Crystallography News

British Crystallographic Association

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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.

Contents

This month's cover:

Pictures of ECM31 by Lucy Saunders and Andrew Maloney; Prof. Yoshinori Fujiyoshi at eBIC

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From the President

BACK in the June heat wave, I spent a rather sweaty, but enjoyable, few days at the UKSR50 meeting in Liverpool, basking on the sun-drenched shores of the Merseyside riviera. UKSR50 was a celebration of 50 years of synchrotron radiation (SR) in the UK, covering both the history and current advances, as well as including a hearty slice of crystallography. The meeting brought together an interesting group of VIPs, visionaries from the early days of the field, and current research leaders. The list of achievements is stunning, not least in crystallography.

The NINA synchrotron was built in 1964 at the Daresbury Laboratory as a research tool for nuclear physics. The SR produced was a by-product, and regarded as a nuisance by the nuclear physicists. **Ian Munro**, a lecturer in the Department of Physics at the University of Manchester, wrote a letter to the director at Daresbury in 1967, suggesting that the SR could be useful for experiments requiring intense beams of electromagnetic radiation, such as X-rays (and, obviously, crystallography). In response to this visionary suggestion, beamlines were built on NINA, and trial experiments took first beam in 1968. These were so successful that they led to the construction of the first of the second-generation sources dedicated to SR, the Daresbury Synchrotron Radiation Source (SRS) that took first beam in 1980. The successes of the SRS, and its illustrious successor Diamond Light Source, are now accepted as commonplace by crystallographers. In my own area of biological crystal structures, five Nobel prizes have been awarded that depended critically on the use of SR. The first of these was to **John Walker** for the structure of ATPase done, of course, at the SRS. The protein crystallographers were enthusiastic early adopters of SR, rapidly populating new synchrotrons worldwide with beamlines able to cope with large unit cells and rapid X-ray damage. Small molecule crystallographers and materials scientists joined in, with the high photon flux allowing for data collection from small, weakly diffracting samples, as well as the tuneable wavelength capability allowing for discrimination of heavy atom oxidation states, the ability to collect data fast enough to allow *in situ* dynamic studies, and study of materials under extreme conditions.

While listening to the talks I mused on the interesting history of detectors in crystallography. Fast and sensitive X-ray area detectors have been critical to the success of SR, but the history of detectors in crystallography has cycled back and forth between different technologies. The first detector was photographic film (and here I apologise to younger crystallographers with mobile 'phones and digital cameras who have probably never seen it). This was what **von Laue** used to show that crystals could generate X-ray diffraction patterns. The **Braggs**, however, used an X-ray spectrometer to measure the diffraction from NaCl and show how crystal structures could be determined. This instrument was essentially a single-counter X-ray diffractometer. The first four decades of crystallography were, however, dominated by the use of X-ray film again, both for the smaller molecules studied initially, and for the more complex biological molecules, such as penicillin and insulin by **Dorothy Hodgkin** and haemoglobin by **Max Perutz**. In the late 1940s, **Uli Arndt** built a powder diffractometer with a Geiger counter detector, followed by a single-crystal linear diffractometer at the Royal Institution, aimed at obtaining accurate intensities from protein crystals. He went on to develop the single counter four-circle diffractometer, with **Terry Willis**, which rapidly became popular for both large and small molecule data collection with neutrons and X-rays. As the macromolecular crystallographers moved on to larger proteins with larger unit cells, the inefficiency of measuring one reflexion at a time, when a number were in the diffracting position, drove them back to film (again), using the screenless rotation-oscillation camera, another **Uli Arndt** design (with **Alan Wonacott**). This allowed large numbers of reflexions to be recorded simultaneously, but the films needed processing and they are not simple photon counters. Crucially, this also coped with the huge increase in flux at synchrotrons. The small molecule community stuck with the diffractometer, since fewer reflexions were available simultaneously from smaller unit cells so there was little to be gained from film. This divergence was maintained when the image plate came along, and replaced film in the rotation camera. The ideal detector, however, is a position-sensitive electronic area detector (real-time electronic film), and these soon came along, first as multiwire chambers (essentially 2D Geiger counters) with limited dynamic range, then CCDs, which are not photon counters, and now the latest range of pixel detectors, such as the Pilatus, able to cope with enormous fluxes from SR stations and free-electron lasers. These are also good for small molecules, so the two communities have finally reunited. History clearly has a habit of repeating itself in X-ray detectors as in human affairs, but at least the crystallographers are making forward progress.

I am delighted to announce that, following nominations from the membership, Council has decided to award **John Helliwell** and **Sandy Blake** Honorary BCA membership. These awards have been made in recognition of significant contributions by the recipients, both to crystallographic science and to the work of the BCA. Congratulations are also due to **Sir Gregory Winter**, **George Smith** and **Frances Arnold** on the award of the 2018 Nobel Prize for Chemistry, recognising their work in using molecular evolution to generate novel synthetic antibodies and enzymes. You may wonder what this has to do with crystallography, but crystal structures were key to the work. Greg and Frances may not be card-carrying crystallographers themselves, but each has a good clutch of crystal structure entries to their name in the Protein Data Bank.

I am pleased to report that nominations have been received for the all the positions in the Council membership elections. I would encourage all members to use their votes, having read the candidates' statements. Electronic voting is easy. I should also remind you to register for the BCA 2019 Spring Meeting in Nottingham.

Simon Phillips

BCA Council 2018

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

From the Editor

BECAUSE of two cataract operations I didn't indulge in my usual peripatetic lifestyle of conference-going this past summer. Therefore I couldn't give you a travelogue through parts of North America, Europe and crystallography. I am very grateful to the authors who have contributed words and pictures about the conferences and schools that they have attended. For a lot of BCA members the "Big Event" was the European Crystallographic Meeting in Oviedo, Spain. Lucy Saunders contributed the pictures of the venue and the meeting along with culture and scenery of Asturias that appear on the cover and on an inside page. You can see the modernistic conference centre, the cultural entertainment in the opening ceremony featuring traditional musicians playing the Spanish version of bagpipes, Christer Aakeröy giving a particularly stimulating keynote lecture on "Transforming co-crystals from form to function", a classic Asturias dish of cachopo (breaded meat layered with cheese and served with different toppings), the beautiful classical concert associated with the conference and the CCDC leader board ranking diversity in CSD entries. Participants weren't confined within the city; the conference excursion took them to the spectacularly beautiful Lago de Enol (pictured) in the Picos de Europa. Remembering my organic chemistry, I did wonder if there is also a Lago de Keto. Once again the energetic Young Crystallographers held a stimulating satellite meeting, which Andrew Maloney tells us about.

Recognition for the greatest distance covered goes to **Richard Cooper**, who reports on the Zurich School. You may think "Zurich isn't that far away"… but this is their "branch office" in Tianjin, China! Despite the distance, it featured a stellar array of European tutors along with enthusiastic and diligent Chinese students. **Brian Tanne**r brings us news of another important meeting in a relatively far-away corner of Europe: XTOP2018 "14th Biennial Conference on High Resolution X-ray Diffraction and Imaging" in Bari, Italy.

There was one important event that I was very glad to have attended: the official opening of eBIC, the electron Bio-Imaging Centre at the Diamond Light Source. One might have worried that Diamond, with its massive investment in apparatus and personnel for synchrotron science, could have been sceptical about, or even hostile to, this alternative method of structure elucidation. Far from it! Recognising the substantial commonality in software and in infrastructure for running a user service, the Diamond leadership took cryo-EM on board. One reason that our field is so successful is that crystallographers have never been Luddites. During my years as a graduate student, direct methods began to show their structure-solving power. Eminent scientists who had developed amazing ability to interpret Patterson maps and seemed as much at home in vector space as in real space, may at first have regarded direct methods as witchcraft but soon adopted them as first-choice methodology.

Issues of equality and diversity have been in the news lately, and they affect the BCA as well. In this issue we have a statement of the BCA Equality and Diversity Policy as updated at the AGM. I also am pleased to provide a report by **Simon Coles** and **Anna Warren** on their experiences of the childcare facilities at the recent European Crystallographic Meeting in Oviedo. The ECA had made extra efforts to facilitate participation by crystallographers with children. Attendance at conferences is important for all crystallographers, but especially so in their early career, enabling networking with colleagues and providing feedback on research results before definitive commitment to a journal article. I well remember how becoming a widower in 1993 with three sons in their sub-teen and teen years affected my attendance at conferences. I was still able to attend BCA Spring Meetings because my lovely mother-in-law was willing and able to look after the boys for the short duration of those meetings. However, I gave up attending ACA meetings until a few years later, eventually taking my sons along to the meetings in St Louis, MO and Arlington, VA. Because all three were contemplating careers in science and the ACA didn't have strict door controls in those days, I could smuggle them into some lectures. Fortunately, crystallography is such a pictorial subject that my sons enjoyed them even when unfamiliar with details. Besides, all the museums of Washington DC were available just across the river from Arlington. The only feeding issues I faced were teen-agers' typical aversion to vegetables. I can only imagine what it would have been like to try to feed infants, and I doubt if even the most precocious toddler would have enjoyed taking part in a Transactions Symposium!

Next year's BCA Spring Meeting is taking shape nicely, as shown by the updated programme. Then the ACA will meet in Covington, KY from 21-24 July, followed by the ECA in Vienna from 18-23 August. I am sorry to say that, growing up in Ohio, I developed an arrogant attitude about Covington. It is just across the Ohio River from Cincinnati, whose German-American roots gave it seriousness of purpose and a love of culture, including the culture of brewing. On the other hand, Kentucky is conflicted. It is regarded as part of the Bible Belt, with corresponding hostility to alcohol, but it also makes top-quality bourbon whiskey. While Cincinnatians could consume their beer during generous but rigorously enforced hours, the laws in Kentucky about alcohol sales and other pleasures too were stricter, but enforcement was lax. We regarded Covington as the Tijuana of Cincinnati. Then Joan and I actually went to Covington for a previous ACA meeting and were very impressed. The conference centre is pleasant and efficient, there are good shops and restaurants, and one can easily cross the Ohio River to Cincinnati on the nearby Roebling Suspension Bridge, an engineering landmark of 1866. As for Vienna, what do I need to say? The meeting will be held at the renowned University, the city is full of great cultural monuments but peaceful scenery in the surroundings is easily reachable by public transport, and it is a happy accident of the German language that the words for Vienna (Wien) and wine (Wein) are so similar.

Carl Schwalbe

BCA Corporate Membership

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

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

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- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

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

Puzzle Corner

THE 2019 European Crystallographic Meeting will take place in a city much loved for its New Year's Day concert. By tradition the musicians give a greeting to the audience near the end of the concert. Use your knowledge of the elements and their symbols, admixed with a little group theory and linguistics, to construct it here.

__ __ To an inorganic chemist, a rare-earth metal. To an organic chemist, C_3H_7-

__ This makes what's above turn professional.

__ __ Together with what's just above, this makes sand.

__ Schoenflies symbol for a tetrahedral group.

…

__ An amine wouldn't be the same without this.

__ __ Named for a continent that has this city near its centre.

__ __ An enthusiastic "yes" in German.

__ The first one of its kind (and the lightest).

__ To an organic chemist, like the very first clue but completely general.

Answers to September 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?

There is one clear winner: Toronto. After that, there is a 5-way tie for second place. We can be proud that the UK has more of these venues than any other country.

Bol (33%) – Hot Topics in Contemporary Crystallography

London (33%) – BSG Autumn Meeting

Moscow (33%) – Biomembranes 2018

Oviedo (33%) – ECA

Oxford (33%) – S R School

Toronto (43%) – ACA

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.

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

Monday 15th April:

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.

Tuesday 16th April:

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

This session looks at all the excellent ways both outreach and social media can have an impact on science. How can we access a wider community? How can we inspire the next generation?

Plenary: **Tim Easun**

Parkin lecture: (to be confirmed)

Lonsdale lecture:
Professor George Sheldrick (University of Göttingen)

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

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

Tuesday 16th April:

CCG plenary:
Carl Henrik Görbitz (University of Oslo)
(Chair: Iain Oswald)

"Slippery when hot: temperature-induced sliding phase transitions in amino acid crystals"

BSG:
Novel data collection strategies
(Chair: Ramona Duman)

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!
(Chair: Anuradha Pallipurath)

In this session we showcase the many applications of the CCDC tool Mercury. How users in the community are delving deeper into visualising their systems to gain better insights into its chemistry.

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.

Keynote: **Dr Karen Johnston** (Durham)
"Probing ion mobility mechanisms in solid electrolytes using solid-state NMR spectroscopy"

BSG:
Complementary Structural Biology techniques
(Chair: James Garnett)

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

Keynote: **Dr Dmitri Svergun** (EMBL)

CCG:

Neat structures
(Chair: Lucy Saunders)

This session celebrates structure and is a chance to share yours with the community; think those with interesting structural features, properties or behaviour.

Keynote: **Michaele Hardie** (University of Leeds)

PCG/IG:

Surfaces of alloys and glass
(Chairs: Tony Bell and Lewis Owen)

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"

Wednesday 17th April 2019

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:

Novel 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)

Ensuring a sustainable energy supply is a pressing global issue. Advances in materials for energy applications are urgently needed to increase renewable-energy usage, and address current concerns about declining fossil fuel reserves and climate change arising from CO2 emissions. Diffraction plays a key role in understanding the structure-property relationships of materials for energy applications, including in operando studies. This session will examine recent developments in this field and contributions, oral or poster, are invited from across the diverse range of energy materials including batteries, fuel cells, solar and energy harvesting.

Keynote: **Dr Eddie Cussen** (University of Strathclyde)

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.

Keynote: **Dr Linda Seton** (Liverpool John Moores University)

Early career prize lectures

BSG:

Computational structural biology
(Chair: Shozeb Haider)

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.

Keynote: **Dr Gianni de Fabritiis** (GRIB Barcelona)

CCG:

Chemistry of voids
(Chair: Hamish Yeung)

Voids in crystal structures, whether discovered by chance or incorporated by design, result in a range of interesting properties. In this session we celebrate the exciting chemistry that occurs in the spaces between the molecules, and the possibilities that lie beyond. Think storage, rearrangement, reactions, flexibility and more...!

Keynote: **Professor Andy Weller** (University of Oxford)
"Solid-State OrganoMetallic (SMOM) Chemistry and Catalysis using Single-Crystal to Single-Crystal Solid/Gas Reactivity"

IG:

Prediction and modelling of surfaces
(Chair: Helen Blade)

Keynote: **Professor Mike Anderson** (University of Manchester)

BCA prize lecture:

Professor Clare Grey
(University of Cambridge)
Title TBC

BCA AGM and conference dinner followed by ceilidh.

Thursday 18th April 2019

BSG Plenary: TBC

BSG:

CryoEM and crystallography
(Chair: Chris Savva)

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
(Chair: Helena Shepherd)

This session is aimed at the wider community of chemists, doing all sorts of weird and wonderful things in their labs. We aim to open up a broader discussion in this session looking at how crystallography contributed to completing a research puzzle.

Keynote: **Professor Lee Brammer** (University of Sheffield)

PCG:

Magnetic structures
*(Chair: **John Claridge**)*

Research work on magnetoelectrics, multiferroics, magnetocalorics, skyrmions, or any kind of functional magnetic material is welcome. Characterisation of all forms of magnetic structures, and their correlation with their physical properties. Special focus will be given to the most recent approaches.

BSG (joint with RaMP):

EU Network for Rationalising Membrane Protein Crystallisation
*(Chair: **Arwen Pearson**)*

This session will discuss some of the new approaches being developed by the EU network RaMP to rationalise membrane protein crystallisation thereby improving the crystallisation hits and facilitating structure determination of otherwise difficult membrane protein targets.

Keynote: **Professor Adrian Goldman** (University of Leeds)

PCG/YCG:

In-situ methods
*(Chairs: **Hamish Yeung** and **Tom Wood**)*

Increasingly *in-situ* methods are being used to probe materials under non-ambient conditions. This session will highlight recent progress in both fundamental structural insight as well as that pertinent to real-world applications from biological systems through to solid state technology.

Keynote: **Dr Steve Hull** (ISIS neutron and muon source)

PCG:

Topologically interesting materials
*(Chair: **Alex Gibbs**)*

Topological materials host a surprising range of unusual physical phenomena and are believed to provide a pathway to further intriguing electronic phases. Well known examples are topological insulators such as Bi_2Se_3 and topological Dirac semimetals. Their topological nature is ultimately facilitated and controlled by specific crystal and/or magnetic symmetries in combination with effects such as spin-orbit coupling. A key focus of the current intense study of these materials is the exploration of new physics driven by combining topology with magnetism and electron-electron interactions. They provide a large playground for fundamental research whilst also providing potential for transformative future technologies. This session will focus on the prediction, discovery and study of such topologically interesting materials (e.g. topological insulators and Dirac and Weyl semimetals) with a wide range of tools including e.g. crystal and magnetic structure analysis, electronic structure calculations and physical property measurements.

Keynote: **Professor Maia Garcia Vergniory** (Donostia International Physics Center and University of the Basque Country, Bilbao, Spain)
Title TBC

The 2019 Annual General Meeting of the British Crystallographic Association will be held at the University of Nottingham at 18:00 on Wednesday 17th April, 2019.

Draft minutes of the British Crystallographic Association Annual General Meeting 2018

6pm March 28th 2018, Lecture Theatre 3, Sciences Building, University of Warwick.

1. **Approval of the Agenda –** proposed by Jeremy Cockcroft and seconded by Pierre Rizkallah and approved by the meeting.
2. **Apologies for absence –** no apologies received.
3. **Minutes of the 2017 AGM**
   The minutes had been circulated previously, published in *Crystallography News* and are available in the members area of the BCA website. Proposer Moreton Moore and seconded by Claire Murray and accepted without any changes.
4. **President's report**
   The President, Lee Brammer, started with noting the death of B.T.M. (Terry) Willis (1927-2018). Terry Willis's career was largely at Harwell and Chem Cryst in Oxford and he was well known for his work on neutron diffraction and instrumentation and the understanding of thermal motion. He established the on-going schools on neutron scattering and was a Founder and Honorary member of the BCA.

   The President thanked Leo Brady, the Programme Chair and also Richard Cooper for his valuable contribution, the Programme Committee, speakers and chairs and Hg3 for an excellent meeting.

   The Spring meeting in 2019 will be held at the University of Nottingham, 15-18th April and Emma McCabe, University of Kent is the Programme Chair. The President said that planning for the meeting would start with a meeting at 8am the following morning and encouraged everyone to provide input on the meeting to the Programme Committee.

   Congratulations were given by the President to Richard Henderson, MRC Laboratory of Molecular Biology Cambridge for the Nobel Prize for Chemistry in 2017 and to Andrew Goodwin, Oxford University, who has been honoured with the inaugural Blavatnik Award, Chemistry Laureate 2018.

   At the end of his term as President, Lee took the opportunity to reflect on the previous 3 years. He started by mentioning that the BCA president twitter account had been handed over to him by Dave Keen, the outgoing President, at the dinner following his election. It has 365 followers and has become a more and more important outlet for the organisation. The most liked tweet was a periodic picture of rhubarb!

   In terms of what he felt the BCA Council had accomplished during his term he reflected that he took the attitude that the BCA was not broken and to hand it back in good shape was good but he was hopeful that there was more to it than that. He chose to flag three changes: the revised election procedure with the nominating committee and electronic ballot, the establishment of a more formal nomination process for the main awards and Honorary members and the introduction of an Equality, Diversity and Inclusivity Policy.

   Lee concluded his report by saying that his term as President had been really quite enjoyable with bursts of hard work and giving thanks to the following people: BCA Officers: Richard Cooper, Claire Wilson, Pamela Williams and Elizabeth Shotton; the members of BCA Council for their input, enthusiasm, and willingness to endure long Council Meetings; *CN* Editor Carl Schwalbe, commenting that writing the President's column had been a very challenging role; Education and Outreach Officer, Simon Coles; Nicola Hardaker and all the team at Hg3 and to all the BCA members for their continued support for the Association.

   Simon Coles, Education and Outreach Coordinator gave a short presentation. He explained that in 2013 and 2014, with the IYCr and the Bragg centenary, there had been a number of large events such as the Big Bang Fair and the funding available for them. This was no longer the case and he was now looking at how to continue the good work but for smaller, local events. The aim is to resource and motivate people to be involved and a system is being set up to provide a repository for resources for local outreach that can be added to and used. These can be physical or electronic resources, for example giving guidance or kits that can be used with information on suitable age range and level of audience and is on the learn.crystallography.org.uk site. This is financially supported through bursaries, one cycle ran last year, offering £300-500 to buy materials up to £2500 for an internship and anything in between. The outputs will be available to everyone and there will be an annual call for proposals. Simon Coles proposed using Ada Lovelace day on October 9th to focus activities, develop resources on women in crystallography possibly through presentations, posters, short movie etc and asked people to contact him.

   The President thanked Simon and encouraged everyone to get involved.
5. **Secretary's report.**
   There was nothing to report.
6. **Hg3 report**
   Lee Brammer presented the information provided by Nicola Hardaker at Hg3. It was reported that the number of registrations for the Spring meeting on March 19th 2018 was 218 (186 in 2017) with 150 on the full residential package, 44 as day delegates and 16 exhibitors (11 in 2017). There were 95 delegates for the YCG satellite meeting. A list of Corporate members and current advertisers in *Crystallography News* was also provided. Membership on 19th March 2018 was reported as 691.
7. **Treasurer's report**
   The Treasurer, Elizabeth Shotton, started with a reminder that the reporting period is from January 1st to December 31st 2017. Elizabeth explained that the previous Treasurer, Pamela Williams, had largely prepared the accounts and she would do her best to reply to any queries. A full breakdown of the accounts is included in the BCA annual accounts available via email or online at the Charity Commission website and a summary was provided.

   It was commented that the major difference between 2017 and 2016 is due to the CCG Intensive course running in 2017 and not in 2016. There were also increased membership subscriptions and *Crystallography News*

income. The Spring meeting showed a small surplus in 2017 and we are in line to make a better surplus this year.

Charitable expenditure is dominated by subscription to the IUCr with 49% contributed by the Royal Society. We provided support to a crystallography school in Senegal as part of the crystallographic initiatives developing in Africa and we continue to award bursaries to BCA students and fund educational outreach activities.

In summary the Treasurer stated that the BCA continues to try and reduce governance costs and maintain a cautious, balanced investment of funds. Overall the total BCA income rose over the year to £279,277 (2017). The Treasurer concluded with thanks to Hg3, Council members, particularly Pamela Williams, BCA group treasurers, Charles Stanley Bank and the Young Company accountants.

Elspeth Garman thanked Pamela Williams, the previous Treasurer, for a fantastic job over 8 years. Lee Brammer agreed and commented that Pamela was also thanked at the previous AGM when she completed her term and had kindly agreed to be co-opted to stay on until the new Treasurer could be found. He was very grateful to Elizabeth and Pamela for the smooth handover.

There was a question pointing out that there was no Hg3 fee under the Spring meeting and Elizabeth Shotton replied that the costs are given under administration fee and expenses.

8. Acceptance of the Accounts for 2016. Proposed Elspeth Garman, seconded by Mike Glazer and accepted.

9. Appointment of examining accountant The Young Company were appointed as the examining accountant for 2018, fee £5400 a small increase on £5100 last year), proposed by Jeremy Cockcroft and seconded by Elliot Carrington and approved.

10. **Elections to Council**
This was the first year with the new mechanism for elections. Nominations were put forward by the newly established Nominating Committee in addition to the usual route of nominations from members by the earlier deadline of 30th September 2017. Candidate statements were published in the December issue of *Crystallography News* and voting was by electronic ballot during January. The nominees were restated and the results of the elections, which had also been emailed to members previously, were as follows: Simon Phillips was elected as President, Simon Coles as Education and Outreach Coordinator for a second term, Cheryl Doherty as Ordinary Member, Elizabeth Shotton has been co-opted to Council as Treasurer and Hazel Sparkes has been co-opted to replace Stephen Moggach who is stepping down as an Ordinary Member.

Some voting statistics were presented showing peaks in voting when it opened and following reminders and 150 votes were received in total. After initially feeling disappointed with this number Lee commented that when considered relative to the AGM attendance it is a good level and he expects it to increase as the process beds in. The motivation had been to allow involvement of the membership beyond those attending the AGM and to provide some distance from the current Council. Lee Brammer said he was very grateful to the Nominating Committee who had done a great job. The composition of the nominating Committee with the past president plus members representing the 4 groups of the BCA would continue with a new IG rep to replace Paul Fewster. Lee thanked all the candidates and stressed that it was very important that people were prepared to stand.

Simon Phillips was unable to attend the AGM as he was in Australia on a visit planned before his nomination but had provided a statement which was presented at the meeting thanking members for giving him the opportunity to serve as President.

In 2019 the posts of Vice-President and Secretary will be open for election and neither of the current post holders will be eligible for re-election. One Ordinary Member position will also be open for election when Anna Warren completes her first 3-year term.

11. **Honorary Life Members**
The President explained that Honorary members are chosen for their contributions both to crystallography and to the BCA. The nomination deadline for 2019 Honorary Life members will be August 31st, 2018 and nominations should be sent to the BCA President along with a short case for support of not more than 400 words. Nominations will be considered at the September Council meeting. New Honorary memberships are not necessarily awarded every year and can be awarded to a maximum of two people in one calendar year. He was very pleased to announce that the Honorary Life memberships awarded for 2018 were to Elspeth Garman and Carl Schwalbe. Prior to presenting certificates to Elspeth and Carl, Lee confessed that last year when Honorary Life memberships were awarded to Eleanor Dodson and Olga Kennard, who were not able to attend last year, he had intended to send them certificates and had not done so and as Eleanor was present this year he asked her to join Carl and Elspeth for the presentation.

12. **Membership, annual subscriptions and subventions**
BCA membership numbers at December 31st were presented for 2017 and 2016 and were as follows: Total membership 664 in 2017 (733 in 2015) with the following breakdown (2016 figures in parentheses): BSG 171 (177), CCG 215 (225), IG 58 (62), PCG 81 (97), YCG 143 (163), Corporate 10 (9), unknown/not verified 139 (154).

Elspeth Garman clarified that the numbers had dipped to under 400 members in 2012 but when the membership administration was taken on by Hg3 it was found that the previous figures included many people who were in fact not paid up members. Bill Clegg commented that Elspeth had led a successful drive to recruit members. It was commented that the membership numbers are in fairly good health and we will always aim to do better.

There had been an extensive discussion of membership fees at the AGM 2 years ago and there was strong approval for maintaining the category 5 membership of the IUCr and the decision was made to make modest increases to the membership fees. While it is not expected to be increased every year, with no increase last year, this year a small increase was proposed to cover running costs and continue to have funds to support outreach activities. Mike Probert asked whether corporate members had been asked about the increase and the reply was that there hadn't been a discussion with them but the increase was modest and reflected that the BCA values the support of corporate members.

The revised fees were proposed by Mike Glazer and seconded by Mike Probert and approved with no votes against.

Membership fees for 2019 were set at £40 for full membership, £20 for concessions, student (four years) £65, overseas member (5 years) £175 and corporate members £800.

13. **Equality, Diversity and Inclusivity Policy**

Lee Brammer said that this had been discussed within BCA Council for the last year or so and had now been developed through to a policy in this area. Although we often reflect that crystallography has good gender diversity with well known, prominent female members of the community there is a need to look at the numbers. At the IUCr general assembly there were discussions about this and Lee Brammer thanked Elspeth for initiating this.

Lee Brammer presented the Equality, Diversity and Inclusivity policy agreed at Council on Monday and invited comments and questions.

There was a question as to why we are not extending this to nominations, for example there was an all-male candidate list for President. Lee Brammer said that the nominating committee were advised to heed this policy and that it was also challenging to find people willing to stand for these positions at a particular point so it is not always possible to enforce balance but is encouraged. Elspeth Garman, commented some female candidates were approached. It is hard to achieve balance with small numbers but by reporting on it we highlight if there are imbalances. Elspeth Garman was asked if she was lonely as the only woman on the nominating committee. There have only been two female BCA presidents and in the first instance the nominating committee was largely drawn from past presidents.

Richard Cooper commented that by committing to recording and reporting the data we are open to scrutiny and questions and if the balance is not correct then we will address what is needed to be done.

Anthony Phillips questions when this was really a policy as it gives a series of aims. Lee Brammer replied that it is a directive to those involved that this needs to be taken into consideration and that statistics will be reported and raise people's awareness.

A suggestion was made to include age explicitly and encourage wide range of ages and career stages.

Lee Brammer commented that the wording was not perfect and that was why feedback was being sought. It was agreed that age should be included, and it was pointed out that age is a protected characteristic. Bill Clegg commented that it was an excellent beginning and that publishing it and inviting feedback is welcomed.

Statistics were presented on the gender balance of the membership and overall is 29% female, with higher percentages for student members (46%) and non-student Young Crystallographers (36%). For the Spring meetings from 2014-2018 the gender balance of the programme committee, plenary speakers, keynotes, speakers and chairs were presented. It was commented that although the information has not been previously formally recorded we had attempted to extract the information from past programmes and for this meeting information on age and gender had been requested on a voluntary basis. The BCA Equality, Diversity and Inclusivity policy is given on the BCA website.

14. **AOB**

Mike Glazer proposed a vote of thanks to Lee Brammer for his work as President over the last three years which was heartily applauded.

There was no other business and the meeting closed at 19:30.

BCA Equality, Diversity and Inclusivity Policy

The BCA Council is pleased to announce the adoption of the following policy:

Conference Policy

The BCA recognizes the positive impact that a conference speaking opportunity has on an individual's track record and visibility. We also recognize that some sections of the scientific community are often under-represented in conference programmes, and that this can affect diversity in the long-term. Our policies are intended to ensure quality and equality.

Speaker Invitation Policy

The programme chairs will ensure the highest quality scientific programme, with speakers that represent the broad diversity of our community. We aim to achieve a speaker and programme chair balance that reflects the make-up of our community without bias with regard to gender, sexual orientation, race, religion, disabilities, age, geography, or national origin.

Reporting Policy

We will report and review statistics on the gender balance of the membership, the composition of committees and of invited speakers, selected speakers, session chairs, and attendees of the BCA Spring Meeting.

Feedback

We welcome feedback to **president@crystallography.org.uk** on this policy and how it might be improved for future conferences to better ensure equality and diversity.

This policy was approved by the BCA Council Meeting on 26th March 2018.
Version 2: Policy modified to include age in list of criteria in section on SPEAKER INVITATION POLICY following discussion at BCA AGM on 28th March 2018.

Membership statistics (estimated from 2017 data)

Students – 50 female and 59 male: 46% female.

YC (not including students) – 20 female and 36 male: 36% female.

Standard members – 147 female and 355 male: 29% female.

Spring Meeting statistics

The following table gives the fraction of each role filled by women for each year (as a percentage).

Main Meeting	2014	2015	2016	2017	2018
Programme Committee:	53%	44%	27%	27%	27%
Plenary speakers:	0%	0%	25%	25%	75%
Keynotes:	17%	28%	11%	18%	28%
Speakers:	12%	35%	31%	24%	38%
Chairs:	53%	22%	23%	42%	43%

YCG Meeting	2014	2015	2016	2017	2018
Plenary speakers:	50%	50%	50%	0%	50%
Teaching session:	n.a.	0%	0%	66%	n.a.
Speakers:	31%	38%	62%		29%
Chairs:	67%	60%	40%	40%	33%

BCA Council Elections – Candidate Statements

FOLLOWING the procedure for elections to the BCA Council adopted at the AGM in April 2017, nominations for the following positions on Council were invited from the Nominating Committee and from members of the BCA by the nomination deadline of September 30th: Vice-President, Secretary, and Ordinary Member. Elections will be held by electronic ballot of the BCA membership, with voting available until the end of January 2019. The outcome of the election will be announced and confirmed at the AGM during the Spring Meeting in April 2019. Each nominated candidate has been asked to provide a short CV and candidate statement; these appear below.

Vice-President Candidates

Simon Coles

Current Position:
Professor of Structural Chemistry, Director of the UK National Crystallography Service and Director of the UK Physical Sciences Data-science Service, Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton.

Professional Activities:
Since 2015 I have been a member of the RSC Local Section committee, since 2013 Director of an MSc in Instrumental Analytical Chemistry and since 2010 Director of Southampton Diffraction Centre. I am a visiting academic at the Universities of Cagliari (Italy), Gebze (Turkey) and Sydney (Australia). I am an Editorial board member for 4 journals (Crystallography Reviews, Supramolecular Chemistry, Chemistry Central & International Journal of Digital Curation) and my peer review panel membership has included EPSRC, ARC, JISC, ISIS, Diamond and ALS. I also serve as a member on 8 large project and facility management steering groups (external and internal to my university).

BCA positions held:
2015-Current, BCA Education and Outreach Coordinator; 2013-2015 Chair, Chemical Crystallography Group; 2011-2013 Vice Chair, Chemical Crystallography Group; 2009-2010 Chair, Spring Meeting Programme Committee; 2006-2008 Chair, Young Crystallographers Group; 2000-2003 Ordinary Member, Chemical Crystallography Group Committee; 1995 Member Local Organising Committee BCA Spring Meeting.

Research Interests:
I am author on around 850 publications in journals, conference proceedings, periodicals and books, with an H-Index of 48 and >10000 citations. A significant proportion of these arise from being at the leading edge of service crystallography since the early 1990's. However, my research interests beyond service crystallography are numerous, as illustrated by recently becoming the Director of a second national facility devoted to chemical and physical sciences data. Structural chemistry research interests include the study of solid-state reactions and transformations, structural systematics, the determination of charge density distributions and their application to solid state reactivity and behaviour, discovering and investigating structure-property relationships and crystal growth. In the last 15 years I have diversified my research from conventional crystallography into interdisciplinary work with Libraries & Information Science, Archaeology, Statistics, Computer Science, Physics and Engineering. This has resulted in working in CT Imaging, SHG Laser Spectroscopy, Dynamic Light Scattering, Computational Modelling, Additive Manufacturing, Formulation, eLearning, Data Management, Data Science and Chemical Informatics areas.

Statement:
I am committed to ensuring the continued efficient operation of the BCA and maintaining its profile as a professional organisation that works for the benefit of its members and the crystallographic community as a whole. I am exceptionally familiar with the operation of the BCA, having served in numerous committee positions and attended every Spring Meeting since 1992!

This position is primarily concerned with the functional operation of the BCA and I have considerable experience in coordinating activities and organisations at this level. I have served on BCA Council in a number of different roles over the years, as Spring Meeting Programme Chair, Education & Outreach Officer and representative for both the CCG and the YCG. I also understand the roles and operation of the BCA groups, having worked through the different levels of the CCG and having been involved in getting the YCG established. Finally, as a Director of two National Research Facilities, I am fully aware of what is involved when it comes to actually putting proposals and recommendations into practice!

There are two further aspects I would like to touch on to illustrate what I would bring to the post.

Crystallography Education: I am passionate about enhancing education and understanding of chemistry and crystallography at all levels and to the broadest possible audience. I have spent time making sure education and outreach is firmly knitted into the agenda, infrastructure and working of the BCA and developed routes by which more members can get involved with education and outreach. I will ensure that we can put even more effort into these activities.

International Recognition: My personal research collaborations are global and I feel it is vital that the BCA is not only represented at this level, but that it is also seen to be internationally leading – I would strongly contribute to this agenda. I have participated in the IUCr General Assembly and am a very active member of the IUCr CommDat (Committee on Data) and as an ECA & ACA member I am involved in their meetings and Special Interest Groups. Working as a member of the Scientific and Local Organising Committees for the PCCr2/AFLS (Pan-African Conference on Crystallography joint African Light Source) conference, I have been very active in promoting British crystallography as a way to help developing nations. This involves talking to politicians as well as scientists!

I will bring all this background and experience to the position and relish the opportunity to be fundamentally involved in operating the BCA.

Simon Parsons

Current Position:
Professor of Crystallography and Director of The Centre for Science at Extreme Conditions, The University of Edinburgh.

Education and Career:
BSc(Hons) Chemistry, University of Durham (1987). PhD in synthetic inorganic chemistry, University of New Brunswick (1991). EPSRC Post-doctoral Fellowship, University of Oxford (1991-1993). I joined The University of Edinburgh in 1993, first as a post-doctoral fellow, then manager of the Crystallography Service, lecturer and reader, becoming Professor of Crystallography in 2007.

Professional Roles:
Deputy Chair, then Chair of the CCG (2003-2007). Chair of Organising Committee, BCA Spring Meeting, Loughborough, 2009. BCA Council, Ordinary Member (2012-2015). Co-editor of Acta Cryst. Section B and member of CrystEngComm and Acta Cryst. Section E Advisory Boards since 2008 and 2014. Tutor or lecturer at the Durham X-ray Structure Analysis School since 1995, Chair of programme committee since 2011.

Research Interests:
Since joining the University of Edinburgh in 1993 I have developed a research programme in crystallography and structural chemistry, with ca 600 publications and an h-index of 81. I am ranked 22nd in the list of contributors to the Cambridge Database. My research interests focus on molecular solids and their response to external conditions, particularly pressure, making extensive use of Daresbury SRS, Diamond Light Source, ALS, ISIS and ANSTO. My group aims to combine experimental structure determinations with computational simulation, to derive a complete thermodynamic model of the system under investigation. Over the course of this work I have developed crystallographic methodologies for extreme conditions research, treatment of twinning, absolute structure determination and single-crystal neutron diffraction. In addition to this 'personal' research activity, I was until 2009 manager of the Crystal Structure Facility in the School of Chemistry at The University of Edinburgh, supporting our highly prolific synthetic research groups with crystal structure determination. I was honoured to receive the Lonsdale Lectureship from the BCA in 2015.

Statement:
One of the biggest challenges that the BCA faces is the diminishing numbers of attendees at the Spring Meetings. Perhaps this reflects a certain degree of conference fatigue and the decline in numbers of research groups in universities who define themselves in terms of crystallographic research. Yet this is one of the most exciting periods that I can recall for advances in crystallography. Not only have laboratory sources become much more versatile, but central facilities such as Diamond and ISIS are upgrading and making ever more powerful techniques available to researchers, XFELs are bringing previously inconceivable time resolution to diffraction experiments and electron crystallography has revolutionized macromolecular crystallography and is set to do the same for small molecule work as well. Theory is being applied much more widely using accessible codes; reliable structure prediction is becoming a reality and the Cambridge Database is about to add its millionth structure. In the UK we have one of the most active crystallographic communities in the world – and some of the very best crystallographers. As vice president of the BCA I would be a member of the programme committees responsible or organizing Spring Meetings, providing continuity from year to year. I see this as a great opportunity to encourage engagement with other related disciplines and societies, bringing new members, and growing and diversifying the Spring Meeting.

Secretary Candidate

Alex Stanley

Current position:
Marketing Director at Rigaku, October 2017 – present.

Education and Career:
Product Manager at Rigaku, 2015-2017; Sales Representative at Rigaku, 2012-2015; Single crystal X-ray diffraction Application Scientist at Oxford Diffraction, 2009-2012; PDRA on Single Crystal Beamline at STFC Daresbury, 2007-2009; Ph.D. in Chemical Crystallography at Bristol University, 2007; MChem. at Bath University, 2003 with Industrial Placement at GSK crystallography department in 2002.

BCA roles:
BCA Council Member and Bursaries Coordinator, 2009-2018;
CCG Treasurer Secretary, 2007–2010;
Program Committee BCA Spring Meeting 2007;
YCG Secretary, 2006–2007;
CCG Co-opted Student on BCA council, 2005–2007.

Statement:
It was thanks to a fortuitous placement at GSK with Dr. Roy Copley during my undergraduate studies, which first gave me my first taste of the beautiful world of crystallography. In my final year I was excited to pursue a research project supervised by Prof. Paul Raithby before moving on to a Ph.D with Prof. Guy Orpen in crystal engineering. Alongside the research, the BCA played an ever-present role in life and I still claim to this day, that you will never be lonely for long at a BCA meeting. I find it a friendly and welcoming community, one that I hope will continue for many years to come.

Working for a corporation can appear to outsiders as a shift away from the field of scientific research, however, the ethos at both Rigaku and formerly, Oxford Diffraction, has always been to pursue the boundaries of science. Employees are actively encouraged to keep up-to-date with the latest technology and research interests so that instrumentation can keep pace with new and exciting developments in the field of crystallography.

Whilst trying not to extoll the virtues of a company to gain advantage or encourage favour at the expense of the BCA, having the opportunity to actively work in this industry for the last sixteen years has really opened my horizons to the wide and varied research that takes place every day in the most far flung corners of the globe. The world of crystallography is a very small, but powerful, entity indeed and many countries in

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this scientific arena look to the BCA and the UK crystallography teachings as a model for their own organisations.

Having been a member on the council for a number of years, I have a broad understanding of how our association is run and the opportunities that may exist to encourage membership expansion. The nomination for Secretary of the BCA Council comes as an honour and I am confident that I have the necessary skills to do the role justice.

Ordinary Member Candidates

Helen Y. Playford

Current position:
Instrument Scientist on the Polaris powder diffractometer at ISIS (2013-present).

Professional Activities:
Member of the British Crystallographic Association. Secretary of the Physical Crystallography Group & Group Representative to BCA Council (2016-2019). Member of programme committee for the 2019 BCA Spring Meeting. Organiser of annual Physical Crystallography "Winter Meeting" with the ISIS Crystallography User Group.

Research interests:
I would describe myself as a keen scientist with a short attention span! Luckily as an instrument scientist I am privileged to be involved with a diverse community of facility users and there are always new problems to sink my teeth into. My main research interests involve the hydrothermal or solvothermal synthesis of disordered crystalline materials, as well as the analysis of their structures using powder diffraction and total scattering techniques. I am one of the developers of the RMCProfile software for the analysis of total scattering data, and am always keen to push the limits of the technique to find out just how much information is contained within the "wiggly lines" that come from our diffractometers!

Statement:
I am pleased to stand for election to the BCA Council as an Ordinary Member. I have been involved with the Physical Crystallography Group (PCG) for several years now, and have enjoyed contributing to the research community in this way. As the PCG representative to Council I have attended council meetings which has allowed me to strengthen my involvement with the association. I believe that the strength of an organisation such as the BCA is in the dedicated individuals that run it, and I really appreciate the opportunity to be part of it. I also believe that as an Instrument Scientist I have a unique perspective with a good understanding of the research interests of a large user community, as well as the ability to promote BCA activities amongst this community.

Kenneth Shankland

Current position:
Associate Professor in Pharmaceutics, School of Pharmacy, University of Reading.

Education and Career:
BSc (Hons) Pharmacy, University of Strathclyde; Pharmacy Pre-registration, Stobhill Hospital, Glasgow; PhD in Nanoparticle Size Distributions, University of Strathclyde; PDRA to Prof. Chris Gilmore, Chemistry Dept., University of Glasgow; Member of, and ultimately Group Leader of the Data Analysis Group, ISIS Facility, STFC Rutherford Appleton Laboratory; Associate Prof. of Pharmaceutics, University of Reading; Director of Pharmaceutics and Pharmaceutical Chemistry (2011-2017), University of Reading.

Professional Activities:
Joint organiser of "Structure Determination from Powder Diffraction Data – An International Workshop" (Oxford, July 1995); joint organiser of first electronic abstract submission for IUCr XVIII (Glasgow, 1999); regular member of programme committee for ICDD's "Pharmaceutical Powder Diffraction" conference series (US/Europe, 2000-2015); organiser (with Prof. Bill David) of the 44th Erice International School of Crystallography – "The Power of Powder Diffraction" (Erice, 2011); member of the IUCr Commission on Powder Diffraction (2008-2016); member of the IUCr Calendar Committee (2014 to date); invited referee for ETH (Zurich) Medal Award (2016). Invited speaker at more than 50 national and international conferences.

Research Interests:
My main research interest is the use of powder X-ray diffraction (PXRD) for the crystal-structure solution of molecular organic materials. The origins of this interest lie in applying the MICE maximum entropy and log-likelihood gain approach to PXRD data whilst I was a PDRA. Broadening out from just data analysis to collecting high-resolution diffraction data with a view to applying direct methods of structure solution, I then switched to the use of global optimisation methods (initially genetic algorithms, then simulated annealing). This resulted in the development of the DASH structure determination program, which has been further developed and marketed by the CCDC since the year 2000. Aside from using DASH to solve challenging crystal structures, I have helped drive its development to enable it to cope with the increasingly large structures that are of interest to academic and industrial solid-state scientists. Whilst at ISIS, the Data Analysis Group developed not only new methodologies for structure solving, but also implemented efficient computational approaches to coarse-grained parallelisation, such as local clusters and GRID computing. The latter proved valuable not only in structure solving, but also in running Monte-Carlo codes for neutron facility instrument design. Latterly, my interest in computing meant that our group interacted strongly with the E-science Centre, resulting ultimately in the ICAT open-source metadata management system for large facilities. Since moving to Reading in 2009, my research has focussed on further extending the power of DASH, particularly with laboratory-based PXRD data; for example, by utilising CSD data in structure solution, and solving the structures of MOFs and their intermediates formed during mechanochemical synthesis. I am also now applying PXRD to a much broader range of materials, including, for example, chocolate crumbs, with a view to their characterisation by multi-phase Rietveld refinement. I

am also a regular user of single-crystal X-ray diffraction, providing crystal-structure determination services to synthetic chemists.

Statement:
My decision to switch from physical pharmacy to crystallography was rooted in an opportunity given to me by Chris Gilmore at University of Glasgow, who took a chance on hiring me (as a PDRA) as someone who knew very little crystallography, but who could program in FORTRAN. Chris was a great believer in sending PDRAs and PhD students to conferences, both to present and to learn. I attended a great many BCA meetings, and vividly recall the excitement of seeing so many "big names" whose work I was aware of, and having the opportunity to hear them speak about their work in person. Moving south to the Rutherford Appleton Laboratory a few years later, and working with Bill David, this trend continued and I really came to understand not only the value of meetings organised by the BCA, the ACA, the IUCr and others, but the incredible hard work that goes into funding, planning and running them. This came into particularly sharp focus in the lead-up to IUCr 99 in Glasgow, where it was my privilege to be asked (along with Tony Csoka) to set up a database-driven online system for the submission of abstracts for the meeting. Another major challenge was organising and running (along with Bill David) the programme for the prestigious 2011 Erice Summer School on Powder Diffraction, which was very hard work but incredibly rewarding.

Serving on both the CPD and IUCr's Calendar Committee has given me tremendous insights into not only how crystallography is being promoted in developing countries, but also the tensions between large-scale crystallography conferences and smaller, highly-specialised meetings. At a time where exciting developments in (for example) XFELs and electron diffraction are pushing the limits of structure characterisation, it is important that the fundamentals of crystallography continue to be promoted both at home and abroad.

I would be honoured to serve as an ordinary member of the BCA council. Having benefited greatly from BCA and BCA-related activities, my aim would be to help others benefit similarly, via contributions to education, outreach, industrially relevant activities and conference organisation.

Anna Warren

Current Position:
Senior Support Scientist on the VMXm beamline at Diamond Light Source (May 2015 – Present).

Education:
MChem degree, Chemistry (2007), University of Bath; PhD in Chemistry, University of Bath (2011).

Professional Activities:
BCA ordinary member (2016-2019). YCG committee member from 2008-2014, chair (2012-2014), secretary/treasurer (2010-2012) and ordinary member (2008-2010).

Member of the organising committee for the 2014 Spring Meeting and the inaugural European Young Crystallographers Satellite Meeting (2013).

Education and Outreach Coordinator (2014-2015).

Research Interests:
Since finishing my PhD I have been working at Diamond Light Source working on several of the beamlines, including for small molecule and macromolecular crystallography. Since 2015 I have worked on helping to build the new microfocus macromolecular crystallography beamline, VMXm, which is due to take first users in Autumn 2018. My research during this time has focussed on method and beamline development to aid with data collection from challenging protein crystals, ranging in size from 10s of microns down to 1 micron. This has involved having to develop new mounting techniques for such small crystals, as well as using scanning electron microscopy to aid with sample visualisation.

Statement:
I am delighted to have been re-nominated for a position on the BCA council, having already served a term as an ordinary member over the last 3 years. I joined the BCA as a first year PhD student attending my first Spring Meeting in 2008. It was great being able to attend the Young Crystallographers Satellite meeting, which was such an important forum for early career researchers to get together and discuss their research. Having seen the significant work of the YCG in bringing young crystallographers together, I joined the committee the same year. I was then involved with committee business for 6 years working my way up to chair the committee for a term. During this time as a committee, we were involved with organising the first European Young Crystallographers meeting at ECM28 in Warwick. This satellite meeting has since been present at all subsequent ECM meetings. I have been heavily involved with the BCA council over several years, and have also been on the organising committee for the 2014 Spring Meeting, as well as chairing sessions in many other Spring Meetings.

I have a background in both chemical and macromolecular crystallography from my PhD in framework materials to my current beamline scientist position for VMXm. This broad disciplinary background and my vast experience in committees, organisation and planning I believe will benefit the BCA council. I would be thrilled to have the opportunity to serve on the BCA council for another term.

ECM31 Oviedo, Spain

THE ECM 31 was a brilliant meeting held in Oviedo in the beautiful region of Asturias, Spain. Those attending were treated to fantastic hospitality in a very friendly city with delicious food and drinks to try.

The conference kicked off at the Palace of Exhibitions and Congresses (PEC) of Oviedo on Wednesday 22nd August with the European Young Crystallographers satellite meeting. The friendly atmosphere hosted a keynote from **Peter Spackman** followed by lots of great talks from the YC members. Attendees were also treated to a picnic lunch under the Oviedo sun.

The opening ceremony followed in the evening with the traditional ECM committee welcome, led by chair Prof **Santiago Garcia Grande** and followed with an inspiring talk given by **Sine Larsen**, the recipient of this year's Max Perutz Prize Lecture. To kick off the festivities, Oviedo style, a bagpipe ensemble took to the stage treating the audience to some traditional local music before everyone spilled into the Exhibition hall for delicious local nibbles and to meet new faces.

The four days of the main meeting followed with a great range of plenaries and microsymposia to attend. It wasn't just scientists enjoying the atmosphere either; this year's ECM saw the welcomed inclusion of family members helping many more attendees to get to the conference and to share their scientific world with those closest to them. Women in crystallography were also celebrated with a dedicated symposium and a new range of t-shirts leading to an appearance in the local newspaper.

As well as attending the conference, participants could explore Oviedo after hours discovering local specialities including cachopo, local seafood and of course cidre (served in every way imaginable)! On the Friday night there was also the chance to go to a special concert given by the Symphony Orchestra of Asturias at the Auditorium Príncipe Felipe and was a very impressive evening of music.

The meeting finished with a conference dinner in the beautiful location of the Castillo Bosque de la Zoreda, on the outskirts of Oviedo. A swing band accompanied the aperitifs adding to the bustling atmosphere before guests sat down for their evening of dinner and dancing. Those staying to the very end got up bright and early the next day for the conference excursion to the Picos de Europa. The trip passed first to Covadonga to see the impressive mountain church and holy cave. The next stop was into the Picos de Europa national park to walk around the lakes of Lago de Enol and de La Ercina, a beautiful stop for lunch! The last stop was a trip to the estuary town of Ribadesella for a quick swim in the sea before going home.

Overall, this was a brilliant and varied meeting with lots to attend, people to meet and culture to enjoy!

Lucy Saunders
Diamond Light Source

NOW in its fourth iteration since starting off in Warwick in 2013, the European Young Crystallographers Satellite Meeting seeks to give the early career researchers in the ECA region the opportunity to present their work in a less formal environment than the main meeting, as well as to get to know each other before the conference starts proper.

On a gloriously sunny Wednesday morning in late August, a group of young scientists from all over Europe and Africa (and even further afield) descended on the Palace of Exhibitions and Congresses in Oviedo. Our goal? To talk about the research that we've been at the forefront of while getting to know some new faces.

The opening presentation was given by **Peter Spackman** (University of Southampton, UK) who told us about the latest work that he has been doing with CrystalExplorer. We were treated to an excellent overview of the processes involved in a Crystal Structure Prediction calculation, before diving into how the lattice energies calculated in CrystalExplorer can be applied in this ever-expanding field. **Filip Topić** (McGill University, Canada) went on to talk about mechanochemistry and how crystallography proves itself to be invaluable in understanding the stepwise mechanism in the formation of halogen bonded cocrystals. In the final talk before coffee, **Vittoria Marzaroli** (University of Parma, Italy) showed us some beautiful structures of porous metallacrowns and explained how they can find uses as highly responsive luminescent or magnetic probes.

Reenergised by coffee and pastries, **Alix Volte** (Institut de Physique de Rennes, France) kicked us off again by taking us into the realms of physical crystallography with photo-induced phase transitions from ultrashort laser pulses. Using synchrotron radiation, it is possible to carry out time-resolved diffraction experiments to understand the processes that govern elastically driven cooperativity. From physics we went to biology, and **Elisabeth Damisch** (University of Graz, Austria) presenting her work on the surface layer proteins of *Lactobacilli* species. These cell components are responsible for vital tasks like bacterial adherence to other cells, and so understanding their structure/property relationships is very important. Our final talk of the morning shifted the topic to materials science with a talk from **Laura Folkers** (Lund University, Sweden). Her variable temperature studies had shown an interesting "sibling"-like relationship between AuIn and PdBi alloys, raising the question as to how many other similarly related intermetallates exist?

Lunch followed, with an opportunity to wander round the posters and chat to the other satellite participants. In particular, I enjoyed a long discussion with **Soufiane Zerraf** (University Hassan II of Casablanca, Morocco) about his thorough analysis of L-arginine phosphate monohydrate.

After lunch it was the turn of **Jonathan Richardson** (University of Edinburgh, UK) who explained his role in the studies of CO_2

uptake in the metalorganic framework Sc_2BDC_3. By combining X-ray diffraction, *ab initio* calculations and GCMC simulations, the fascinating behaviour of this system is starting to be very well understood, particularly its selectivity of CO_2 uptake over other gases such as methane.

After some final rambling from myself, the European Young Crystallographers satellite was over for another year, and it was time for the opening ceremony of the main meeting. It's always excellent to see such a diverse range of scientists from all over the world coming together to share a common theme of crystallography. Long may such meetings continue!

Andrew Maloney
CCDC

ECM31 – a family friendly conference

Anna's Story:

AFTER receiving an invitation to speak at ECM 31 in Oviedo, Spain, I didn't want to turn down the opportunity, but it would be the first time attending a longer conference since returning from maternity leave. After investigating on the ECM website it became clear that this year they were really promoting a child-friendly conference, and had come up with a number of initiatives to aid conference delegates to bring their children along.

A number of initiatives were put in place by the ECM31 organising committee, focussed around gender balance, one of which included creating a family friendly conference. Primary caretakers of children will often forgo attending conferences due to childcare responsibilities, and this can have a detrimental impact on people's careers.

With this in mind, ECM31 had free registration for children, as well as for one accompanying person. They were providing onsite childcare during the conference, which involved a number of activities taking place in a large designated room at the conference venue as well as organised family tours. Children were allowed to attend all sessions, including the poster, coffee and lunch breaks.

The children's room at the conference venue was great, there were a number of trained professionals present to look after the children, as well as copious amounts of toys and books for the children to play with. They also organised several different activities on each day, and often took the children outside to play. The room felt safe and secure, they had taken all of our details in advance, and the staff were very experienced and caring with the children. You were able to leave the children there on their own, but the room was closed over the lunch break period of the conference.

All in all, I found having these facilities available really useful while attending the conference. The conference was definitely a different experience to what I had been used to, but being able to attend gave me the opportunity to present about my research and talk to potential collaborators. Although we didn't leave our son on his own in the room as he was still relatively young, having the facilities there for him was really useful. I believe that for older children that could be left more routinely alone, the room was much more useful. Promoting the conference in this way gave caregivers the confidence to bring their children along, and this can only be of benefit to the conference and the crystallography community!

Simon's story:

I DON'T often pay much attention to conference email circulars that are sent >1 year in advance of the actual event, but back in 2017 there was one that did particularly register with me. There was just one sentence in the ECM31 advanced circular, stating that it would be a child friendly conference and this stuck in my mind. I immediately followed the conference on Twitter – and for the next few months thought nothing more of it. When Twitter told me that the ECM31 website was live, my memory was jogged. The skeletal website had the same statement committing to supporting the attendance of those with families. I am a divorced parent of a 6-year old, with 50% caring responsibilities and it was just this sentiment from the ECM organisers that gave me the resolve to attend the conference. Furthermore, my enthusiasm for this initiative was so strong it didn't take much to persuade my partner, a non-scientist, that we should all go to Oviedo in August 2018, despite the fact that I would be attending a conference for a significant part of the trip. Free registration for children and an accompanying adult and the promise of childcare facilities was definitely a further incentive. I registered as soon as I could.

When it got closer to the time and we had to think about logistics, we decided to rent an apartment for accommodation which distanced us from the conference proceedings a little and actually meant my family did not attend as much as might have otherwise been necessary. Nevertheless, the childcare room was very well staffed and had plenty to entertain children – we used it a couple of times, but only when I was juggling attending lectures with family time. However, what really made the difference was the relaxed attitude towards children that was generated by the organisers and certainly seemed to rub off on most delegates! We found it really helpful that children were allowed into the coffee breaks, posters, etc which meant that I could blur the boundaries a bit and also that my family weren't left hanging around outside the entrance when I failed to get out of a lecture or stop networking at the time I had promised when I left the apartment in the morning. My partner was not so comfortable taking the tours organised by the conference, however they provided great inspiration and we made our own way on a couple of outings very similar to those that the conference put on – these were well supplemented by excellent advice from the local tourism office that had a stand in the exhibition.

In summary, I didn't take as much advantage of the great facilities and opportunities that the organisers provided as I could have, however I was certainly given the confidence to attend the conference with my family in the first place. Once at the conference, even though the family was only dipping in and out, it was so relaxed that it meant I could mix the two activities without having that extra bit of pressure. The organisers have to be congratulated for generating an environment that enabled this to happen – and for the next few years of my life it will certainly be a factor that I will consider when selecting conferences that I wish to attend.

Can we learn anything from this so BCA Spring Meetings are attractive to a more diverse audience?

The conclusion from our experiences is that taking a child to a conference is a very different experience to that which you would have if going on your own. However, what ECM31 did were fantastic steps that really enable people with children to attend a conference. It is important to note that the conference itself also benefits by being able to include people in this demographic – remember many of our most vibrant and driving colleagues, i.e. members of the Early Career Researcher community, find themselves in this position. Creating the right attitude is the first, and most key, step. This is what will attract those who wouldn't otherwise be able to readily attend. From this the right environment can be generated…

The BCA for example could explore options for free registration for children (and possibly accompanying adults) that would enable access to networking and exhibition areas along with coffee at break times. Other possibilities could also include a 'family package' which could provide an independent space that can be used during session times for entertainment, baby care etc. There are a range of possibilities that the BCA could consider and Council would welcome input from the membership as this becomes a topic on its agenda.

Opening of the Electron Bio-imaging Centre (eBIC) at Diamond

AS a humble small-molecule crystallographer I felt privileged to get an invitation to this exciting event, which took place on 12th September. I think it must reflect the high esteem in which *Crystallography News* is held, rather than any special merit on my part. Participants were treated to a series of stimulating lectures by very distinguished speakers, along with a chance to view an impressive set of shiny new kit. Notably, the Diamond staff welcomed this technology in a spirit of warm collegiality.

After a greeting from **Andrew Harrison**, CEO of Diamond Light Source, Nobel laureate **Richard Henderson** (Cambridge) gave the keynote lecture. He described the technological developments that enabled cryo-EM to achieve the resolution needed for much research in structural biology. One important technique is plunge-freezing in liquid ethane of a thin sample deposited on a grid, pioneered by Dubochet and colleagues. It converts the water in the sample to amorphous ice, limits mobility and minimises radiation damage, and protects the sample from the high vacuum of the electron microscope. The TEMAFS1.0 detector designed in the UK at RAL/STFC also represented an important advance. Sophisticated software is essential to make best use of the images obtained. The growing usefulness of cryo-EM is highlighted by a comparison of annual deposits to the Protein Data Bank of structures determined by NMR / cryo-EM / X-ray crystallography: 965/19/6,148 in 2007 *versus* 457/408/10,019 in 2016. Furthermore, the structures determined by cryo-EM are often bigger and therefore "more interesting". Recently published structures which would have been intractable without cryo-EM include gamma-secretase and mitochondrial complex 1. We are doing well, but there still are unanswered questions. When frames are taken as a movie, the first ≈5 images tend to be of low quality. This could be the result of differential thermal contraction between protein and amorphous ice and support, introducing strain. Once this has relaxed, the quality is highest until radiation damage sets in. By the end of exposure about ¼ of mass is lost by efflux of species including H_2, CH_4 and C_2H_6.

David Stuart (Oxford and Diamond) spoke next about the "Vision for integrated structural biology at Diamond". In his opinion structural biology "came of age" with the publication in 2016 of *Molecular Biology of Assemblies and Machines*. There are many good reasons to include cryo-EM in a synchrotron facility. About 50 % of Diamond users come to do life science research. The mission of Diamond has always been twofold, to provide a user service and to develop technology. Diamond's user facility is well established and provides access efficiently and fairly. Technical expertise now existing at Diamond in engineering, computing and software development is transferable to cryo-EM, which is being rolled into Diamond's budget from 2019. Now that atomic detail relevant to drug design is achievable, industry is becoming very interested. This new demand is to be satisfied by the installation of 2 machines in partnership with Thermo Fisher. The 4 high-end machines already in use have been heavily oversubscribed; 2/3 of the users are UK based, and 2/3 of the remainder are EU based. The group making the greatest use is the Henderson group. Important technical advances are also taking place in macromolecular crystallography. Beamline I23 is held under vacuum, allowing long wavelength X-rays to be used with no air scattering. Thereby, anomalous scattering can be measured from S and P atoms in native proteins and polynucleotides. The XFEL Hub extends Diamond's dual mission of user service and technology development to free electron lasers, providing training and sample preparation facilities to help users to access existing FELs, and developing hardware and software for the European X-ray Free Electron Laser.

Two "Ignite" talks before lunch showed how eBIC has already provided structural information about important biological mechanisms.

First, **Alessandro Vannini** (Institute of Cancer Research) examined the mechanism of RNA III polymerase. Purified from yeast, the pre-initiation complex consists of 26 subunits with a total mass around 1.5 MDa. With a fully complementary DNA scaffold the native PIC could be studied without crosslinking. The mechanism of DNA opening involves movement of the template strand into the pocket provided for it. Alessandro also discussed sensing of DNA opening. Novel protein interfaces have been identified which could serve as targets for anticancer drugs.

Xiaodong Zhang (Imperial) has already obtained 10 unique structures from eBIC, concentrating on DNA processing enzymes involved in bacterial transcription regulation and in eukaryotic damage repair. Cryo-EM reconstruction of the RNA polymerase – σ^{54} complex partially explained inhibition, and X-ray crystal structure determination at 3.8 Å completed the explanation. The molecular mechanism of DNA damage repair goes through steps of sensing, signalling, site exposure and repair.

The morning session concluded with the formal unveiling of a commemorative plaque.

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We were ready for the very pleasant buffet lunch that was provided in the airy Atrium and featured a wide variety of food items to satisfy the full range of tastes and metabolisms. Afterwards we were divided into small groups, each with a knowledgeable "native guide", to give us some much-needed postprandial exercise and show us the equipment that we had heard about in the morning. We visited the cryo-EM control suite and got as close to the actual equipment as was permissible and safe. Our tour included beamline I23 as well.

Well-fed and exercised, we reassembled for another keynote lecture. This time **Yoshinori Fujiyoshi** (Nagoya) presented cryo-EM from a Japanese perspective. Japan has a distinguished history of innovation in cryo-EM, and an 8th generation is under development. Results presented on aquaporins (AQP) made us glad that we had stayed sober! To date, 13 types of aquaporin have been identified, with water channels that allow proton permeation by domino toppling not requiring the migration of any individual H^+. Results on AQP0 and AQP1 show the importance of the helix dipole. Consumption of alcohol elicits AQP4 expression in the brain, allowing cerebral oedema to develop. Since the brain is confined within a rigid box, this can be fatal. In an example of "drug rescuing", acetazolamide (AZA), used to treat glaucoma, epilepsy and altitude sickness among other conditions, has been found to inhibit expression of AQP4. In mice it cut the death rate from 15 % to zero. Successive structural analyses of the relevant complex with AZA steadily provided more information. At 5.0 Å resolution the binding position could be discerned. At 3.4 Å a rough map could be obtained. At a

resolution of 3.0 Å a map of the inhibitor appeared plausible but led to an incorrect conclusion, which was corrected when the resolution was improved to 2.8 Å. At the highest resolution a particular conformation was clearly shown to be cis; previously, in the absence of such clear evidence, it had been assumed to be the normally more stable *trans*.

After some well-chosen concluding remarks we were able to disperse in time to beat the worst of the Oxfordshire rush-hour traffic.

Carl Schwalbe

Publication Announcement

WE imagine readers of *Crystallography News* would like to know of the just published Royal Society Biographical Memoir for Durward Cruickshank (7 March 1924—13 July 2007). The abstract is reproduced here.

Durward Cruickshank was an eminent crystallographer and structural chemist, whose mathematical abilities transformed the precision of the molecular structures determined in three dimensions by X-ray crystal structure analysis. This technique is very widely applied to determine the three-dimensional (3D) shapes of molecules of importance in biology, chemistry, mineralogy, materials science and physics. Durward's first publication was on this topic, with Sir Gordon Cox. It represents a lifelong interest of Durward in the precision of crystal structure analysis and extended also to gas-phase electron diffraction. His research publications spanned an amazing 60 years and he had a direct influence on over 900 000 chemical crystal structures, the number currently determined and held in the Cambridge Structure Database alone. Proteins took his attention for research in his last decade, and his diffraction precision index (DPI) indicator of the precision of a protein structure is added regularly to entries in the Protein Data Bank. In his 'retirement' he contributed, with one of the authors of this memoir, J.R.H., and various colleagues in the UK and the USA, to the development of the 'Laue diffraction' white beam synchrotron method, applied today to sub-nanosecond X-ray crystallography measurement techniques, and also to study micron sized, i.e. tiny, crystal samples. The method has also led ultimately to more effective exploitation of neutron beams from research reactors for crystallographic studies of the hydrogenation details of molecules.

The weblink to the article is here:-
http://rsbm.royalsocietypublishing.org/content/roybiogmem/65/71

John R. Helliwell

Zurich School of Crystallography 2018 in Tianjin, China

THE eighth Zurich School of Crystallography (ZSC) pitched tent at Tianjin University from June 17-28 following an invitation by Prof. Jay Siegel, Dean of the School of Pharmaceutical Science and Technology (SPST). The school was attended by 20 handpicked participants, 9 from the Tianjin area, 8 from various other parts of China, 1 from Hong Kong and 2 from Thailand. Of these, 2 are studying towards an MSc, 11 are PhD students, 2 are Postdocs and 5 are young academics. Seven of the long-time Zurich School tutors from the universities of Zurich, Bern, Prague, ETHZ and EPFL took up the invitation, namely Tony Linden, Olivier Blacque, Hans-Beat Bürgi, Lukas Palatinus, Michael Wörle, Bernd Schweizer and Gervais Chapius. Richard Cooper from Oxford University, Ian Williams from Hong Kong University of Science and Technology and Junliang Sun from Peking University completed the team, thereby ensuring our usual and popular 2:1 student:tutor ratio. The goal of the school is to equip each participant with enough theory and practice to be able to determine small-molecule organic and inorganic crystal structures and to recognize difficulties that require help from a more experienced specialist. The encounter of the mostly western teachers with the Asian students was both interesting, at times somewhat challenging, but in the end very rewarding.

The programme followed our well-tried format, usually with two hours of lectures followed by two hours of practical work during the mornings and afternoons. The participants had to solve at least three set structures and could then work on their own data set collected from a sample they provided. The specially selected set structures provide increasing levels of complexity. The first one is straightforward and allows the participants to learn the general procedure from structure solution through to a completed and validated structure report using the program package *Olex*^{2}. The second one requires some chemical knowledge for proper atom assignment, while for the third one the chemist's guess of the structure is largely wrong and the actual molecular structure has to be found using a combination of chemical, crystallographic and geometrical logic and even databases. Examples involving severe disorder and solvent molecule handling were also demonstrated.

The SPST is well equipped with three recently installed Rigaku diffractometers: a Synergy-S and a XtaLAB Synergy Custom FR-X Rotating Anode system with two ports. In addition, we had access to a Rigaku SuperNova diffractometer at the School of Science, Tianjin University, thereby allowing the participants adequate opportunity to gain hands on experience with data collection procedures using their own samples. **Yan Zier** from Rigaku China was on hand to assist with the brand new instruments and his expertise was highly appreciated. Structure solution, refinement and analyses were done in a fully equipped computer room, which provided a workstation for each participant and tutor.

We found that the student-tutor interaction in China is somewhat more reserved than what we are used to in Zurich and this was particularly noticeable during the lectures. Although the participants spoke good English, their pronunciation sometimes needed getting used to. We also learned that the Chinese language has technical terms that are very different from the English ones and it was here that the help of our Chinese colleague **Junliang Sun** was invaluable, as he usually untangled communicative roadblocks with a single, short sentence in Chinese. Some of the lecturers felt at times that their message did not get through, but as the school proceeded it became increasingly clear that the participants understood enough of the lectures to be able to consult their Chinese text books and discuss the day's material together at the hotel in the evening. Thanks to the 2:1 format during the practical work, the interaction between the participants and the tutors became increasingly more relaxed. The very successful outcome of the final two-hour written exam showed how really hardworking everybody was. When **Lukas Palatinus** from Prague started playing the guitar after the final dinner, everybody joined into the singing and the two cultures had definitely merged into a single, merry group.

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On the rest day, the tutors were taken to the Huangyaguan Pass section of the Great Wall and almost had the wall to themselves during the strenuous 2.2 km walk along the ridge and down to the river. It was a great experience.

Professors **Jay Siegel**, **Kim Baldridge** and **SPST** made an enormous effort to provide a congenial atmosphere for the school and excellent accommodation. We are especially grateful to **Jun Xu** who did most of the local organization, including initial data collections and structure solving for the crystalline samples contributed by the participants, thereby ensuring that they did not have to work on didactically unsuitable structures. Without the efforts of **Ying Wei**, the Europe-China communication, transportation and visa arrangements would have been significantly more difficult. Vice Dean **Zhou Yan** acted as the local coordinator and organizer. The directors and local organisers very much appreciate the willingness of the tutors to undertake this adventure. Tianjin University, The Health Sciences Platform of Tianjin University and Rigaku Oxford Diffraction supported the school financially. We also wish to thank the Cambridge Crystallographic Data Centre and the Fachinformationszentrum Karlsruhe for permission to access their databases during the school. Last but not least, the tutors are very grateful to the volunteer students who accompanied them between the hotel and the university and made sure that we did not get into difficulties in a country where we knew only a handful of words. Xiè xiè!

Hans-Beat Bürgi, **Tony Linden**, School Directors

The Zürich School of Crystallography 2018 – Report from a participant

The Zürich crystallography school (ZSC), 2018 in Tianjin is a great surprise for Chinese scholars. I would say joining this school is one of the best things I've ever done. I can feel how considerate ZSC is. We had a Chinese tutor this year for dealing with language issues which turned out to be a very wise and helpful decision.

Tutors are kind, patient and knowledgeable. What impressed me most was their open-mindedness and enthusiasm towards a new culture. They adapted themselves so quickly to China's environment by learning Mandarin and gestures, using Wechat and climbing the great wall in Tianjin.

Another thing to be mentioned is the 2:1 student:tutor combination which is the most beneficial and effective part of this course. Chinese students tend to keep quiet in discussions, which may be inefficient for feedback and interactions. But within a small group, I felt free to ask whatever I wanted, meanwhile, my tutor would try his best to answer my questions, no matter how trivial or how strange they were.

The ZSC covered everything I can imagine about crystallography, from fundamental background to the practical operation of solving structures, including the introduction to the instruments and the output of the final report. No wonder it is so intense. Fortunately, the theoretical concepts were taught repeatedly during the whole course and externalized in the practical sessions. I have a systematic map in my mind with more confidence and ability to work on crystals after the school.

I had a great time during the school, where I met many people around China and made two friends from Thailand. The final banquet was full of joy and music; I enjoyed it very much.

In the end, I appreciated everyone who contributed to this school and made it so successful and meaningful. I strongly recommend ZSC to anyone who are interested in this area. This will be a good opportunity to immerse yourself in the ocean of knowledge.

Mengsi Lu, Tianjin University, China

If you are you interested in the next school, see
The Zürich School of Crystallography
University of Zürich, June 16-27, 2019
http://www.chem.uzh.ch/linden/zsc

XTOP2018 14th Biennial Conference

High Resolution X-ray Diffraction and Imaging

3rd-7th September 2018, Bari, Italy

IT is rare that potential delegates have to be turned away from a scientific conference, but such was the popularity of this meeting that the attendance limit set by the size of the lecture room was exceeded by mid-August. With 185 delegates, the 14th XTOP was the largest in the 26 year history of the series, which began in 1992 in Marseille. In 1992, there was a focus on diffraction imaging and promotion of the capability of the new imaging beamline ID19, then being constructed at the ESRF in Grenoble. Over the years, the focus shifted towards phase imaging and high resolution diffraction of nano-systems. At one point, it appeared that the specific niche that the conference series occupied was being squeezed by other meetings and there was debate about the series' future. The Bari meeting completely dispelled such thoughts. There was a new and exciting focus on imaging (if readers will pardon a pun) with novel work on coherent imaging a highlight. There was a renewed energy apparent in the meeting, reflected by the large numbers of young crystallographers who were present.

Delegates assemble for the obligatory conference photograph.

As has become the tradition, the first day was devoted to a tutorial school, designed to introduce PhD students to some of the topics to the presented later in the conference. As has also become commonplace, this school-day was attended by a considerable number of more experienced researchers, such was the clarity of the six presentation given by **Ullrich Pietsch**, University of Siegen "X-ray diffraction in Nanoscience"; **Gilles Renaud**, Univ. Grenoble Alpes "Hard X-ray surface science methods"; **Oliver Bunk**, PSI, Villigen, "Scanning imaging methods"; **Gerardina Carbone** -MAX IV, Lund, "Science opportunities at new generation X-ray sources; **Tilo Baumbach**, KIT, Karlsruhe, "Full Field Imaging"; and **Vladimir Kaganer**, Paul-Drude-Institut für Festkörperelektronik, Berlin "X-ray scattering from imperfect crystals".

Invited key-note speakers in the main conference were **Andrei Benediktovitch**, DESY, Hamburg, "X-ray diffraction from imperfect crystals theoretical approaches applied to laboratory measurements"; **Peter Cloetens**, ESRF, Grenoble, "A journey in space and time using X-ray full field microscopy"; **Ana Diaz**, PSI, Villigen, "X-ray imaging with coherent X-rays"; **Erik Lauridsen**, Xnovo technology, Køge, "Nondestructive Materials Characterization in 3D by Laboratory Diffraction Contrast Tomography – Applications and Future Directions"; **Marianne Liebi**, Chalmers University of Technology and MAX IV Laboratory, Göteborg, "Scanning Small-Angle X-ray Scattering from 2D to 3D"; **Stefano Marchesini**, Lawrence Berkeley Lab, "High Throughput Phase Retrieval"; **Maksym Myronov**, Warwick University, "X-ray diffraction from advanced epitaxial group-IV semiconductor structures"; **Henning Friis Poulsen**, Department of Physics, Lyngby, "X-ray diffraction microscopy"; **Pantaleo Raimondi**, ESRF, Grenoble, "Status update of the ESRF's Extremely Brilliant Source project to design and build a low-emittance, high-brilliance storage ring, opening up new horizons for accelerator science", **Marie Ingrid Richard**, Institut Matériaux Microélectronique et Nanosciences de Provence, "In Situ & Operando X-Ray Investigation of Single Nanoparticles", **Raj Suryanarayanan**, University of Minnesota, "Pharmaceutical Applications of Powder X-ray Diffractometry" and **Tao Zhou**, ESRF, Grenoble, "Grazing Incidence X-ray Scattering and Full Field Diffraction X-ray Microscopy for in situ and operando studies".

A high point was the talk of **Robert Feidenhans'l** of the European XFEL, Schenefeld, on "The European XFEL – a powerhouse for new X-ray Science". Robert presented us with the first results from the XFEL – experiments that had either appeared in Nature that week or had been accepted by Nature that week. It was immensely stimulating, truly indicating the start of a new era of diffraction physics applied to a wide range of scientific problems.

The oral sessions were full, the poster sessions lively and the social activities friendly and relaxed. The environment, a hotel converted from a large villa with cool, spacious gardens, was wonderful. The sun shone, but not too fiercely. The food was excellent and taken in the garden. **Cinzia Giannini**, of INSTM and CNR-IC, Bari is to be congratulated on organizing such a truly magnificent conference.

Cinzia Giannini, Chair of the conference.

If there is one down-side of a wonderful week it was the very few UK papers that were presented. In addition to the one invited paper, there were only two other UK oral presentations. It is a pity that a long and distinguished contribution of the UK to high resolution diffraction and imaging appears to be dwindling away.

Brian Tanner
Durham University

Diamond shines its light on Moon Rocks from Apollo Missions

NEARLY 50 years after our first steps on the Moon, rock samples from the Apollo missions still have a lot to tell us about lunar formation, and Earth's volcanoes.

An international collaboration involving scientists in Tenerife, the US and the UK, are using Diamond, the UK's world class synchrotron, to investigate Moon rocks recovered during the Apollo Missions in a brand new way.

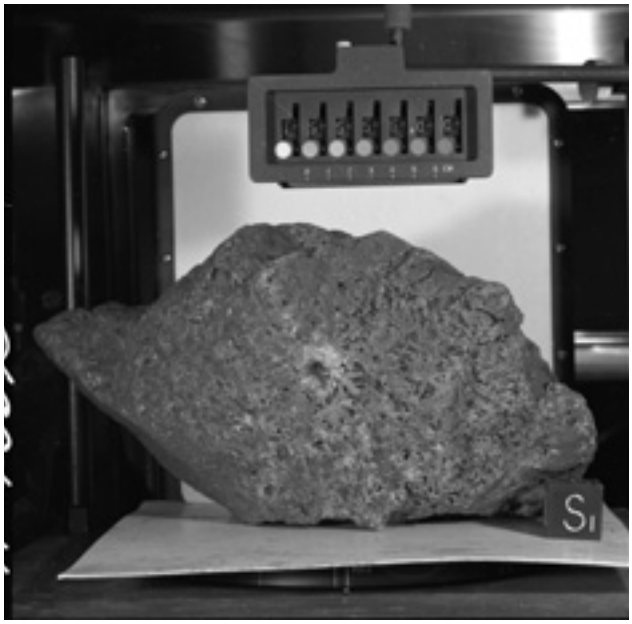
Dr. **Matt Pankhurst** of Instituto Volcanológico de Canarias and NASA lunar principal investigator explains; *"We have used a new imaging technique developed at Diamond to carry out 3D mapping of olivine – a common green mineral found in the Earth's sub-surface and in these Moon rock samples. These maps will be used to improve understanding of the Moon's ancient volcanic systems and help to understand active geological processes here on Earth.*

With this new technique, our team may be able to recover from these Moon rock samples information such as what the patterns of magma flow within the volcanic system were, what the magma storage duration was like, and potentially even identify eruption triggers. The data will be analysed using state-of-the-art diffusion modelling which will establish the history of individual crystals."

When early astronomers looked at the Moon, they mistakenly thought that the darker areas they could see were seas, and named them *Mare*, the Latin for sea. Around 16% of the lunar surface is covered in this dark material, which we now know is basalt, a volcanic rock. Before the Apollo missions, we believed that these areas meant that they were young, but when the rock samples brought back from the Moon were examined, they were shown to be ancient; the youngest volcanic Moon rock sample is nearly 3 billion years old.

The team have examined samples from the Apollo 12 and 15 missions, using an advanced X-ray speckle imaging technique developed on Beamline B16 at Diamond Light Source. As Dr. **Hongchang Wang**, Senior Optics Scientist, explains: *"Combined with the recently developed fast fly-scan tomography and novel white beam camera, the X-ray speckle imaging technique has allowed us to swiftly and effectively collect 3D information of olivine inside of the lunar rock in* much more detail than ever before." This new technique does not damage the lunar samples.

Dr. Pankhurst continues; *"Nearly 50 years after the first humans landed on the Moon, there is still a lot we don't know about how the Moon formed, and the nature of lunar volcanic activity. We know that, on Earth, volcanic eruptions can be triggered (or ended) by changes in magma (molten rock) in or beneath the planet's crust. The cause of these changes is often thought to be a result of the mixing of different batches of magma in the 'plumbing system' below the volcanoes. Volcanologists are working on detecting and understanding these changes, by examining volcanic rock samples, with the aim of being able to accurately forecast future eruptions."*



The same techniques are now being applied to lunar rock samples, which will provide new insights into how the Moon was formed, and its volcanic history.

In magma, the ratio of iron to magnesium in olivine changes over timeframes ranging from hours to months, and these changes are 'locked in' to the mineral as the magma cools. Accurate 3D images of the iron distribution within olivine in the Moon rock samples will 'unlock' information about the volcanic processes in which they formed.

NASA has approved the use of 18 lunar samples for these experiments, and similar, well-characterised terrestrial samples have also been scanned, and used to verify the chemical composition of olivine. Samples are loaned to scientists who wish to study them, a process overseen by NASA's Apollo sample curator, **Ryan Zeigler**. As a scientist who understands the trade-off between studying the samples and preserving them, a balance must be struck in experiment design. These decisions are becoming easier as we develop more powerful, non-destructive techniques. He comments: *"The researchers are now using state-of-the-art diffusion modelling to establish the history of individual crystals of olivine from 3D images. These techniques will be applied to the new data gathered during this beamtime. The results will add to our understanding of lunar and planetary formation, topics which have been continually debated since the samples were first returned to Earth."*

Prof **Andrew Harrison** CEO at Diamond Light Source concludes: *"A successful demonstration of the new technique at B16 will pave the way, we hope, for extended collaboration with NASA and maybe next No10 Downing Street and the Natural History Museum might be interested in loaning us their own samples."*

Diamond has a huge amount of experience of investigating priceless heritage items, and gaining new insights from them. Using these techniques, we could study the UK's Moon rock samples in new ways, and these fresh images would give them more meaning and inspire the next generation of scientists and engineers.

Isabelle Boscaro-Clarke and **Lorna Campbell**
Diamond Light Source

Who were the astronauts behind the rocks studied at Diamond?

Everyone can name the first two people to step on the Moon, but the Moonwalkers from the later Apollo missions are less well known. During Apollo 12, Mission commander **Charles "Pete" Conrad** and Lunar Module Pilot **Alan L. Bean** collected 35kg of samples in an area of the Ocean of Storms (*Oceanus Procellarum*) that had previously been visited by several unmanned missions, and was therefore named *Mare Cognitum* (Known Sea). For Apollo 15, Commander **David Scott** and Lunar Module Pilot **James Irwin** spent three days near Hadley Rille, in an area of the *Mare Imbrium* called *Palus Putredinus* (Marsh of Decay). They used the first lunar rover to travel much further, and collected 77kg of samples.

These rock samples are so precious that they are kept in a special building, the Lunar Sample Laboratory Facility at NASA 's Johnson Space Center (JSC) in Houston. They have been housed in a clean environment for nearly 50 years.

Not all Apollo samples are still in Houston, however. From the 48lbs (nearly 22kg) of rocks that **Neil Armstrong** and **Buzz Aldrin** brought back from their Apollo 11 Moon landing, plaques were prepared with four pieces weighing 50 milligrams. The White House presented these as goodwill gifts to the leaders of 135 countries, the United Nations and all 50 American states.

* The UK's Moon rock gift was presented to Prime Minister **Harold Wilso**n by President **Richard Nixon** in 1970. It went on a tour of museums around the country, starting at the Science Museum in London, returning to Downing Street in 1973. In 1979 an aide to Margaret Thatcher revealed to her that the Moon rocks had been languishing in a cupboard for several years! Since then they have been on display in Downing Street and the Natural History Museum.

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.

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/

2-9 December 2018
Fifth Joint DLS/CCP4 Workshop, Didcot.
https://www.diamond.ac.uk/Home/Events/2018/Diamond-CCP4-Data-Collection-and-Analysis-workshop.html

7 December 2018
Nanostructures at soft interfaces: technology and biophysics, Cambridge.
https://www.iopconferences.org/iop/frontend/reg/thome.csp?pageID=755901&eventID=1237&traceRedir=2

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

19-21 December 2018
2nd BornAgain School and User Meeting, Garching, Germany.
https://indico.frm2.tum.de/event/150/

8-10 January 2019
2019 CCP4 study weekend entitled "Integrated, Rational Molecular Replacement", Nottingham.
http://www.cvent.com/events/ccp4-study-weekend-2019/event-summary-3372f50a47c74742afc6e001881e38de.aspx

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

2-8 February 2019
3rd NEUBIAS Conference, Luxembourg City, Luxembourg.
http://eubias.org/NEUBIAS/neubias2020-conference/luxembourg-2019/

6-8 February 2019
Cryo-EM in Industry & Academia, Heidelberg, Germany.
https://www.embl.de/training/events/2019/CPP19-01/

12-14 February 2019
BioXFEL. 6th International Conference, San Diego, CA, USA.
https://www.bioxfel.org/events/details/1183

2-6 March 2019
Biophysical Society Annual Meeting, Baltimore, MD, USA.
https://www.biophysics.org/2019meeting#/

7-8 March 2019
Microscopy characterisation of organic-inorganic interfaces – 2019, Berlin, Germany.
https://mcoii-2019.mpikg.mpg.de/

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/

17-22 March 2019
School and Conference on Analysis of Diffraction Data in Real Space, Grenoble, France.
https://workshops.ill.fr/event/133/

25-28 March 2019
27th Annual Meeting of the German Crystallographic Society (DGK), Leipzig, Germany.
https://www.dgk-conference.de/

6-14 April 2019
17th BCA/CCG Intensive Teaching School in X-ray Structure Analysis, Durham.
https://community.dur.ac.uk/durham.x-ray-school/general.htm

9-12 April 2019
21st International Conference on Microscopy of Semiconducting Materials (MSM-XXI), Cambridge.
http://msmxxi.iopconfs.org/Home

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

15-18 April 2019
ISSC-22. Interdisciplinary Surface Conference, Swansea.
http://issc-22.iopconfs.org/home

22-26 April 2019
2019 MRS Spring Meeting & Exhibit, Phoenix, AZ, USA.
https://www.mrs.org/spring2019

5-10 May 2019
RapiData2019, Menlo Park, CA, USA.
http://smb.slac.stanford.edu/news/rapidata/rapidata-2019/

31 May – 9 June 2019
Cryo 3D Electron Microscopy, Erice, Italy.
https://crystalerice.org/2019/

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

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

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

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

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

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

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

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

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

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

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

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

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