prizes were awarded to **Amy Danson** of the University of Reading, **Marston Bradshaw** from the University of Bristol, and **Rhys Dunphy** from the University of Bath. The meeting also included a round table discussion of topics of interest to structural biologists at all career stages which included industrial colleagues. Workshops on the latest CCP4 software developments regarding DIALS and GUI2 from Luis Fuentes-Montero and Kyle Stephenson were well received. The SWSBC meeting especially acknowledges the generous sponsorship from CCP4, and from the commercial exhibitors who attended the meeting. We look forward to the 2019 SWSBC meeting, which will be held at the University of Reading.

Nic Harmer and **Jenny Littlechild**
University of Exeter

Dr Bertram Daum (right) presented poster prizes to (l-r) *Amy Danson*, *Marston Bradshaw* and *Rhys Dunphy*.

1st Intensive School in Physical Crystallography

1st Intensive School in Physical Crystallography: From Phonons to Phase Transitions, 18th – 21st June 2018.

THE Physical Crystallography Group (PCG) of the British Crystallographic Association was pleased to be able to offer its first residential school in physical crystallography in Abingdon, Oxfordshire, UK in June 2018. Planning for the School started back in January 2017 when the organising committee consisting of myself, **Mike Glazer**, **John Claridge** and **Nick Funnell** undertook the initial task of shortlisting topics for the school. We quickly homed in on the key material that we felt would be most beneficial to the community, from which everything else followed naturally. We decided for the first run of the PCG School we would focus on phase transitions since the study of this topic is what unites all physical crystallographers. We were keen to include topics such as phonons and Landau theory in this that are not so commonly taught as part of postgraduate courses. We were delighted that **Martin Dove** and **Michael Carpenter** were willing to take on these topics and keen to be involved in this new project. The course was structured to follow the path of a soft mode phase transition, with the final line-up of Mike Glazer for a review of symmetry and reciprocal space, Martin Dove for phonons, myself for irreducible representation analysis, Michael Carpenter for Landau theory and John Claridge for incommensurate phase transitions. Our ambitious plan was now to fit this program into a 3.5 day intensive residential school. We were very fortunate in receiving substantial sponsorship from The ISIS Neutron and Muon Source, as well as contributions from Diamond Light Source and the Institute of Physics. This meant that we could hold the event with a substantially reduced residential registration fee of £240, whilst still being able to make use of STFCs unique Cosener's House venue situated in the picturesque town of Abingdon-on-Thames. A special thanks goes to Nick Funnell here, who took on the bulk of the local organising leading to a seamlessly run school.

On midday on the 18th of June 2018, after months of planning, we were finally ready to welcome the 40 school participants, many who had travelled from afar. Registration for the School had far exceeded our expectation, making it a tough process shortlisting the candidates for the school. The final list or course participants included PhD, Post docs and early career academics from the Netherlands (5), Germany (2), USA (1), South Korea (1), Australia (1) Spain (1) France (1), Republic of Ireland (1), with the rest coming from all around the UK.

continued >>>

Science & Technology Facilities Council
ISIS Neutron and Muon Source

diamond

IOP Institute of Physics

S
P C G
M
P

Mike Glazer opened the school with a review of point group and space group symmetry for his first lecture, before developing the idea of reciprocal space, the appreciation of which would be crucial for the students' understanding in the following lectures. After a coffee break during which the sunshine and beautiful surroundings of Cosener's House could be enjoyed, it was back to work. Mike had prepared a lovely practical exercise helping the students gain familiarity in identifying symmetry elements, and helping them appreciate how the International Tables of Crystallography Volume A is constructed.

As we had promised the students, the school would be intensive, which meant that after a three-course meal served back in the main building of Cosener's House, we returned to work. This time it was a poster session giving students the chance to present their work to each other, and it was also a great chance for the lecturers to get an idea of the research areas that the students were working in. I particularly enjoyed this session and was impressed by both the breadth and diversity of research topics covered by the course participants, and by how many students stayed on well past the point at which the free drinks ran out!

One Tuesday morning, fuelled by a full English breakfast, **Martin Dove** took the reins. He started out with a nice historical introduction to the field of lattice dynamics, before diving into the detail behind phonons and normal modes. The links between the theory of soft phonon mode phase transitions and Landau was beautifully made, and Martin finished his lectures with some nice example of the effect of rigid unit mode motion on phonon dispersion and diffuse scattering. This tour de force, followed by a practical session using GULP, took the student through from 9 am to 5pm – interspersed with plenty of breaks of course!

I was up next. I was a little nervous, not least as I had scheduled my lectures for the shift before and after dinner in what I appreciate was already a very long day for the students. My goal was to describe the language through which symmetry-breaking events can be classified according to irreducible representations. I was keen for the students to grasp that this symmetry-breaking could be instantaneous, such as the dynamic fluctuations induced by phonons, or that it could be related to the order parameters describing the long-range ordering occurring at phase transitions. My tutorial session, which saw the students return fresh-faced on the Wednesday morning, sought to reinforce these concepts through several exercises, using ISODISTORT to analyse phase transitions and degeneracy in phonon dispersion curves.

It was then over to **Michael Carpenter** who gave a very nice illustration of how the coupling between primary order parameters and strain can be used to study the nature of phase transitions, within the framework of Landau theory. As well as providing practice at performing this kind of analysis, the tutorial sessions explored how, once the Landau potential has been constructed, a host of other thermodynamic quantities can be derived and interrogated. It was particularly impressive to see the enthusiasm and stamina of the students throughout these sessions, who, even come the evening, were still working hard at problems and asking questions.

We felt it was also important for the students to appreciate how experimental measurements probing lattice dynamics can be made and interpreted, and in this respect we were very lucky to have two guest speakers on Wednesday afternoon from the ISIS Neutron and Muon Source. **David Voneshen** and **Matthias Gutmann** talked about their research interests around inelastic neutron scattering and diffuse scattering, providing an extra dimension to the school's curriculum. Even after such an action-packed Wednesday, I was pleased to see that a substantial number of students found the energy to soak up the last rays of sunshine by the river Thames, over a drink or two at the Nags Head Pub.

On Thursday morning it was over to **John Claridge** who gave an introduction to the superspace formalism and incommensurate crystallography, before diving into many intriguing examples of incommensurate phase transitions in functional materials. These ranged from site occupancy modulation in thermoelectrics, to lone pair and incommensurate tilt ordering in ferroelectric materials. For the final tutorial session, the students were let loose on refining incommensurately modulated structures in the program Jana2006.

As lecturers, we were very impressed by the calibre of the students, and their enthusiasm which was sustained up until the final session. For me, this is what really made the school so special. We hope to return for the 2nd PCG School in Physical Crystallography in 2020, but in the meantime the lecture material is available online for all to enjoy:

https://pcgschool2018.wordpress.com/lecture-notes/

Mark S Senn
University of Warwick, UK

Free, Unified Deposition and Access of Crystal Structure Data

THE Cambridge Crystallographic Data Centre (CCDC) and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karlsruhe) announced the launch of their joint deposition and access services for crystallographic data across all chemistry. These services will enable researchers to share data through a single deposition portal and explore all chemical structures for free worldwide.

"With this joint depot, FIZ Karlsruhe supports the community's need for a reliable infrastructure for research data from crystallography." says **Sabine Brünger-Weilandt**, CEO from FIZ Karlsruhe. *"Providing freely available research data for all chemistry is in line with our claim to Advancing Science. The announcement of the cooperation between CCDC and FIZ Karlsruhe was already enthusiastically received by the community. We are convinced that we can meet the high expectations with the new joint depot."*

The Chair of Trustees for the CCDC is equally excited about the impact of this launch to researchers worldwide: *"All information users, whether they admit it or not, wish that all of the information that they require was in a single location. Failing that, they are searching for a "magic bullet" that will hit exactly what they want; they want to be able to use a simple interface and locate all of their information needs. By unifying the deposition and access of organic, metal-organic, and inorganic crystal structures we get a little closer to that magic bullet, at least in the area of crystallography, and make researchers' lives that much easier."* says **Judith Currano**, Chair of Trustees for the CCDC and Head of the Chemistry Library at the University of Pennsylvania.

Recent advances in chemistry have meant that the distinctions between inorganic and organic structures have become blurred, for instance through research to design new batteries, gas storage systems, zeolites, catalysts, magnets, and fuel additives. This, coupled with the desire from researchers for more integrated databases, has been the driving force behind the development of these joint services.

As a result, researchers and educators worldwide, working across all fields of chemistry, are able to explore over one million crystallographic structures through a joint Access Structures service enabling them to view and retrieve deposited datasets associated with structures in the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD).

Crystallographers can deposit organic, inorganic and metal-organic structures through a unified deposition service. This features a streamlined online portal for easy submission and integrates a variety of checks to alert researchers about the validity, integrity and originality of their data. Additional features include the rapid assignment of deposition numbers and the ability for depositors to choose to share their data immediately through an appropriate database. Alternatively, data destined for inclusion in a scientific article is automatically shared at the point of publication through workflows with most major publishers. Anyone looking for structures previously stored in the FIZ Karlsruhe depot can still find them using the published depot number.

All of the existing expert data curation and publishing processes will remain in place, ensuring that users will still have access to the high-quality data and advanced analysis capabilities on which they can depend. The highly curated CSD and ICSD databases and their associated advanced software will continue to develop and to be available independently from the CCDC and FIZ Karlsruhe, respectively.

To use these joint services go to:

www.ccdc.cam.ac.uk/structures for access

www.ccdc.cam.ac.uk/deposit for deposition

For more information about these joint services, please go to the CCDC or FIZ Karlsruhe websites:

www.ccdc.cam.ac.uk

www.fiz-karlsruhe.de

And for more information about this announcement please contact:

Suzanna Ward
CCDC ward@ccdc.cam.ac.uk

Helmut Mueller
FIZ Karlsruhe Helmut.Mueller@fiz-karlsruhe.de

The CCDC welcomes Jürgen Harter as CEO

THE CCDC is pleased to announce that Dr Jürgen Harter has accepted the position of CEO of the Cambridge Crystallographic Data Centre (CCDC). Jürgen is a highly commercially driven scientist, who has acquired more than 20 years of life sciences, information technology, and big data expertise in the biopharmaceutical domains by working at companies such as Horizon Discovery Group plc, ExcoInTouch Ltd., CambridgeSoft Ltd., Abcam plc and BioWisdom Ltd.

Jürgen holds a PhD in organic chemistry from the University of Cambridge (Whiffen Lab – Prof. S. V. Ley), and carried out his postdoctoral research at the Unilever Centre for Molecular Informatics Cambridge (UCC) on eScience and chemical information management (Prof. R. C. Glen/Prof. P. Murray-Rust).

In his most recent role as Global Head of IT & Informatics, Jürgen grew and managed several teams and integrated the IT infrastructure and system landscape of the various acquired biotech companies into Horizon Discovery Group plc. On a company-wide level he has been instrumental in establishing, delivering and evolving a range of complex commercial and scientific systems with corresponding processes and workflows. Some examples are Horizon's global ERP deployment, the CRM, a new eCommerce platform and consolidated website, the gene editing cloud platform and a number of underlying databases containing bioinformatics and genomics data. In his work as Director of Business Development at ExcoInTouch, Jürgen drove the incorporation of innovative digital engagement and data capture solutions (mobile-first) into major pharmaceuticals and CROs for the efficient running of clinical trials and the handling of big clinical data. This included deployment of cloud-based mHealth platforms, placing patients at the heart of every program. While working at CambridgeSoft (later Perkin Elmer Informatics), he orchestrated a number of ELN / LIMS deals, pushed superior lab automation methods, and generally drove the sale of a suite of software products (e.g. ChemBio Office) & services. Prior to that, Jürgen headed Abcam's scientific business development department, managing collaborations and networking activities, and setting scientific strategies for core research areas. This included the building and utilisation of an expert system to help predict commercial intelligence and scientific advances. As Senior Chemistry Analyst at BioWisdom, he engineered and automatically produced the content of a chemistry ontology, integrating it into a huge and dynamic life sciences knowledge map.

The Board of Trustees is delighted with the outcome of the search and looks forward to working with Jürgen in the coming years. Jürgen cares passionately about digital transformation, big data (particularly generating value and insights), knowledge management and scientific and business intelligence. He has worked on complex projects with most of the Top 20 pharmaceutical companies and has a wide global network of connections in both the biotech and pharma sectors. This is combined with links to information management and software development companies, where he is keen to utilise their transformative and innovative technologies to the CCDC's advantage and to create further value and growth over the years to come.

In response to his appointment, Jürgen stated, *"I would like to stress that it will be an absolute privilege to lead the CCDC into the future and to serve the world-wide science community where crystallography data and its related software play an important role. I am very happy to bring to bear all my experience and network to help the Centre and its employees, and to work on fulfilling its vision and mission. I am very excited to be joining such a great team of people with excellent science and gold-standard data behind them."*

Please join us in welcoming Jürgen to the CCDC family!

Judith Currano
Chair of Trustees
Cambridge Crystallographic Data Centre

Meetings of interest

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

3-6 September 2018
Photon 2018, Birmingham.
http://www.photon.org.uk/516760

3-7 September 2018
EChemInfo workshop. Training and Innovation Course in Drug Design, Didcot.
http://www.echeminfo.com/events/echeminfo-oxford-2018

3-7 September 2018
XTOP2018. XIV Biennial Conference of High Resolution X-ray Diffraction and Imaging.
http://www.ba.ic.cnr.it/xtop2018/

3-7 September 2018
Synchrotron Radiation and Neutrons in Art and Archaeology, Portsmouth.
http://www.diamond.ac.uk/Conference/SR2A-2018.html

3-14 September 2018
22nd Laboratory Course Neutron Scattering, Juelich and Garching, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html

9-13 September 2018
29th Annual Meeting of the European Society for Biomaterials (ESB2018), Maastricht, Netherlands.
http://www.esb2018maastricht.org/

9-14 September 2018
19th International Microscopy Congress. IMC19, Sydney, Australia.
http://imc19.com/

10-11 September 2018
Scottish Centre for Macromolecular Imaging – Symposium and opening, Glasgow.
http://www.facebook.com/SCMICryoEM

12-14 September 2018
First Serial Millisecond Crystallography (SMX), Paul Scherrer Institut, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?confId=6479

13-14 September 2018
10th International Workshop on Radiation Damage to Biological Samples, Brookhaven, Upton, NY, USA.
http://www.bnl.gov/rd10/

13-16 September 2018
ESCG2 Second European School on Crystal Growth, Varna, Bulgaria.
http://escg2.eu/

16-19 September 2018
8th Conference on Electron Tomography, Les Diablerets, Switzerland.
http://www.colorado.edu/symposium/etm2018/

16-19 September 2018
Neutrons and Biology, Carqueiranne, France.
http://sites.google.com/view/bioneutrons2018

16-20 September 2018
ECCG6 Sixth European Conference on Crystal Growth, Varna, Bulgaria.
http://eccg6.eu/

16-21 September 2018
Synchrotron Radiation School (SR school 2018), Oxford and Diamond Light Source.
http://www.diamond.ac.uk/Home/Events/2018/SR-Summer-School.html

16-21 September 2018
SSC2018. 13th International Conference on Solid State Chemistry, Pardubice, Czech Republic.
http://www.ssc-conference.com/2018/

17 September 2018
2018 E-MRS Fall Meeting and Exhibit, Warsaw, Poland.
http://www.european-mrs.com/meetings/2018-fall-meeting

20-22 September 2018
HEC 21. 21st Heart of Europe Bio-Crystallography Meeting, Quedlinburg, Germany.
http://hec21.uni-halle.de/

22-25 September 2018
SEG2018. Metals, Minerals and Society, Keystone, CO, USA.
http://www.seg2018.org/

23-27 September 2018
Hot Topics in Contemporary Crystallography – HTCC, Bol (island of Brač), Croatia.
http://htcc2018.org/

24-28 September 2018
ICDD Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

24-28 September 2018
MDANSE: Molecular Dynamics and Lattice Dynamics to Analyse Neutron Scattering Experiments, Puerto de la Cruz, Tenerife, Spain.
http://www.isis.stfc.ac.uk/Pages/MDANSE-2018.aspx

26-29 September 2018
7th Murnau Conference on Structural Biology, Murnau, Bavaria, Germany.
http://www.murnauconference.de/conference_2018/index.php

1-5 October 2018
4th Biannual international Conference "BIOMEMBRANES 2018", Dolgoprudny, Moscow region, Russia.
http://biomembranes2018.ru/

5-7 October 2018
9th International Conference of the Hellenic Crystallographic Association, Patras, Greece.
http://sites.google.com/view/hecra2018/home

7-12 October 2018
SAS2018. XVII International Conference on Small-Angle Scattering, Traverse City, MI, USA.
http://sas2018.anl.gov/

8-14 October 2018
ASMOSIA XII – Association for the Study of Marble & Other Stones in Antiquity XII, Izmir, Turkey.
http://asmosia2018.com/

16-19 October 2018
Neutrons and Food 5, Sydney, Australia.
http://www.ansto.gov.au/Events/Neutronsandfoodconference2018/index.htm

29 October – 1 November 2018
JCNS Workshop 2018, Tutzing, Germany.
http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/JCNSWorkshops/2018Workshop/_node.html

31 October 2018
BCA Chemical Crystallography Group Autumn Meeting, Belfast.
http://ccg.crystallography.org.uk/

5-6 November 2018
BCA Physical Crystallography Group Autumn Meeting, Didcot.
http://www.pcg-scmp.org/Main_Page

11-13 November 2018
Protein Structure Determination in Industry. PSDI2018, Versailles, France.
http://www.synchrotron-soleil.fr/en/events/psdi-2018-26th-protein-structure-determination-industry-meeting

13-14 November 2018
BCA Industrial Group Autumn Meeting, Durham.
bca@hg3.co.uk

2-5 December 2018
AsCA 2018/Crystal32: 15th Conference of the Asian Crystallographic Association and 32nd Conference of the Society of Crystallographers in Australia and New Zealand (SCANZ), Auckland, New Zealand.
http://asca2018.org/

17 December 2018
BCA Biological Structures Group Autumn Meeting, London.
http://bsg.crystallography.org.uk/

28 January – 2 February 2019
2nd Pan African Conference on Crystallography (PCCr-2), Accra, Ghana.
http://www.pccrafrica.org/

11-22 March 2019
50th IFF Spring School: "Scattering! Soft, Functional and Quantum Materials", Jülich, Germany.
http://www.fz-juelich.de/pgi/EN/Leistungen/SchoolsAndCourses/SpringSchool/

15-18 April 2019
BCA Spring Meeting, Nottingham.
http://www.crystallography.org.uk/spring-meeting-2019/

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

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

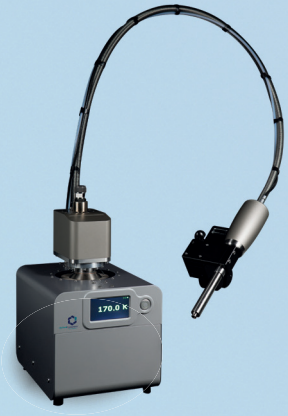
17th Intensive School on X-Ray Structure Analysis

Durham, UK, 6th April – 14th April 2019

https://community.dur.ac.uk/durham.x-ray-school/

The renowned Intensive Schools on X-ray Structure Analysis provide participants with a fantastic opportunity to gain a breadth and depth of crystallographic knowledge that they may previously have thought unattainable within a warm and collegial atmosphere.

Information about next year's school can be found on the website detailed above. The timing of the school is particularly convenient as the school will finish on the 14th of April 2019, and the BCA Spring meeting will commence, with the YCG Satellite Meeting, on the afternoon of the 15th of April in Nottingham.



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