Crystallography News

British Crystallographic Association

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Scenes from ECM28

Photos by Katharina Fromm, Minmin Yu and Carl Schwalbe

Next BCA Spring Meeting: April 2014

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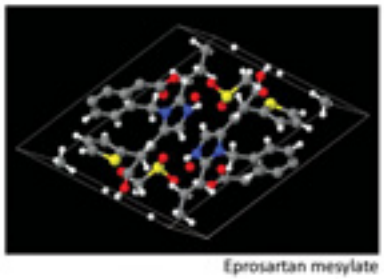

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Please ensure that items for inclusion in the March 2014 issue are sent to the Editor to arrive before 25 January 2014.

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As required by the DATA PROTECTION ACT, the BCA is notifying members that we store your contact information on a computer database to simplify our administration.

These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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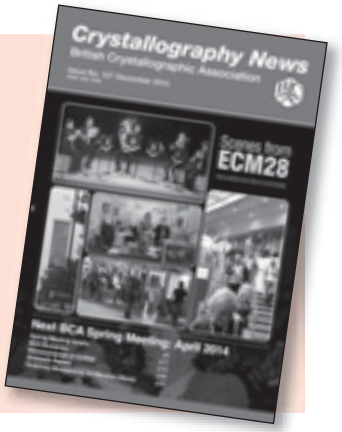
This month's cover:

ECM28: opening concert, IUCr stand, poster session, participants "in the pink"



From the President

PERHAPS appropriately, given this nostalgic Bragg Centenary year, I have recently been returning to my crystallographic beginnings and the delights of the rocksalt structure. Rocksalt itself was the first structure ever determined using x-ray diffraction, by William and Lawrence Bragg in 1913. And rocksalt-structured silver bromide was the first material that I tackled crystallographically during my PhD. I am perhaps displaying my physics background somewhat here by declaring a fondness for such a simple structure (indeed several more knowledgeable crystallographers delight in telling me that physicists recognise only two crystal types, those that are cubic and those that are complicated) but it is the disorder that develops within the structure that fascinates me, from the ionic mobility in AgBr to the recent reports of transient molecular dipoles in thermoelectric PbTe. Rocksalt is also one of the few crystals that I have actually successfully grown…

Crystal growing is one of those 'kitchen science' experiments that has particularly wide appeal. We had an entertaining and light-hearted discussion on the subject at our recent Council meeting. In fact I confused some by saying that you could – with time – get crystals from tomorite; they thought it was some unfamiliar mineral! That old forgotten tin of maple syrup at the back of the cupboard can be a good source of sweet crystals. It is therefore not surprising that there will be a number of crystal growing competitions sprouting up around the world as part of the International Year of Crystallography. For example every primary school in Oxfordshire will be sent a crystal growing kit next year, organised by Diamond and funded by STFC, so that the children can see and understand how crystals grow. The best ones will be displayed in central Oxford and suitable prizes awarded. Please let me know of other similar events that may be happening around the country – it would be great to see photos of the results!

Of course other crystallography-based public-engagement activities are continuing apace for the Bragg Centenary and IYCr2014. Thanks to a grant from STFC, the Royal Institution is producing a Celebrating Crystallography Collection on their online RiChannel.org that, as well as other content, already includes the very popular animation explaining the origins of crystallography. This particular clip has already received 21,198 views on YouTube. Please do take a look at this if you haven't already done so. I'm also really pleased that there will be a crystallography stand at next year's Big Bang Fair, to be held in the NEC in Birmingham, 13-16 March 2014. The stand is again sponsored by STFC with support from Diamond and with the BCA responsible for the content and stand volunteers. Those who helped this year already know what a great event it was to be a part of, and I am confident that there will be no shortage of volunteers when Anna, Claire and Lynn (our Education and Outreach Co-ordinators) come calling for your help in the near future. Please also consider whether you might like to attend and support the IYCr2014 Opening Ceremony to be held at the UNESCO building in Paris 20-21 January 2014 – see www.iycr2014.org/opening-ceremony for more details.

Many of us will have been in Warwick in August for the European Crystallographic Meeting. It was a fantastic event, enhanced by the Two Braggs exhibition and the many incidental events and meetings. One highlight for me was the lunchtime lecture by **Jenifer Glynn** on her sister **Rosalind Franklin** (of DNA fame). She finished her talk by showing the Quentin Blake cartoon of the discovery showing Franklin studying the DNA molecule whilst Crick and Watson are propped up on the double helix chatting and drinking beer! (See www.cambridge-news.co.uk/Whats-on-leisure/Books/The-unsung-heroine-of-DNA-remembered-17082012.htm.) I was also pleased to see how well attended the very prominent BCA stand was, with many people using it as a meeting place throughout the meeting. Thank you to all those who provided the posters in a very short time-scale and especially to **Anna Warren** for arranging their printing and transportation.

An evening picture of the BCA Stand at ECM28 in Warwick, showing a rare moment when it wasn't surrounded by people

We also held the 2013 Annual general Meeting of the BCA in Warwick and I am pleased to welcome **Richard Cooper** as our new Vice President and **Andrea Thorn** as an Ordinary Council Member, and to formalise **Claire Wilson**'s position as Secretary. I also want to again thank those council members who have 'retired' from their respective roles, to **Arwen Pearson**, **Dave Allan** (as Vice President), **Georgina Rosair** (as Secretary) and Elspeth Garman (as Past President). Thanks are especially due to Elspeth and Georgina who together have served the BCA in different roles for many years, and to Dave Allan who has supported me and Elspeth as Vice President, his last duty being to

Post AGM photograph of BCA President David Keen honouring Elspeth Garman (past President, left), Georgina Rosair (after long-service as Secretary, middle) and Moreton Moore (newest Honorary Member sporting an early BCA logo'd T-shirt, right).

source flowers from within walking distance of the Warwick University campus for Elspeth and Georgina (see photo above).

It was also a great privilege to award **Moreton Moore** with a BCA Honorary Membership at the AGM. Moreton has been a fantastic supporter of the BCA over many years and has been to nearly all BCA Spring Meetings. He has been the editor of several crystallographic journals, including a Founding Editor of Crystallography Reviews as well as carrying out a strong crystallographic research career starting in Cambridge and Bristol before settling at Royal Holloway. Please congratulate him (again) when you next see him!

I hope that you enjoy the festivities over Christmas and New Year and are looking forward to next year's crystallographic events: IYCr2014; BBF; BCA Spring Meeting; IUCr Congress; etc. etc. The BCA will have a busy and very enjoyable 2014!

I commend this edition of Crystallography News to you.

David Keen

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

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From the Editor

UNDOUBTEDLY the big event of our year has been ECM28. The London Olympics showed the world that Britain could successfully host a major international event and do it with efficiency and style. ECM28 provided confirmation. We have long known that Sandy Blake and Elspeth Garman are talented and enthusiastic crystallographers; now we have seen how brilliant they are as organisers and, in Elspeth's case, as impresario of a great little concert as well. In fact, there was so much going on that it would have been all too easy to miss an interesting and important event. By reminding us at breakfast of the day's schedule, the Newsletter provided by Paul Raithby and Richard Cooper was just what we needed to avoid such mistakes. The "Two Braggs" exhibition was a particular highlight. As I sit comfortably in front of a laptop computer whose software does its best to anticipate my wishes and correct my errors, I recall with boundless admiration the fiddly ionisation spectrometers that gave vital data with totally manual operation, and the precise handwriting in which the Braggs recorded and communicated their results. Thanks are due to Northern Networking for their administrative support from beginning to end; and Warwick University gave us comfortable accommodation and good food at a fair price. The weather matched one's ideal of a balmy English summer. However, this highlighted the one and only drawback I could find: the boldness of the Warwick wasps. The warm sunshine prompted many of us to eat our packed lunches outdoors. Importantly, we had a wide choice of lunch items; but whatever we chose, it delighted the wasps!

Gently but irresistibly, Sandy persuaded the majority of session chairpersons to provide concise summaries of their microsymposia at ECM28. These summaries and associated pictures are featured in this issue. I hope that they will rekindle interest in the excellent presentations that so many of us witnessed. We may well wish to revisit the abstracts, and these will be forthcoming in a special issue of *Acta Crystallographica*.

A forward look to 2014 shows that plans are well advanced for our Spring Meeting at Loughborough University. Details appear in this issue. Now it is up to you, our readers, to provide the all-important contributed abstracts. Please note that the deadline is 17 January 2014.

Of course, 2014 will be a very special year for another reason: the Congress of the International Union of Crystallography in the International Year of Crystallography. It promises glorious cutting-edge science allied to sagacious historical perspectives. Even better, the meeting will be held in Montreal, a city where the eminence of Mount Royal overlooks the mighty St. Lawrence River and where abundant fresh North American food is cooked with French panache. For people like me whose skills at conversational French are rather lame, the Quebecois are very helpful. In my experience they are willing to speak French slowly and distinctly when necessary to help foreigners who are making an effort.

While most of the BCA Groups will already have held their Autumn Meetings by the time this issue appears, the onset of winter will bring out our hardy Biological Crystallographers (is this another example of cryoprotection?). The BSG Winter Meeting on "New X-ray developments and macromolecular structures in the Bragg Centenary year" will be held at King's College London on Monday, December 16. Then, in Nottingham on January 3-5, the CCP4 Study Weekend will provide an opportunity to learn about Complementary Methods. I don't think this term means improving the happiness of your crystals by acupuncture or reflexology. Instead, it involves biophysical techniques, SAXS, new mounts, EM and dynamics.

I am delighted that this issue carries the announcement of the election of **Moreton Moore** to Honorary Membership of the BCA. Initially, Moreton had aspirations to become an astronomer, but fortunately he lowered his gaze to terrestrial matters and became a physical crystallographer. Moreton has loyally served the BCA in many important ways. As the first editor of *Crystallography News* he set a standard that subsequent editors have to work very hard to match. Much of Moreton's most important research has been on the structural properties of diamonds. Although he showed that diamonds tend to have defects, he himself remains a "diamond geezer".

Readers who scrutinise the Council Page with the same care they apply to a difference map will have noticed that **David Allan**'s term as Vice President has come to an end. I am particularly grateful to Dave for his contributions to *Crystallography News*. One of my ambitions is to publish articles of lasting value that readers will want to keep. Dave's articles about the National Facilities were exactly what I had in mind. Recently Dave started providing backup for me as Editor, and I am delighted that he will continue in this role. As well as contributing an extra pair of eyes to proofread each issue, Dave will ensure that an issue appears in timely fashion even if I were to suffer a major mishap.

It just remains for me to wish all our readers a happy and productive Year of Crystallography.

Carl Schwalbe

BCA Council 2013

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

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

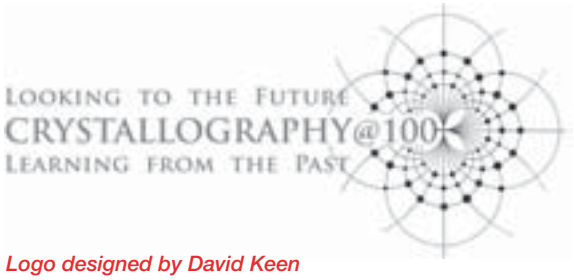
BCA Annual Spring Meeting

University of Loughborough
8-10 April 2014

"Crystallography@100: Looking to the Future, Learning from the Past"

CRYSTALLOGRAPHY is in a period of centenary celebration, looking back at the foundations of the field with the first observation of diffraction and von Laue's Nobel Prize (1912), followed by the first crystal structure determinations using diffraction conducted by W.H and W. L. Bragg, which led to their Nobel Prize in 1915. Next year has been designated the International Year of Crystallography (IYCr) by UNESCO, and the IUCr will initiate a year of activities intended to showcase crystallography with the official Opening Ceremony of the International Year of Crystallography, which will take place at UNESCO Headquarters in Paris on 20-21 January 2014.

The annual spring meeting of the BCA will be very forward looking, reflecting the health and future of the field 100 years on from its origins, but will also provide an opportunity to reflect on where the field has come from over the past century. This balance is reflected in the theme for the meeting.



Logo designed by David Keen

The format of the meeting will be very similar to previous years, with a 1-day Young Crystallographers Satellite meeting preceding the 2-day main meeting. It will be a pleasure to welcome you to Loughborough.

The BCA is pleased to host the **Bragg Lecture**, this year presented by Prof. **Judith Howard**, FRS (Durham University) whose lecture topic is in tune with the meeting theme, "Exploring a century of reciprocal space: same old theory – endless new results." The Lonsdale Lecture opens the main meeting and will be presented by Prof. **Henry Chapman** (Center for Free-Electron Laser Science, DESY, Hamburg).

There will be four further plenary lectures associated with the BSG, CCG, IG and PCG. On the middle Wednesday (April 9) there will be a session devoted to winners of the prizes for early career scientists. Details of the CCG prize, sponsored by the CCDC, PCG prize sponsored by PANalytical, the IG/YCG prize and the newly announced BSG prize, can be found via the BCA web pages.

Prof. ***Judith Howard***
Bragg Lecture

Prof. ***Henry Chapman***
Lonsdale Lecture

The overall theme of the meeting is very forward looking and focuses on the development of crystallography away from purely structure determination towards crystallography under non-ambient conditions, crystallography at different timescales, combining crystallography with other diffraction and non-diffraction techniques (e.g. spectroscopy, computation), and applications of structural science.

Confirmed sessions are:

- ***Non-ambient Diffraction***
- ***Complementary Non-Diffraction Methods***
- ***Dynamic Processes and Reactions***
- ***Neutron Diffraction in Chemical Crystallography***
- ***Magnetic Structure Determination***
- ***Crystal Engineering***
- ***XRD in the Pharmaceutical Industry***
- ***Getting a Job in Industry***
- ***Pushing the Limits: Faster***
- ***Pushing the Limits: Slower - the X-ray limits***
- ***Pushing the Limits: Larger***
- ***Pushing the Limits: Smaller***

Each session is listed with a short description and any confirmed speakers in the programme outlined below.

The Young Crystallographers Satellite meeting (April 7-8) is expected to be as vibrant as ever and this year concludes with a provocatively entitled session "Are Crystallographers Still Necessary?" Plans are in place to cancel the main meeting should the answer to this question turn out to be "No".

The meeting space at Loughborough has been improved since the last BCA visit. There is more seating available for informal discussions in a combined space, adjacent to the three lecture theatres, where the Exhibition and the poster sessions will also be held. There will be a late-night bar on campus to facilitate further informal scientific discussions.

The **Exhibition**, comprising a wide range of companies and organisations, will run throughout the meeting and will be featured along with the main **poster session** and buffet dinner on the evening of Tuesday April 8. Wednesday evening (April 9) will include the AGM of the BCA, which will follow the Bragg Lecture at 6pm. The Conference Dinner will be at 7.30pm followed by a Ceilidh, back by popular demand.

The programme committee look forward to seeing you in Loughborough in April.

Lee Brammer
(University of Sheffield)
Programme Chair

Registration and Abstract Submission

Meeting website:
http://crystallography.org.uk/spring-meeting-2014/

The registration is now open and the early bird deadline is **7 March 2014**.

The deadline for both oral and poster submission is on **17 January 2014**.

This deadline cannot be postponed due to the tight schedule surrounding printing the abstract book.

Young Crystallographers Satellite Meeting

Monday 7 April

1:00-3:00 pm YC Session 1
YC Chemical Plenary
Iain Oswald (University of Strathclyde)
Title: TBC

3:30-5:00 pm YC Session 2
YC Biological Plenary
Elspeth Garman (University of Oxford)
Triumph over Adversity: structure solution of M. tuberculosis NAT, 'difficult' throughout

5:30-7:00 pm YC Session 3
YCG AGM
Poster flash presentations

7:00-9:00 pm
Poster Session with dinner and wine

Tuesday 8 April

9:00-10:30 am YC Session 4
Parkin Lecture

Nominations should be sent to **Lauren Hatcher** (leh29@bath.ac.uk) no later than **17 January 2014**.

10:30-11:15 am YC Session 5
Are Crystallographers Still Necessary?

Simon Coles (University of Southampton): **Yes**
Graeme Winter (Diamond Light Source): **No**

Abstract deadlines for the YC Satellite
Oral presentations and Posters:
17 January 2014

Abstracts can be submitted at:
http://crystallography.org.uk/spring-meeting-2014/

Meeting Highlights

Tuesday 8 April

12.00-12.50 pm **Lonsdale Lecture**
Speaker: **Henry Chapman** (Center for Free-Electron Laser Science, DESY, Hamburg)
Title: TBC
Chair: **David Keen** (ISIS and University of Oxford)

1.30-2.20 pm **PSG Plenary**
Speaker: **Malcolm McMahon** (University of Edinburgh)
Extreme Crystallography in a Flash
Chair: TBC

6.10-7.00 pm **CCG Plenary**
Speaker: **Paul Raithby** (University of Bath)
Understanding the solid-state into the next 100 years
Chair: **Simon Coles** (University of Southampton)

Wednesday 9 April

9.00-9.50 am **IG Plenary**
Speaker: **Joel Bernstein** (NYU Abu Dhabi)
Title: TBC
Chair: TBC

10.15am-12.15 pm **Early Career Scientist Prize Lectures and Awards Ceremony**

Award of the CCDC CCG Young Scientist Prize, the PANalytical PCG Thesis Prize, the Young Crystallographers Industrial Group Prize and the BSG Prize.

5.10-6.00 pm **Bragg Lecture**
Speaker: **Judith Howard** (Durham University)
Exploring a century of reciprocal space: same old theory – endless new results'
Chair: TBC

Thursday 10 April

9.00-9.50 am **BSG Plenary**
Speaker: **Neil Isaacs** (University of Glasgow)
Title: TBC
Chair: TBC

Scientific Programme

Tuesday 8 April

2.30-4.00 pm and 4.30-6.00pm
Non-ambient Diffraction

The behaviour of many functional materials is influenced by changes in environment, and so understanding the structure-property relationships in these various conditions (e.g. temperature, magnetic or electric fields, pressure, atmosphere) is crucial. This session will cover a range of materials and illustrate the diverse environments now available for *in situ* diffraction studies.

Chairs: **Emma McCabe** (University of Kent) and **Ivana Evans** (Durham University)

Bill David (ISIS and University of Oxford)
Title: TBC

Stephen Hull (ISIS)
In situ studies of batteries and fuel cell materials

Andrzej Katrusiak (Adam Mickiewicz University, Poland)
Title: TBC

2.30-4.00 pm
Crystal Engineering

The self-assembly of building blocks into the solid-state is a powerful means of designing in function or improving the physical properties of materials. This session will demonstrate the use of crystal engineering techniques in both framework and molecular systems with a range of application areas.

Chair: **Lynne Thomas** (University of Bath)

Neil Champness (University of Nottingham)
Crystal Engineering Strategies for Functional Materials

Colin Pulham (University of Edinburgh)
Crystal engineering of energetic materials – a step change in the design of safer explosives and propellants?

4.30-6.00 pm
Application of neutron diffraction in chemical crystallography

In this session the complementarity of neutron and X-ray diffraction for single crystal and powder samples will be explored across a variety of materials, thus highlighting the diverse range of research within chemical crystallography that can be facilitated by neutron diffraction.

Chair: **Samantha Callear** (ISIS)

Amber Thompson (University of Oxford)
Small Molecules at Big Facilities

Dominic Fortes (University College London)
Chemical substitution yields new hydration states in $MgSO_4$ hydrates and related analogues

Wednesday 9 April

1.30-3.00pm
Magnetic Structure Determination

The emphasis of this session is on recent research, focusing on examples for which a thorough understanding of magnetic structure and symmetry has given an insight into the factors that stabilise the magnetic structure, and a deeper understanding of the behaviour of the material.

Chair: **Emma McCabe** (University of Kent)

Andrew Wills (University College London)

Paolo Radaelli (University of Oxford)
Titles: TBC

1.30-3.00 pm
XRD in the Pharmaceutical Industry
This session focuses on the use of x-ray diffraction and crystal structures within the pharmaceutical industry. The majority of marketed drugs are delivered in the crystalline state and so the use of XRD to determine crystal structures is extremely important. XRD can of course also provide information on other aspects of condensed matter that are relevant to pharmaceuticals such as bulk properties, disorder and amorphous forms. Topics that may be covered include: advances in technology, new experimental and computational methodologies, how crystal structures are used within the industry as well as an outlook on how XRD and crystal structures may be used in the future.

Chairs: **Cheryl Doherty** (Pfizer) and **Peter Wood** (CCDC)

Andrew Dobson (Astra-Zeneca)
Title: TBC

1.30-3.00 pm
Pushing the limits: Faster
Free-electron lasers and single-shot synchrotron

Chairs: **Henry Chapman** (Center for Free-Electron Laser Science, DESY, Hamburg) and **Peter Moody** (University of Leicester)

Speakers and titles: TBC

3.30-5.00 pm
Dynamic Processes and Reactions
In this session developments in time resolved techniques that can be applied to crystallography and related diffraction and spectroscopic methods will be discussed. By combining the techniques it will be possible to study the dynamics of chemical processes right across the time range from nanoseconds to milliseconds and to make molecular movies of these processes!

Chair: **Paul Raithby**

Mark Warren (Diamond Light Source)
Collecting time-resolved data on I19

John Evans (University of Southampton)
Time resolved XAFS and X-ray Studies on Catalysts

3.30-5.00 pm
Pushing the limits: Smaller
Micro/nano-focus beams

Chair: **Gwyndaf Evans** (Diamond Light Source)

Colin Nave (Diamond Light Source)
Title: TBC

Robin Owen (Diamond Light Source)
Title: TBC

3.30-5.00 pm
Getting a job
This session is aimed at younger career researchers who will be interested to hear about the job opportunities that are open to them. There will be three short presentations from speakers representing academia, a small company and a larger multinational company, followed by a panel discussion with these speakers.

Chairs: **Elizabeth Shotton** (Diamond Light Source) and **Anna Warren** (Diamond Light Source)

Andy Doré (Heptares Therapeutics)
Title: TBC

Thursday 10 April

10.15-11.45 am and 12.00-13.30 pm
Complementary Non-Diffraction Methods
This session will illustrate the use of experimental and computational methods complementary to diffraction, which provide unique insight into the structural properties of functional materials studied.

Chairs: **Ivana Evans** (Durham University) and **Graeme Day** (University of Southampton)

Yaroslav Khimyak (University of East Anglia)
Probing intermolecular interactions and dynamics in porous host-guest systems using solid-state NMR

Joke Hadermann (EMAT, University of Antwerp, Belgium)
Mapping of chemical order in inorganic compounds

Martin Dove (Queen Mary, London)
Reverse Monte Carlo method: coupling scattering data with computer simulation

Lyndon Emsley (Ecole Normale Supérieure, Lyon, France)
Title: TBC

10.15-11.45 am
Pushing the limits: Larger
Viruses, complexes.

Chair: **John Schwabe** (University of Leicester)

Speakers and titles: TBC

12.00-13.30
Pushing the limits: Slower – the X-ray limits
The paradigm of "structure is needed to define function in biology" leads to a thirst via appropriate techniques to achieve this, irrespective of sample state. Thus crystal structure analysis by X-rays works well in furthering this paradigm but hits limits. It is not effective in many cases, becoming slow or obviously impossible to give the desired structural details. Neutrons are exquisite probes of proton ionisation states of amino acids. Cryo EM and single particle imaging can free up the need for crystals. Atom and molecular dynamics also can underpin function. Solid-state NMR finds application in defining ligand dynamics in membrane targets. This session brings together experts spanning these techniques and their applications.

Chair: **John Helliwell** (University of Manchester)

Matthew Blakeley (Institut Laue Langevin, Grenoble)
Neutron macromolecular crystallography: current developments and highlight applications

Alan Roseman (University of Manchester)
What to do with non-homogeneous molecular populations: complementing crystallography with EM

Anthony Watts (University of Oxford and Rutherford Appleton Laboratory)
Functionally relevant dynamics of bound ligands at their target sites in membrane proteins

Young Crystallographers Satellite Meeting

THE next Young Crystallographers Satellite Meeting (YC2014) will take place prior to the main BCA Spring Meeting from 1 pm on Monday 7 April until 11.15 am on Tuesday 8 April at the University of Loughborough.

Following the established format there will be three sessions of oral presentations – a superb opportunity for Young Crystallographers to present and discuss their work in a friendly and relaxed environment. More senior crystallographers are of course welcome to attend, but we respectfully request that difficult questions are kept to a minimum. The poster session will commence on Monday evening together with the buffet dinner and drinks.

This year there will be two plenary lectures, with a chemical and biological theme looking at difficult data. There will also be a debate session entitled 'Are crystallographers still necessary?' This will be a light-hearted look at the ways in which automation has affected the way we collect and process data, and conversely at the traps that await those who believe too literally what their computers tell them. And of course we confidently expect the answer to be a resounding "yes"! The third Parkin lecture will also be awarded to a Young Crystallographer who will then present their work at this satellite.

The Parkin Lecture, the prize lecture of the YCG, was established in recognition of the outstanding contributions of the late Dr **Andrew Parkin** to the YCG of the BCA. The candidate should be a Young Crystallographer (undergraduate or graduate student or a crystallographer within five years of graduation), who has been recognised for outstanding contributions to any of the following:

- **Promoting science**
- **Raising public awareness of science**
- **Teaching crystallography/science**
- **Originality in outreach and teaching activities.**

If you think you know of a Young Crystallographer who has excelled in any of these areas then why not nominate him or her for the Parkin Lecture!

The rules for the Parkin Lecture, details regarding the nomination process and nomination form can be found under the prizes section on the YCG website (**http://ycg.crystallography.org.uk/prizes/**). The nomination form should be sent to the YCG Secretary **Lauren Hatcher** (leh29@bath.ac.uk) no later than **17 January 2014**.

At the main meeting there will also be a joint session with the IG entitled "Getting a Job." This is aimed at younger career researchers who may be interested in staying in science but are unsure of the different routes that may be open to them. This will be held on **Wednesday 9 April at 3.30-5:00 pm**.

Dinner and registration for the YC2014 will be free for those attending the whole Spring Meeting. There is the option to only attend the YC2014 and not the main meeting, but a fee will be charged. There are a limited number of bursaries available and applications should be made online via the BCA webpage.

The deadline for abstracts to be considered for oral presentations and posters is **17 January 2014**. Submissions should be made via the main meeting abstract submission webpage using the template available there. The AGM will again include elections to fill the YCG Committee vacancies, which will be advertised nearer the time. For more information about the YCG have a look at the YCG website (**http://ycg.crystallography.org.uk/**).

YCG Committee

BCA Bursaries

BCA Bursaries: How to apply

VARIOUS bursaries are open to members of the BCA. They are summarized here, together with eligibility criteria and application deadlines:

Arnold Beevers Bursary Fund (ABBF):

Bursaries sponsored by the ABBF are available for BCA members to attend BCA Spring meetings and other crystallographic meetings. The ABBF was set up in 2001 by the BCA council in honour of Dr **Arnold Beevers**. Arnold was a firm believer in the free and open exchange of scientific ideas and information. He was also a founder member of the BCA and thrived on getting together with people of all ages at BCA, IUCr and ECM meetings. For more info see the June 2001 issue of *Crystallography News*: http://crystallography.org.uk/wp-content/uploads/77JUN.PDF

The ABBF is supported by proceeds from the BCA and several generous donations, which it gratefully acknowledges. Further contributions to this worthwhile cause are always welcome.

ABBF – BCA Spring Meeting Bursaries

Up to six bursaries are available for those attending the BCA Spring Meeting, each up to the value of £200. The deadline for applications coincides with the abstract deadline for the next meeting; **17 January in 2014**.

ABBF – General Bursaries

Bursaries to attend other crystallographic related meetings are also available. In 2014 the deadlines for applying are **17 January**, **2 May** and **30 September**. Applications will only be considered for meetings/conferences, which begin at least six weeks after these deadlines.

Eligibility and Conditions for ABBF sponsorship

1. The bursaries are primarily intended to support bona fide research students and postdoctoral workers who are BCA members. Applications from those with more senior non-tenured positions, and from those in junior permanent positions where university or industrial funds are unavailable, may be supported at the discretion of the BCA Bursary Committee if BCA funds are available.
2. Applicants must normally have been a member of the BCA for 3 months before applying.
3. Applicants will not normally be considered if they have been awarded a general bursary in the previous two years.
4. Preference will be given to applicants who have attended a BCA meeting and also if they are contributing with a talk or poster.
5. Applications must be received at least 6 weeks before the date of the meeting/visit. No retrospective applications are possible.
6. The recipient must contribute an article about the meeting to Crystallography News. Photographs are welcome in addition to the article.

Other Bursaries – External Sponsor Bursaries

The ABBF is limited, and often the BCA find that they cannot support all applicants attending the BCA Spring Meeting. We are fortunate that external sponsors have been willing to sponsor those not receiving ABBF assistance. Applications for these should be made in the same way as for ABBF with the deadline being the **17th January in 2014**.

Application form for all Bursaries:
http://crystallography.org.uk/about/bursaries/

Microsymposia at ECM28

ECM28 – Thank you

WE would like to thank everyone, particularly BCA Members, for all their help in making ECM28 a success. Many of those who contributed to the organisation of the Meeting are listed on the committee pages at http://ecm28.ecanews.org/organisers. The very positive feedback we have received suggests that delegates very much enjoyed the ECM, including the scientific programme, the informal meetings and the social events.

ECM28 attracted 850 delegates from over 50 countries, making it one of the largest ECMs to date. It featured several unique events, including the inaugural meeting of the European Young Crystallographers Group, a special Bragg Symposium, the Two Braggs Exhibition and a Nobel Lecture by **Dan Shechtman**.

We would like to thank Northern Networking Events for all their contributions as our professional conference organiser, and Warwick Conferences for providing the excellent conference venue and facilities. Finally, we are extremely grateful to the Trustees of the ECM28 Company.

We wish the organisers of ECM29 in Rovinj, Croatia, all our best wishes for 2015!

Sandy Blake and **Elspeth Garman**
Chair and co-Chair of ECM28

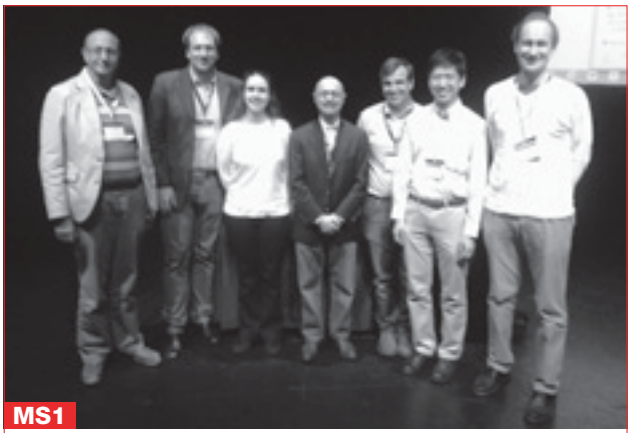
Microsymposia at ECM28

THE chairpersons of the relevant microsymposia are to be thanked for compiling the following reports. The layout and text have been lightly edited by Sandy Blake and Carl Schwalbe.

MS1 "XFEL and time-resolved crystallographic methods"

Co-chairs: **John R. Helliwell** and **Victor Lamzin**

The selected speakers came from Europe, the USA and Japan. The first, opening, talk was given by **Lars Redecke** (Hamburg and Lubeck Universities) and entitled "Free Electron Laser radiation and *in vivo* grown nano-crystals open new routes in structural biology and options for time-resolved experiments". Lars described the use of very tiny, in vivo grown crystals, with a typical volume of just ~4 μm^3, of *Trypanosoma brucei* cathepsin B (TbCatB), a protein that is important in structure-based drug discovery aimed at eradicating sleeping sickness. This was one of *Science* magazine's 'top 10 discoveries of 2012'. As well as its technical cutting edge nature the electron density map contained new extended features readily interpretable and thereby not showing any serious disruption of these atoms' X-ray scattering factors; this had been a serious anxiety in the whole field of applications of X-ray lasers in structural biology. Obviously a distinctive feature of this successful study was the use of femtosecond X-ray pulses. To date, studies of time-resolved evolution of small changes in a protein crystal structure extend into the sub-nanoseconds regime (typically 100 picoseconds) using synchrotron X-ray radiation. The use of X-ray lasers should now allow such studies to be expanded into the femtosecond regime. The second talk was delivered by **Abbas Ourmazd** from the University of Wisconsin, USA entitled "Single-particle structure and dynamics". Using mathematical techniques



L-R: *John Helliwell, Lars Redecke, Catherine Dejoie, Abbas Ourmazd, Jose Trincao, Atsushi Nakagawa, Victor Lamzin.*

Abbas cogently and imaginatively argued that sparsely photon-populated diffraction patterns should be amenable to structure analysis. He advanced the view based on manifold techniques that the X-ray photons per pulse of 10^{12} would be adequate for structure analysis of most, perhaps all, envisaged samples in protein and virus structure studies with XFELs. This produced a vigorous discussion on the pulse fluxes required for biological FEL-based imaging.

The third talk was given by **Catherine Dejoie** (ETH Zurich and Paul Scherrer Institute, Switzerland) and entitled "Using a non-monochromatic microbeam for serial snapshot crystallography". By using such a pink Laue method more reflections from a given nanocrystal could be obtained and a more efficient diffraction data acquisition would be possible, allowing for a lower X-ray flux per pulse whilst preserving an equally strong diffraction pattern. The fourth presentation was made by **Jose Trincao** (Research Complex at Harwell and University of Bath, UK) and entitled "Dynamic Structural Sciences Consortium – diffraction methods". Jose described the strengths of the co-location of the Central Laser Facility, with its wide range of lasers, and the Diamond Light Source as well as the plans to join a consortium to help build and then access a nanocrystal beamline at European XFEL in Hamburg for structural biology. In the final talk by **Atsushi Nakagawa** (Osaka University, Japan) entitled "Coherent diffraction imaging for spherical biological particles" some of the first experiments from the Japanese SACLA X-ray free-electron laser were described looking at very large spherically shaped virus single particles. All speakers were addressed with a wide range of questions from the audience including molecular biology, structural biology, mathematics and X-ray scattering physics. The lecture hall was completely full during the whole session.

MS3 "Hybrid approaches"

Co-chairs: **Bruno Klaholz** and **Guillermo Montoya**

The micro-symposium session comprised oral presentations with some typical examples of data integration such as combined usage of crystallography and cryo electron microscopy, or of novel approaches in SAXS or for *in situ* diffraction tests.

1) **Dale Wigley** (ICR London) presented a multidisciplinary study deciphering the interactions between the nucleosome histone core and Arp8 in the INO80 chromatin remodelling complex. The work combined crystal structures and electron microscopy with biophysical techniques. Taken together, these data provide a novel insight into the stoichiometry, architecture, and molecular interactions between components of the INO80 remodelling complex and nucleosomes, providing a first step toward building up the structure of the complex.

2) **Paula da Fonseca** (Institute of Cancer Research and now Laboratory of Molecular Biology, MRC, Cambridge, UK) presented the structural analysis of the human proteasome. This 2.6 MDa complex recognizes ubiquitinated peptide substrates, within which the 19S cap promotes substrate unfolding and translocation into the 20S core. The sub-nanometric cryo-EM map of the complex was analysed in detail by fitting known and newly determined crystal structures, providing notably a full backbone model of the 19S caps (*Mol. Cell* 2012). Future work points in the direction of substrate complexes.

L-R: *B. Klaholz, D. Wigley, G. Montoya, P. da Fonseca, P. Aller and J. Beale. (Missing: N. Galatanu).*

3) **Nicoleta Galatanu** (Xenocs, Grenoble, France) presented a small-angle X-ray diffraction (SAXS) setup comprising a low-background camera and a micro-source coupled with multi-layer optics providing scatterless collimation. Experimental data using this setup were obtained for a V(1)V(0)ATPase sample at a concentration of 5 mg / ml, after concentration optimization with respect to aggregation (high conc.) or sufficient signal intensity (low conc. limit).

4) **John Beale** (University of Oxford) communicated the structure of the extracellular domain of peptide transporters PepT1 and PepT2. Both are of significant pharmaceutical interest due to their ability to actively uptake a number of clinically important drugs. A combination of SAXS and crystal structures including ab initio modelling and ensemble organisation provide additional insight in the working mechanism of these membrane proteins.

5) **Pierre Aller** (Diamond synchrotron, UK) presented the *in situ* plate screening and data collection when dehydration of crystals is performed through replacement of the reservoir solution by a NaCl solution (0.5-1.5M) and overnight equilibration (*Acta Cryst. D* 2013). Examples were shown where the diffraction, as tested on the I24, I03 of I04-1 beamlines, improved from the range of 2.9-2.6 Å under cryo conditions to 2.8-2.3 Å when freezing after dehydration without additional cryo-protectant, or improvement from 24 Å to 11 Å resolution for a membrane protein.

MS8 "Cell-signalling – Interactions and allostery"

Co-chairs: **Jacqueline Cherfils** and **Remy Loris**

In cells, signals propagate between different biologically active sites of a protein, and from protein to protein within cellular pathways. Allostery, a concept first devised 50 years ago by Monod, Wyman and Changeux in a series of articles whose celebration started in 2013, applies to many regulated signalling networks. Speakers in this session

MS8

L-R: *Jacqueline Cherfils, Marc Delarue, Aude Echalier-Glazer, Karin Kühnel, Valérie Campanacci, Saccas Savvides, Remy Loris.*

presented a variety of studies that illustrate signalling and allostery in their broadest sense.
Marc Delarue (Institut Pasteur, Paris, France) presented an impressive series of crystal structures of pentameric ligand-gated ion channels, which are prototypical allosteric membrane receptors. Notably, he used an engineered bacterial homologue to show that ethanol stabilizes an open form of the receptor, suggesting a structural basis for neurological actions of ethanol in related human receptors.

Savvas Savvides (University of Ghent, Belgium) discussed how cytokines (a diverse group of extracellular signalling molecules) signal to oncogenic class III receptor tyrosine kinases, which he studies by using a combination of biophysical, structural and computational approaches. Notably, he showed that the Epstein-Barr virus intercepts a human cytokine (CSF-1) by allosteric competitive inactivation, rendering it unable to signal to its cognate receptor.

Valérie Campanacci (CNRS, Gif-sur-Yvette, France) presented a structural and biochemical study of AnkX, a *Legionella* effector with a catalytic FIC domain that attaches a phosphocholine moiety to the small GTPase Rab1, thus rewiring membrane trafficking pathways in the infected host cell. This uncovered a conserved enzymatic mechanism common to all FIC domain-containing toxins, which allows them to process diverse diphosphate-containing substrates.

Karin Kühnel (MPI for Biophysical Chemistry, Göttingen, Germany) described structural and biochemical studies of PROPPINS, a family of proteins that are crucial in autophagy, an evolutionary conserved degradative pathway. She showed that PROPPINS have two phospholipid binding sites on its 7-bladed beta-propeller structure that are adjacent but non-overlapping, suggesting how these proteins bind to autophagosome membranes.

Aude Echalier-Glazer (CNRS/University of Montpellier, France) used crystallographic and *in silico* approaches to analyze the regulation of the Cop9 signalosome, a large multiprotein complex implicated in various cellular functions through its role in the ubiquitin-proteasome pathway. Notably, she described the mechanism that triggers the deneddylation activity of the CSN5, a subunit of this complex with isopeptidase activity.

MS11 "Twinning problems and advantages"

Co-chairs: **Pietro Roversi** and **Loes Kroon-Batenburg**

The session saw a lively mix of theory and applications, both from the small molecule and the macromolecular crystallography worlds: it was good to hear about aspects of twinning detection and modelling (**Berthold Stoeger**, **A. David Rae** and **Areej Abuhammad**), and software development to aid twinned data processing (**Harry Powell** and **Martin Lutz**) and realise once more that (perhaps unsurprisingly) the two crystallographic (sub)communities are facing very similar problems and have questions in common.

Moreover, after this session, and when dealing with twinned crystals, the question from Harry Powell's talk will always come to mind: are the Thompson Twins in the Tintin stories really twins, or are they just very much alike and always found together? We shall never think of twinned crystals the same way ever again!

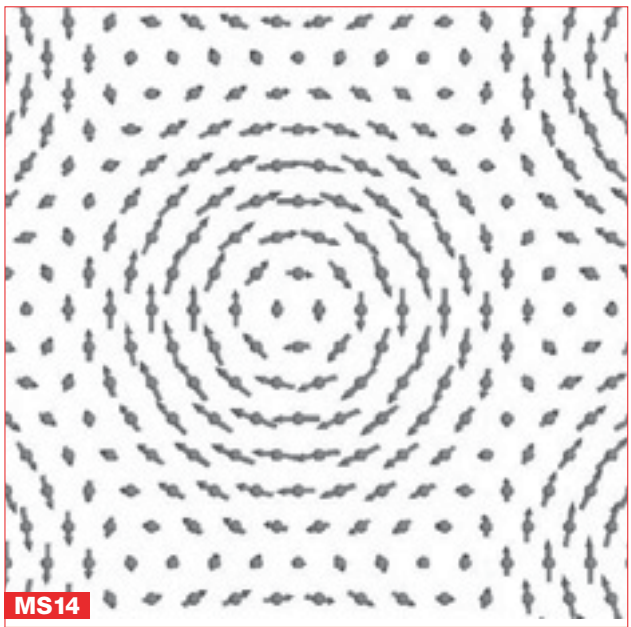
MS11

L-R: *A. David Rae, Areej Abuhammad, Martin Lutz, Berthold Stoeger, Harry Powell*
Chairs (in front): *Pietro Roversi and Loes Kroon-Batenburg.*

MS14 "Aperiodic crystals: structure, dynamics and magnetism"

Co-chairs: **J. Manuel Perez-Mato** and **Marc de Boissieu**

This session, although including in principle all types of structural research on aperiodic crystals, put the focus on research areas that represent at the moment new avenues in the research of quasiperiodic systems, such as epitaxial order on quasicrystals, and incommensurate magnetic structures. The first invited speaker, **Vaclav Petricek** (Institute of Physics ASCR, Praha, Czech Republic), presented the new option developed in JANA2006 for the determination of magnetic structures, both commensurate and incommensurate. The program applies both representational analysis and magnetic symmetry in a combined way. It is the first program that for the determination of incommensurate magnetic structures makes a consistent use of the symmetry associated with such quasiperiodic systems (i.e. magnetic superspace groups). In a second invited talk, **H. Sharma** presented results on the structure of add-atoms on a 5-fold surface of a quasicrystal: a quasiperiodic arrangement of Pb atoms is observed, in good agreement with preferential sites observed on the bare



MS14

Example of skyrmion-type spin ordering shown by H. Stokes.

surface. Subsequently, **Harold Stokes** (Brigham Young University, Provo, Utah, USA) presented new features of the program ISODISTORT, and could show that skyrmion-type spin configurations are simply obtained as incommensurate arrangements caused by the action of a single multi-k irreducible representation (see Figure). **Kirsten Christensen** (University of Oxford, UK) discussed afterwards the regular encounter in a general service diffraction laboratory with modulated molecular structures, and the way they are being investigated. Finally, **Renald David** (Université Lille, France) presented a study on a series of iron compounds that exhibit a complex interplay of structural and magnetic ordering, both commensurate and incommensurate.

MS16 "X-rays and electrons: joining forces"

Co-chairs: **Gopinithan Sankar** and **Xiaodong Zou**

Nine abstracts were received. Two invited speakers and three further oral presentations were selected to cover different approaches of combining X-rays and electrons and applications on various materials covering three-dimensional, layered and disordered materials. Several new electron diffraction techniques including precession electron diffraction (PED), automated electron diffraction tomography (ADT) and rotation electron diffraction (RED) were presented and combined with X-ray diffraction for structure analysis. About 60-80 people attended the microsymposium and showed great interest in the topics. Discussion continued even after the symposium.

The speakers in MS16 were **Ute Kolb** (Johannes Gutenberg University Mainz & Technical University Darmstadt, Germany) who spoke on "Automated Electron Diffraction Tomography (ADT) and X-ray powder diffraction for structure characterization of layered materials"; **Mervyn Shannon** (EPSRC National Facility for Aberration-Corrected Scanning Transmission Electron Microscopy (SuperSTEM) Daresbury, and University of Liverpool, UK) on "Combining X-rays and electrons to characterise disordered inorganic materials; **Oliver Oeckler** (Leipzig University, Germany) whose title was "Combining TEM and synchrotron microdiffraction – a novel lead antimony sulfide telluride, and more examples"; **Holger Klein** (Institut Néel, Grenoble, France) on "Complex Sr64.1Bi27.7Ni8.2Ox revisited and refined" and **Jie Su** (Stockholm University, Sweden) who described "PKU-14: combining X-ray powder diffraction, rotation electron diffraction, NMR and IR spectroscopy".

MS16

L-R: *Xiaodong Zou, Holger Klein, Oliver Oeckler, Gopinithan Sankar, Jie Su, Ute Kolb, Mervyn Shannon.*

MS17 "Combined methods for soft matter and other crystallography"

Co-chairs: **Stavros Nicolopoulos** and **Marco Milanesio**

This session was well attended with more than 50 participants present. The Chairs felt it was a very successful and well-attended microsymposium.

The invited speakers were **Sven Hovmoller** (Stockholm University, Sweden) and **Tatiana Gorelik** (Johannes Gutenberg University Mainz, Germany). In a talk entitled "Single crystal diffraction from powders", Professor Hovmoller presented research results from RED (Rotation Electron Diffraction) tomography techniques in Transmission Electron Microscopy (TEM), for structure determination of various complex materials including zeolites and oxides. Dr Gorelik's presentation "Electron crystallography of molecular crystals" showed research results with ADT 3D (automatic 3D

MS17

L-R: *Marco Milanesio, Richard Beanland, Tatiana E. Gorelik, Stavros Nikolopoulos, Sven Hovmöller, Stef Smeets, Louisa Meshi.*

diffraction tomography technique on TEM) for structure determination of various beam-sensitive organics and various pharmaceutical samples.

In the remaining talks, **Louisa Mesh** (Ben-Gurion University of the Negev, Israel) spoke on "Identification and structure solution of ordered $U(Al_x,Si_{(1-x)})_3$ phase", **Richard Beanland** (University of Warwick, UK) explained "Determining symmetry of ferroelectric oxides at the nanometre scale using 'digital' electron diffraction" and **Stef Smeets** (ETH Zurich, Switzerland) described "Using FOCUS and Superflip to solve structures from 3D electron and powder diffraction data".

MS18 "From nature to laboratory: crystallography of minerals and mineral related materials"

Co-chairs: **Oleg Siidra** and **Biljana Lazic**

The talks and posters in this session covered a wide range of subjects, from mineral classification and structural prediction, over modification of materials to the new techniques for structural solution.

Fernando Camara presented the classification of Ti-silicate minerals into groups with different Ti-Si building blocks. This classification allows establishing relations between structural topology and chemical composition and also prediction of new minerals and crystal structures. **Frederic Hatert** showed how a cation substitution mechanism occurring by an oxidation process in olivine-type phosphates can become the inspiration for development of new cathode materials. **Andrew Goodwin** reported on the recent discovery of extreme negative linear compressibility (NLC) behaviour in a variety of framework materials and general approaches for design to maximize NLC response of metal–organic frameworks. **Olga Yakubovich** presented polysomatic series of layered vanadates, arsenates and phosphates using the modular concept. **Xiaodong Zou** presented some new TEM techniques for solving 3D structures of nanosized and/or intergrown zeolites and minerals.

MS18

L-R: *Oleg Siidra, Biljana Lazic, Andrew Goodwin, Fernando Camara, Olga Yakubovich, Frederic Hatert and Xiaodong Zou.*

MS19 "Heavy crystals: structural crystallography of heavy-element compounds"

Co-chairs: **Olga Yakubovich** and **Marie Colmont**

The session started with two invited lectures given respectively by **Etienne Gaudin** (CNRS, Université Bordeaux, France) and **Oleg Siidra** (St. Petersburg State University, Russia). The first lecture was dedicated to the crystal chemistry of intermetallic compounds assorted to their physical properties whereas the second one gave a general overview of the influence of 'lone-pair' cation (Pb^{2+}, Tl^{+}) on geometry and dimensionality of oxosalt inorganic compounds.

The three selected speakers gave examples of the crystal chemistry of heavy elements in various environments and studies: **Andrzej Grzechnik** (Aachen University, Germany) spoke on the crystal structures and stabilities of $LiCeF_5$ and $LiThF_5$ at high pressures, **Maria Wierzbicka-Wieczorek** (Friedrich-Schiller University Jena, Germany) described novel silicates with the apatite crystal structure, and **Vadim Kovrugin** (Université Lille, France and St. Petersburg State University, Russia) outlined the structural variety of novel Pb and Bi selenites.

MS19

L-R: *Marie Colmont, Olga Yakubovich, Etienne Gaudin, Oleg Siidra, Vadim Kovrugin, Andrzej Grzechnik, Maria Wierzbicka-Wieczorek.*

Through the broad variety of these talks, a general overview of the crystal chemistry of heavy-elements was given, in situation of oxides and non-oxide compounds, with examples of Tl^{+}, Pb^{2+}, Bi^{3+}, lanthanides and actinides. In some cases crystal structures were analyzed under high pressure.

Nevertheless, two small points were very unfortunate: (1) due to the late position of the session in the schedule, the size of the audience was not as big as we could expect with such a broad scientific subject, because a lot of scientists left the conference ending the same evening; (2) the absence of researchers working on uranium element (despite our requests) because of two important conferences taking place in July (Actinides 2013) and in September in Europe.

MS20 "Crystal physics of minerals and materials at variable pressures and temperatures"

Co-chairs: **Anna Gągor** and **Vitali Prakapenka**

This microsymposium was organized by the ECA special interest groups for Mineral and Inorganic Crystallography (SIG5), Crystallography under Extreme Conditions (SIG11) and Crystallography of Functional Materials (SIG12). The first invited speaker, **Gregory Rozenberg** (Israel), reviewed his work on the structural consequences of magnetic/electronic transformations in Fe-based Mott insulators at very high quasi-hydrostatic pressure. He showed main scenarios which strongly correlated systems may undergo on the way to a correlation breakdown. This talk was followed by the second invited speaker, **Ilya Sergeev** (Germany), who presented high pressure studies of magnetism and lattice dynamics in the iron-based superconductors with nuclear resonance scattering – an extremely powerful in-situ synchrotron technique for high pressure applications. **Leonid Dubrovinsky** (Germany) demonstrated that solution of crystal structures, their refinement, and accurate measurements of the thermal equation of state of metals, oxides, and silicates from single crystal diffraction data are possible in a megabar pressure range at temperatures of thousands of degrees with current advances in diamond anvil cell techniques combined with on-line laser heating and synchrotron X-ray probes. By tracking the changes of crystallographic parameters at pressures above 150 GPa and temperatures up to 2200 K, he explored spin transitions in (Mg,Fe)(Si,Al)O3 perovskite – one of the main component of the Earth's interior. **Dean S. Keeble** (Warwick, UK) presented the ergodic to non ergodic transitions in sodium bismuth titanate – which is a relaxor ferroelectric material, studied with powder neutron diffraction. **Valentina Dagtyareva** (Russia) discussed the incommensurate host – guest structures in compressed elements that are stabilized by the Fermi sphere – Brillouin zone (BZ) interactions. Using the BZ concept she showed that in alkali metals the valence electron count increases from monovalent at ambient pressure to divalent or even higher values under pressure.

L-R: *Vitali Prakapenka, Ilya Sergeev, Gregory Rozenberg, Leonid Dubrovinsky, Valentina Dagtyareva, Anna Gągor, Dean S. Keeble.*

MS24 "Organic and inorganic multi-component crystals: structure and properties"

Co-chairs: **Nikoletta Bathori** and **Andrew Bond**

MS24 was opened by **Lee Brammer** (University of Sheffield, UK). The talk focussed on flexibility and chemical transformations in coordination polymers and frameworks, including gas and solvent sorption/desorption processes. The importance of a wide variety of characterization techniques was stressed, including single-crystal and powder diffraction, energy calculations and simulation of spectra. **Chick Wilson** (University of Bath, UK) talked about controlling molecular assembly in the organic solid state, highlighting polymorph control and discovery from multi-component crystallisation environments. The talk also considered the challenges involved with transferring crystal engineering approaches to continuous manufacturing environments. The third talk of the session was given by **Simona Galli** (University of Insubria, Italy) and concerned the use of bipyrazolato ligands for construction of porous coordination polymers. Azole-based frameworks are chemically more stable than low-density MOFs, but can offer potentially comparable gas sorption properties. The use of variable-temperature PXRD was highlighted in particular for measurement of anisotropic thermal expansion properties. **Colin Seaton** (University of Limerick, Ireland) discussed proton transfer in multi-component molecular solids, focussing on the influence of the crystallographic environment on the degree of intermolecular proton transfer. Calculations on isolated molecules and clusters extracted from the crystal structures helped to highlight the influence of intermolecular interactions on the nature of the energy profile for proton transfer in the solid state. The session ended with a talk from **Pete Wood** (CCDC, UK) on the challenges involved with design and prediction of organic salts. The talk covered difficulties associated with crystal structure prediction for salts, and highlighted ways in which the Cambridge Structural Database might be used to approach some of these problems. Overall, the session presented an overview of a broad range of chemistry and analytical techniques, united by the concepts of design and control of multi-component crystalline materials.

L-R: *Chick Wilson, Andrew Bond, Lee Brammer, Simona Galli, Colin Seaton, Pete Wood, Nikoletta Bathori.*

MS27 "Total Scattering"

Chair: **Michela Brunelli**

The Total Scattering microsymposium opened with presentations from two young invited speakers, **Kirsten M. Ø. Jensen** (Aarhus University, Denmark) and **Phoebe K. Allan** (University of Cambridge, UK). Their talks presented achievements of the total scattering approach for challenging crystallographic studies applied to the synthesis of nanoparticles and to the adsorption processes in functional porous materials for medical gas delivery, respectively, both studies followed by *in-situ* diffraction. Kirsten M. Ø. Jensen was also winner of one of the poster prizes awarded during the Closing Ceremony. She will start a post-doc position at Columbia University (NY, USA) in Simon Billinge's group, while Phoebe K. Allan will soon take up a position as an Oppenheimer Research Fellow and Junior Research Fellow at Gonville and Caius College at the University of Cambridge (UK) where she is currently a postdoctoral fellow working with Professor Clare Grey FRS.

Total scattering measurements now span X-ray, neutron, and electron studies of powdered (*i.e.*, Pair Distribution Function, PDF, analysis) or single crystal samples, and a growing range of tools are available to analyse these data including "real space Rietveld", reverse Monte Carlo (RMC), and whole particle modelling and model-independent analysis of real-space features in the data. The three oral contributions represented much variety of research and methodology in this field, with presentations by **Antonio Cervellino** (SLS, Paul Scherrer Institut, Switzerland) on a 3D pair distribution function modelling framework for comparing different local ordering models in single crystals; by **Arkadiy Simonov** (ETH Zurich, Switzerland) on a revised description of the Jahn-Teller symmetry switching in $LaMnO_3$, and finally by **Callum Young** (University of Oxford, UK) on the total scattering structure-microstructure study of Fe_3O_4/gamma-Fe_2O_3 nanoparticles.

With 75 people in the audience, the microsymposium was well attended and the discussion lively.

L-R: *Kirsten M. Ø. Jensen, Phoebe K. Allan, Antonio Cervellino, Arkadiy Simonov, Callum Young, Michela Brunelli. (Not present: Karena Chapman).*

MS29 "Getting more from your electron density"

Co-chairs: **Annamaria Mazzone** and **Claude Lecomte**

Phasing algorithms and charge density studies were the main topic of this symposium. It generated great interest in the subject, and the number of attendees was about 100. The session included two contributions on the application of methods using electron density modification approaches to improve phase estimates from a given structure model, two talks about accurate electron density modelling and one talk on the importance of not restraining a protein model too much.

L-R: *C. Lecomte, A. Mazzone, D. Sisak, O. Sobolev, M. Burla, M. Fronc. (Not shown: M. Kubicki).*

M. Burla (University of Perugia) spoke about the VLD phasing algorithm, which is based on the properties of the difference Fourier synthesis and the joint probability distribution function. The efficiency of the algorithm was improved by introducing the RELAX procedure, and the new procedure has been implemented in SIR2011. Some of the possible applications were exploited as the combination of the VLD algorithm with the hybrid Fourier synthesis for *ab initio* phasing and its integration in a Molecular Replacement pipeline for automatic protein crystal structure solution. VLD was never used for non *ab initio* phasing, where some phase information is available but data resolution is usually very far from 1Å.

D. Sisak (Dectris Ltd) described a new approach for solving polycrystalline materials using charge flipping algorithm. After an introduction on the standard procedure for treating X-ray powder diffraction data (XPD), Sisak presented an approach modification based on using as starting phase sets for charge flipping, approximate structure obtained from direct-space optimization followed by a flowchart that indicates which approach is most suitable for a specific problem, depending upon the structural motif, the types of atoms, the symmetry and the number of atoms.

O. Sobolev (Russian Academy of Science) showed that large distortion of a residue in unrestrained refinement may hint at the presence of alternative conformations (ACs) for this residue. The presented study showed that analysis of atomic shifts in unrestrained refinement may reveal poorly ordered residues that should be checked first with electron density maps for modeling in ACs. This analysis is also sensitive to disordered residues which may be modeled in ACs when better ordered crystals become available.

M. Kubicki (Poznan University) described accurate electron density modeling for crystals of 4-nitroimidazoles; not only important results on the intermolecular interactions like dipole-dipole,weak H bonds and H ..H attractive contacts, but he also showed that these studies led to important methodology problems like anharmonicity and estimation of dipole moment from electron density models. Another important point was that these ultra high resolution measurements up to 1.2 A^{-1} allow the discovery and modelling of organic solid solutions $A_{(1-x)}B_x$ with x smaller than 4%.

M. Fronc (Bratislava University) described his very first results on the electron density modeling of $[Cu_2(\mu_2\text{-}I)_2(2,6\text{-dimethylpyridine})_2]$. This is a very ambitious project due to the presence of the very heavy atom iodine which μ links two copper atoms. The first results on electron density are encouraging.

MS30 "Anharmonic Thermal Motion"

Co-chairs: **Simon Grabowsky** and **Birger Dittrich**

Microsymposium MS30, organized by Simon Grabowsky (Perth, Australia) and Birger Dittrich (Göttingen and Hamburg, Germany), was scheduled for the last day of the conference and attracted a surprisingly large audience. It took place in one of the smaller rooms, providing approximately 60 seats. This room remained full for the whole session, with several people standing. The high attendance came as a nice surprise to Simon and Birger, since during conference organisation and prior to the start of the session several obstacles needed to be overcome. One invited speaker quit on short notice and there was a general lack of submissions that fitted the rather specific topic. Only three of the five scheduled talks were hence on thermal motion, and to fill our slots we extended the session's scope to cover charge-density research in general. As a result an interesting set of talks was given.

The first invited talk was given by **Regine Herbst-Irmer** (Göttingen) on a multi-temperature study on an interesting structure, where two independent molecules, one affected and one unaffected by anharmonicity, provided compelling evidence of the effect and a fitting example for the introduction to the topic. The second invited talk by **Joanna Bak** from Warsaw exploited the most recent unpublished methodological developments, namely the combination of Hirshfeld-atom and X-ray wavefunction refinement. Dr Bak used the quantum crystallography program "Tonto", which can now also treat anharmonicity.

L-R: *Simon Grabowsky, Joanna Bak, Regine Herbst-Irmer, Anna Hoser, Sander van Smaalen, Jozef Kožíšek, Birger Dittrich.*

The third talk was given by **Sander van Smaalen** from Bayreuth, who showed that today's high-resolution protein data contain additional contributions to atomic displacements beyond thermal motion, thereby fundamentally affecting our ability to extract information on static and dynamic electron density distributions. The last two speakers were **Jozef Kožíšek** from Bratislava and **Anna Hoser** from Warsaw, the former focussing on data quality for faithful modelling of the charge density in a copper coordination complex and the latter on structural, energetic and charge density investigations of triptycene and selected derivatives of it.

We want to emphasize that the ratio of male and female contributors was actually in favour of the latter. The quality of talks was very high, leading to vivid discussion; and most of the audience stayed until the end of the last talk of the conference (Professor Kožíšek had to leave for the airport immediately after his talk).

MS33 "Molecular compounds under high pressure"

Co-chairs: **Yaroslav Filinchuk** and **Francesca Fabbiani**

This joint Microsymposium between SIGs 11 and 13 gave a good overview of the latest trends in high-pressure studies of molecular materials. With an average of 60 people in the audience, this Microsymposium was very well attended.

The first speaker of the session, **Elena Boldyreva** (RAS & Novosibirsk State University) gave a talk on "Two-component organic crystals at high pressure". Multicomponent crystals (including salts, hydrates and co-crystals) are attracting considerable attention from both industrial and crystal-engineering perspectives. After a thorough and instructive review of the motivation for studying these materials at high pressure, the speaker explored some case studies of amino acids and pharmaceuticals in more detail, taking examples from her own group's latest research and drawing parallels with the results of other groups. The examples focussed on a variety of pressure-induced phenomena, including mechanisms of phase transitions, proton transfer, order-disorder structural changes and tuning of hydrogen bonds, studied by a combination of single-crystal and powder X-ray diffraction and Raman spectroscopic methods.

The second talk, entitled "Bonding and phase change in ammonia borane and lithium amidoborane under high pressure" was given by **Jiuha Chen** (Florida International University). With the world's increasing fuel demands and limited fossil fuel resources, research on hydrogen storage is currently very topical. Ammonia borane is a very promising material for hydrogen storage, but industrial applications are hampered by a slow and irreversible release of the gas; reversibility of the decomposition reaction could potentially

L-R: *Yaroslav Filinchuk, Elena Boldyreva, Scott McKellar, Iain Oswald, Kamil Dziubek, Francesca Fabbiani.*

be promoted by the application of pressure. The phase diagrams of the title compounds were studied as a function of pressure and temperature: both compounds exhibit a rich phase diagram, as evidenced by a combination of powder diffraction and Raman spectroscopic measurements. Interestingly, at 3.9 GPa opaque samples of lithium amidoborane turn transparent. The lack of dihydrogen bonding in this material, which is present in the hydrogenated parent compound and facilitates hydrogen release, may prove useful for optimising the hydrogen storage properties of this compound.

Kamil Dziubek (Adam Mickiewicz University) presented a very interesting historic perspective on "Volumetric measurements in high pressure crystallography". The historic journey started from experiments on water by Sir Francis Bacon in 1620, through the first patent for a hydraulic pump by Joseph Bramah in 1795, to the wide range of volumetric experiments by one of the fathers of high-pressure research, Percy W. Bridgman, beginning at the end of the 19th century, to the introduction of the diamond-anvil cell in 1958. The speaker presented the design of the piston-cylinder press in use at his home laboratory, which is capable of compressing liquid and solid samples up to *ca.* 2 GPa. Direct compression experiments in the press provide useful and precise information on volumetric properties and phase-transition pressures complementary to diffraction experiments, as demonstrated by a range of experiments on a range of organic compounds, including chloroform and imidazole.

In his talk entitled "Pressure-induced polymorphism in small molecule acrylic acids", **Iain Oswald** (University of Strathclyde) presented the results of thorough structural high-pressure investigations on acrylic acid and methacrylic acid, which are the monomers of the two industrially-relevant polymers. Using a combination of single-crystal X-ray diffraction and neutron powder diffraction (on the ISIS PEARL instrument), the phase behaviour previously inferred by Raman spectroscopy was extended and clarified. For acrylic acid, a phase transition at 0.75 GPa was identified, which is associated with pleating of molecular layers. Further compression to 7.0 GPa results in an increase of the puckering of the layers. For methacrylic acid, two phase transitions could be identified at 0.4 GPa and 1.21 GPa, respectively. Compressing the sample further to 5.0 GPa appears to lead to polymerisation, and further studies are currently being undertaken to confirm this interesting observation.

The current research impetus on MOFs has not escaped the attention of high-pressure researchers. The Microsymposium was rounded off with a talk on these materials by **Scott McKellar** (University of Edinburgh), "The effect of solvent and pressure on the post-synthetic modification of a metal-organic framework". High-pressure single-crystal compression studies on St Andrews MOF-1 (STAM-1) revealed a rich high-pressure behaviour as a function of the pressure-transmitting medium used, including the observation of pressure-induced post-synthetic modification behaviour, in which exchange with a highly labile axial water molecule coordinated to Cu(II) is observed. When methanol or acetonitrile are used, the exchange occurs at pressures below 0.3 GPa and hydrophilic channels are converted to hydrophobic pores. The post-synthetic modification phases are stable on releasing pressure. No ligand exchange is observed in the presence of isopropyl alcohol or ethanol, whilst exchange leads to a strain-induced collapse of the structure to an amorphous phase when using ethanol.

MS37 "The role of crystallography in chemical reactivity / kinetics / catalysis"

Co-chairs: **Simone Techert** and **Marijana Đakovic**

Five speakers presented their current crystallographic activities for studying solid state reactions employing time-resolved X-ray or electron diffraction methods. The first overview was given by **Tomislav Friščić** (McGill University, Canada) who introduced overall solid state reaction methods based on mechanical forces as "green" methodologies for modern chemical synthesis. In situ monitoring of mechano-chemical milling reaction utilizing hard synchrotron X-ray radiation allowed the researchers to study the mechanism of porous (pre)metal-organic frameworks or metallodrugs for the first time. **Jacqueline Cole** (University of Cambridge, UK) presented her pioneering time-resolved investigations on solar-powered molecular motors employing time-resolved in-situ photo-crystallography at home laboratory X-ray sources. As an example for a photo-driven rotor, she introduced $[Ru(SO_2)(NH_3)_4(3\text{-Cl-pyridine})]Y_2$ single-crystal systems, in which a local photo-induced SO_2 isomerism triggers a larger mechanical change in the benzene ring of the anion during the time course of the reaction. A summary over the first time studies of correlated disorder in structured nanodomains of group 4 MOFs was given by **Matthew J. Cliffe** (Oxford University, UK). In the presented system, face-centered cubic like UiO-66 consists of twelve coordinated $Zr_6O_4(OH)_4$ clusters which are linked together by 1,4-benzenedicarboxylate (BDC). Cliffe and coworker could show that from a superstructural point of view, the system (and derivatives) exhibits broad primitive superlattice reflections, which are interpreted as diffuse scattering caused by nanodomains formed through correlated defects in the MOFs. Ultrafast chemical dynamics studies employing state of the art time-resolved electron microscopy (4D UEM) has been introduced by **Renske van der Veen** (California Institute of Technology, USA). In her work she could show that by the unique combination of the time resolution of conventional optical spectroscopy (ultrafast) with the

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L-R: *Tomislav Friščić, Marijana Đaković, Jacqueline Cole, Simone Techert, Matthew Cliffe, Renske van der Veen, Serena Tarantino.*

excellent spatial resolution of electron microscopy, the photo-switching dynamics of individual spin-crossover Fe(pyrazine)Pt(CN)$_4$ nanocrystals could be studied from the time of reaction initiation up to structural processes carrying thermal losses. In the last presentation **Serena C. Tarantino** (University of Pavia, Italy) presented her first structural mechanistic studies on the solid state reaction zinc oxide / aluminum oxide to zinc spinel – combining in-situ X-ray diffraction with atomic force microscopy and Zn-K-edge X-ray absorption spectroscopy. Depending on oxide film preparation, crystal orientation etc., distinguished features of the complex mechanism of spinel formation have been disentangled, including non-equilibrium intermediates and side reaction branches.

MS38 "Molecular recognition and complexation in small molecules"

Co-chairs: **Alessia Bacchi** and **Janusz Lipkowski**

The two invited lectures were given by **Scott Dalgarno** (Heriot-Watt University, UK) on "*p*-Carboxylatocalix[4]arenes: controlled self- and metal-directed assembly" and **Chiara Massera** (Università degli Studi di Parma, Italy) on "Solid state molecular recognition for supramolecular sensing".

MS38

L-R: *Scott Dalgarno, Evgenij Losev, Chiara Massera, Consiglia Tedesco, Alessia Bacchi, Samantha Chong, Janusz Lipkowski.*

Both were very interesting to the audience and had lively discussion. The remaining three shorter presentations by **Samantha Chong** (University of Liverpool, UK) on "Assembling pore networks in organic cage structures using molecular recognition", **Evgeniy Losev** (Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia) on "The effect of water on the outcome of mechanical treatment in L-serine oxalic acid system" and **Consiglia Tedesco** (Università di Salerno, Fisciano, Italy) on "How metallation affects solid state conformation and assembly of hexameric cyclic peptoids" were also very good and the co-chairs are fully satisfied with the choice made.

The microsymposium gathered in total approximately 100 participants, with about 80 at the beginning of the session and then fluctuating afterwards. We could see many young participants attending the session, so the topic seems still hot and interesting to crystallographers. Not all speakers to the session are crystallographers themselves but the content of the presentations was very full of high quality crystallographic information (excellent X-ray structures of complex supramolecular assemblies in talks 1 through 3 and 5, and solid state reactivity in the talk 4).

MS39 "Crystallization and crystal treatment"

Co-chairs: **J. Gavira** and **T. Bergfors**

This session opened with **Dominique Maes**'s presentation about the effect of impurities on crystal growth. Her atomic force and laser confocal microscopy images of growing crystal surfaces showed the dramatic effect of these impurities. The audience learned how important it is to "feed" their crystal with pure protein. Dominique was followed by **Elspeth Garman** a.k.a. Auntie E, acting as agony aunt. She shared typical questions sent to her: "I am in a polycrystalline relationship, and a loop has been hitting on me lately, how do I get out of this" and "I am experiencing embarrassing dryness and skins, what should I do". Auntie E gave wise advice to these crystals on how best to behave under stressful cryoconditions. Her advice is something everyone in the audience can use on their next synchrotron trip. Next up was **Jindrich Hasek** who showed us how polyethylene glycol, polyethylene oxide-type polymers, non-ionic detergents, and carboxylic acids can act as protein-

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L-R: *Jose Gavira, Trixie Wagner, Terese Bergfors, Dominique Maes, Jindrich Hasek, Takashi Kumasaka, Elspeth Garman.*

surface-active molecules. These "sticky" molecules help form interactions on the protein surface that promote crystal contacts. Our fourth speaker was beamline scientist **Takashi Kumasaka** who showed us how we can use polyvinyl alcohol as a non-toxic, sticky glue to stabilize the protein crystal under humidity control and subsequent cryocooling. Finally **Trixie Wagne**r presented GuideX, a database system to keep track of the 6000 or so small ligand compounds that she manages at Novartis.

The Arts Centre Studio lecture room was filled to capacity and our audience could surely go home with many practical tips and information from this session.

MS40 "Crystallography in Art and Archaeology"

Co-chairs: **Carl Schwalbe** and **Massimo Nespolo**

Taken together, the two invited lectures in MS40 examined artworks from the ground up. **Petr Bezdicka** described the analysis by X-ray powder microdiffraction of the ground used to line an entire canvas before paint can be applied. Being required in much greater quantity than any pigment, it was usually sourced cheaply and locally; and its composition gives guidance about the workshop that prepared the canvas. The five main sources in Central Europe of clay, widely used as a ground between the 16th and 19th centuries, can be clearly distinguished. **Alicja Rafalska-Łasocha** then directed our attention to the paint layer. Phase analysis with X-ray powder diffraction (XRPD) gives clues about its origin and provides information about ageing that is useful in guiding conservation. For instance, from about 1750 to 1850 Naples Yellow contained lead antimony oxide mixed with potassium lead sulphate; but in the late 1800s the second component was changed to zinc oxide. Green pigments usually are made from copper compounds, which may degrade over time. The identity of yellow and white pigments shown by XRPD supported stylistic analysis of two portraits of King John III Sobieski, the dynamic leader who drove away the Turks besieging Vienna in 1683, that suggested they could be by the same artist.

L-R: *Davide Viterbo, Carl Schwalbe, Alicja Rafalska-Łasocha, Petr Bezdicka, Massimo Nespolo, Jordi Rius, Laura Holland, photographed by Wiesław Łasocha.*

The first contributed lecture, by **Jordi Rius**, showed how synchrotron radiation made it possible to carry out transmission micro-diffraction experiments on polished thin sections. Typical samples were 15-30 μm thick, mounted on 1 mm glass slides, yielding (possibly overlapped) discrete patterns or Debye rings depending on the number of grains struck by the beam.

The final two lectures addressed another of the arts, namely literature. **Laura Holland** described the "Light Reading" short story competition, **www.light-reading.org** , conceived by Diamond staff to provide wide outreach and to draw parallels between creative and scientific processes. The only requirement was to mention the Diamond synchrotron within the story – the building, the science or the scientists. The first competition, in 2011 and open to adults, attracted over 70 entries from around the world; in 2012 the competition was repeated for 12- to 16-year-olds. **Davide Viterbo** concluded the session by telling us the dramatic life story of the great author **Primo Levi** (1919-1987) and the importance of crystallography in some of his works. Levi's career as a chemist was disastrously interrupted by transportation to Auschwitz in 1944, which fortunately he survived. His 1980 book "The Search for Roots: a Personal Anthology" includes sections inspired by **William Henry Bragg** (his book "Concerning the Nature of Things" also sparked **Dorothy Hodgkin**'s interest in crystallography) along with **Lucretius** and **Charles Darwin**.

MS41 "Crystallographic teaching and education"

Co-chairs: **Annalisa Guerri** and **Elena Boldyreva**

In view of next year's celebration of the "International Year of Crystallography" we invited representatives of different European countries to give to the audience an overview of the different initiatives undertaken by the different nations.

The first speaker, **Jean-Louis Hodeau** from CNRS in Grenoble, France, illustrated the itinerant exhibition "Voyage dans le Crystal" (**http://iycr2014.org/resource-materials/voyage-dans-le-cristal**), in which the crystals are used to travel from prehistoric times to modern days through their beauty, mystery and modern applications.

The second presentation given by **Luc Van Meervelt** from Leuven, Belgium, described the crystal growing competition that has been run for the past thirteen years. The contest is open to pupils of high schools: in five weeks they have to grow crystals of alum, and at the end a commission of experts awards the prize during a public ceremony. The bout will be open worldwide for 2014 to celebrate the International Year of Crystallography.

Anna Warren, from Diamond Light Source, UK, gave a summary of the Big Bang Fair in London, where The Science and Technology Facilities Council and the BCA funded a crystallography stand in collaboration with Diamond, ISIS and the YCG (Young Crystallographers Group). The YCG is very active in the dissemination of crystallographic science also in Bristol (Kitchen Chemistry) and at Diamond where Open Days are often held.

L-R: *Santiago Garcia Granda, Anna Warren, Michele Zema, Annalisa Guerri, Jean-Louis Hodeau, Elena Boldyreva, Luc Van Meervelt.*

The activities in Spain were presented by **Santiago Garcia** Granda. Many outreaches have been organized for the celebration of 2014. The competition for students "Crystallization in the School", active since 2008 in Andalusia, Asturias, Catalonia and Aragon, will be extended to other regions. The program "Science, Crystals and Society" includes a series of activities with which integrate the science of crystallography with the society: short videos showing "What does a crystallographer do?", a "2014 Crystallography Diary and Calendar" (paper and virtual editions), a "Postage Stamps exhibition", the "Virtual Geology Museum".

Italy was represented by **Michele Zema**. He gave an overview of the intense didactic activity of the Italian crystallographic community since the very beginning of the growth of this science in Italy. Among the many schools, in 2014 the "First European Crystallographic School" will be launched, supported also by the ECA and with the help of many renowned scientists.

The microsymposium was very successful: the attendance was very high. The lecture hall was full for the whole session and the audience was also asked to interact by building a unit cell with toothpicks and marshmallows. Hopefully the diverse initiatives would inspire and help scientists of other countries in organizing outreaches not just for the International Year of Crystallography but also to make people more aware about science and its everyday use.

MS42 "The history of the ECA"

Co-chairs: **Sine Larsen** and **Paul Beurskens**

This MS was initiated by the ECA Executive Committee. In spite of the heavily loaded scientific program, this "General Interest" Microsymposium attracted many (about 60) attendees, undoubtedly so because the speakers are well known as the masters in the fields given in the titles of the lectures.

In the lecture by **André Authier** (FR): "Crystallography in Europe in the 1970s – birth of the European Crystallographic Committee" much attention was given to the discussions among individual crystallographers and local crystallographic societies, raised about 20 years after the foundation of the International Union of Crystallography (IUCr) in 1948. The question was whether or not there should be a regional association, and the problem was that the political situation in Europe did not allow an easy decision! In 1972 the European Crystallographic Committee (ECC) was initiated. The audience of this lecture agreed that André Authier was the True Founder of the ECC and thereby of the ECA.

Hartmut Fuess (DLD): "Transition from a Committee to an Association (ECC > ECA)"
The work of the ECC, initially much keyed towards the organisation of European Crystallographic Meetings and improving the cooperation between European researchers, became more and more demanding, leading towards a more structured organisation; and so, discussions arose whether or not we should create a formal association. The writing of the Statutes for the ECA was severely hampered (again) by political issues. Finally, in 1997, the ECA was founded. The speaker, Hartmut Fuess, rightly (!) mentioned that he was registered as IM (Individual Member of the ECA) number 1.

Santiago Garcia-Granda (SP): "ECA recent history: From Leuven to Rovinj and before"
The speaker, Past-President of the ECA, presented an elaborate and still elegant exposition about many things related to the growth in size, power and other achievements of the ECA. Many details were reported, and it is important that the presentation is stored and made available at the ECA – website.

Jan Boeyens (ZA): "Crystallography in Africa"
Crystallography in Africa was first established in South Africa around 1937, but it hardly reached the rest of the continent of Africa. Soon after the birth of the ECA, the IUCr created the concept of "Regional Associates"; and the ECA accepted the responsibility for Africa as part of the Euro-African Region and wanted to cultivate crystallography in Africa. Though partly successful in Northern Africa, the ECA and the IUCr failed to be successful in most of the continent. Political problems are to blame. ECA support needs to be stimulated. The speaker was not very positive about the present political and economic situation, but was not without good hopes for the future.

MS43 "How to" session

Co-chairs: **Céline Mariette** (CM) and **Svend Erik Rasmussen** (SER)

The previous session in the Arts Centre Cinema ended some minutes before MS43 was due to start, which allowed SER to mention that he replaced H. B. Bürgi. The first half of the session began with a contribution by **Thomas Weber**, ETH, Zürich, Switzerland on "Measurement and reduction of diffuse scattering data". The next speaker was **Olivier Perez**, Caen, France, who spoke on "Superspace Formalism. The Swiss Army Knife of the Crystallographer".

In the second half of the session **Martin Adam** from Bruker, Germany, lectured on "Shutterless CMOS detector data processing using the Bruker APEX2 and PROTEUM2 software suites". The final speaker was **Paul Henry**, ESS

MS43

L-R: *Paul Henry, Martin Adam, Thomas Weber, Olivier Perez.*

Lund & Chalmers Göteborg, Sweden, whose talk was entitled: "To deuterate or not to deuterate? That is the question?" Both speakers finished well before time, allowing good time for discussion.

Finally, the session ended on the time scheduled, the speakers were photographed and lively, informal discussions followed.

MS46 "In situ methods and transient effects in chemical crystallography"

Co-chairs: **Simone Techert** and **Marijana Dakovic**

Christian Schimpf (Bergakademie Freiberg, Germany) started MS46 with a first study on the microstructure defects in hexagonal graphitic boron nitride (h-BN) employing line shape analysis on ex- and in-situ XRD data collected at particular crystallographic directions. The studies revealed the creation of microstructures during the h-BN high temperature / high pressure synthesis – one possible source of disorder (in particular in the context of puckering in basal layers). **Giulio I. Lampronti** (University of Cambridge, UK) continued with the presentation of combined powder XRD and chromatography studies in mechanochemical kinetics. He presented a first state-of-the-art case study of base-catalyzed metathesis of aromatic disulfides, where in-situ XRD / chromatography has been employed disentangling quantitatively the structural kinetic differences between three different polymorphs. They are formed as the reaction passes through the reversible covalently bonded intermediates. **Marco Milanesio** (Università del Piemonte Orientale, Italy) followed with a presentation of novel "downshifting" low-cost solar cell materials which are based on organic molecules (naphthalene-based pentanoic acid dyes and squaraine dyes) inserted into hydrotalcite. The organic molecules are intercalated into LDH by liquid-assisted grinding. For characterizing the formation mechanism, principal component analysis and molecular descriptors have been introduced allowing a classification of the studied intercalation reaction schemes. **Iñigo J. Vitórica-Yrezábal** (University of Sheffield, UK) presented his first case studies on gas-solid reactions in non-porous crystalline materials employing in-situ XRPD methods. He studied a series of reactions between non-porous molecular crystals of halide coordination compounds of the type trans-$[CuX_2(n\text{-}Xpy)_2]$ and anhydrous halide gas reacting to $(n\text{-}XpyH)_2[CuX_4]$ salts. Remarkably, for the reactions in-situ XRPD reveals the cleavage of Cu–N bonds and the formation of new Cu–Cl/Br and N–H bonds without the loss of crystallinity. In the final presentation, **Alice Brink** (University of the Free State in Bloemfontein, South Africa) reported on her synthesis of novel $Re[(L,L')(CO)_3(S)]$ model complexes for therapeutic / diagnostic radiopharmaceutical use. Kinetic and crystallographic studies have been performed to determine possible enhanced linker properties between a biomolecule and the present model systems of radionuclide. These properties and their structural impact have been discussed with respect to possible structural linkage mechanisms.

MS46

L-R: *Marijana Đaković, Simone Techert, Alice Brink, Christian Schimpf, Giulio Lampronti, Iñigo Vitórica-Yrezábal, Marco Milanesio.*

The Bragg-Franklin Symposium

ONE of the personal highlights of the ECM was the lunchtime session on the lives of Lawrence Bragg and Rosalind Franklin, entitled 'A Celebration of a Centenary of Crystallographers'. This session focused on the people behind the science, and John Jenkin and Jenifer Glynn were our respective biographers for this.

John Jenkin started with a tribute to the younger Bragg's vital role during WWI and WWII to the development of the military technique of sound ranging. This riveting guide to what many argue was the crux of the allies' victory highlighted Lawrence's struggles both on and off the battlefield. Around this time Lawrence was awarded the Nobel Prize in Physics as the youngest ever recipient at 25 years of age. The juxtaposition of Lawrence receiving the highest accolade in science contrasts greatly with that of his reception as a scientist amongst many of his peers, and John Jenkin took great care to vehemently defend Lawrence's honour and scientific integrity.

A personal overview of Rosalind Franklin's life was presented by her sister Jenifer Glynn. Rosalind made critical contributions to the field of structural biology through her work on DNA, RNA and viruses, but Jenifer's description of Rosalind truly highlighted the person beyond the scientist. The fantastic photos of Rosalind highlighted just how at home she was in both the lab and on the mountains. Her down-to-earth approach meant that she did not seek recognition for herself as a women but instead as a scientist.

This fantastic session was supported by Oxford University Press and the ECM organisers, and it was gripping from start to finish. It is a great pleasure to have been in attendance to hear about the lives of these crystallographers. Further details are available in John Jenkin's book 'William and Lawrence Bragg, Father and Son: The Most Extraordinary Collaboration in Science' and Jenifer Glynn's book 'My Sister Rosalind Franklin: A Family Memoir'.

Claire Murray
Diamond Light Source Ltd.

Photos courtesy of Dr Alicja Rafalska-Łasocha

L-R: *Claire Murray (co-chair), John Jenkin (speaker), Jenifer Glynn (speaker) and Fermín Otálora Muñoz (co-chair).*

John Jenkin shows a picture of Lawrence Bragg with his sound-ranging unit in Northern France.

Jenifer Glynn during her talk with the fantastic Quentin Blake drawings of Rosalind Franklin, Watson and Crick celebrating the discovery of the DNA double helix.

Report of ECM28 Satellite Meeting

Introduction to Software Development for Crystallographers

32 PEOPLE gathered at Warwick University from 23rd to 24th August 2013 for the first ECACOMSIG (aka "SIG9") Computing School, an "Introduction to Software Development for Crystallographers". The School followed the general lines of recent IUCr Commission for Crystallographic Computing (CompComm) Schools, in that the (relatively short) lectures were richly enhanced with longer in-depth tutorials by all the teachers, and discourse between all participants was strongly encouraged. As with the CompComm Schools, teachers were drawn from across Crystallography with the intention of avoiding a strong emphasis on any particular field (*e.g.* protein, small molecule or powder). The School actually started on the evening of the 22nd August, with a visit into Coventry city centre to sample the local West Midlands culinary speciality, a Balti restaurant. Having all participants together the day before the meeting meant that not only could we get to know each other, but also that we were able to fit in two full days of teaching – a real bonus. Following a welcome to the School by the School organisers (**Harry Powell** and **Andrea Thorn**), **Airlie McCoy** gave us an introduction into "Planning my Programming"; **Paul Emsley** followed with his thoughts on "Scripting and Automation of Existing Software"; we are particularly grateful to Paul because he stood in at the last minute as one of our planned speakers (**Santosh Panjikar**) had been unable to obtain a UK entry visa in time for the School. **Eugene Krissinel** gave us a tour round the "Use and Usage of Libraries", using those from CCP4 as particular examples.

Rita Giordano finished the morning session with "Visualising Statistics in R" (a freely available statistical package, which combines accessible statistical analysis functions with publication quality plots and the ability to script together external programs. An afternoon of tutorials (divided into two hour slots) by the first day speakers was followed by **Harry Powell** presenting fundamental guidelines on interface design in his talk on "GUIs and Web Applications".

Day 2 moved onto some core crystallographic topics; **Reinhard Neder** discussed both computational aspects and the mathematical background for dealing with "Matrices and Symmetry", and **Richard Cooper** followed up with "Geometry and Space Groups" and how to implement the methods in programs. **Lukas Palatinus** talked about "Fourier Methods" and their implementation in code, while **Randy Read** finished the lectures with how to deal with "Structure Factors and Likelihood". The afternoon was again given over to tutorials until the evening when the School wound up in time for the younger members of the audience to register for the Young Crystallographers' meeting.

Slides from the talks and some of the tutorials are available on the SIG's website at http://sig9.ecanews.org/sig9_warwick.html. ECACOMSIG is in the early stages of planning another Workshop to be held before ECM29 in Rovinj in August 2015; details will be posted on the SIG's website when they become available.

Harry Powell
MRC Laboratory of Molecular Biology

Bursary Reports

The 28th European Crystallographic Meeting (ECM28)
25 - 29 August 2013, Warwick, United Kingdom

AS a young crystallographer, ECM28 was among the most inspiring conference I have attended. The blend of science, history and literature made this a very unique crystallography conference which I found both, educational and motivational. The celebration of 100 years of crystallography and Bragg centenary along with the Bragg exhibition emphasised our deep rooted understanding, achievements and the significance of X- ray crystallography's contribution to science. I also believe that ECM along with other IUCr conferences provides an unparalleled platform that brings together crystallographers in various fields.

The conference began with the European Young Crystallographers Satellite Meeting on Sunday 25th August, 2013 where PhD and Masters students presented their research work. This event provided young crystallographers with an opportunity to interact and build a network in the crystallography community. This was followed by the inauguration ceremony of ECM28 along with the 7th Max Perutz Prize lecture delivered by Prof. **Randy Read**, a pioneering figure in the field of statistical approaches used in protein crystallography.

The next day began with the Bragg symposium at which, along with other speakers, we got a chance to hear an account of the Two Braggs' life and discoveries from their biographer, Prof. **John Jenkin**. This was followed by keynote speakers and other microsymposia all through the week, at which various crystallographic advances and discoveries were presented by both young and highly established crystallographers. These lectures gave us a chance to understand and appreciate the progress in this field and helped widen our horizon.

Being a young crystallographer who is still trying to learn and understand crystallography, meeting the likes of Prof. **Elspeth Garman**, Prof. **Zbigniew Dauter** and Prof. **Randy Read**, in person, interacting with them and listening to them address our misunderstandings and doubts was a very treasured learning. This gave students an opportunity to meet the authors of books we refer to and of various programs we use, on a regular basis as a PhD student in crystallography.

The lunch time lectures/events, included films such as '50 years a winner' – a film made in 1965 to celebrate the 1915 Nobel prize awarded to the Braggs and 'Hidden Glory' – a play about **Dorothy Hodgkin** by **Georgina Ferry** and lectures by Prof. **John Jenkin** – biographer of The Braggs and **Jenifer Glynn** – biographer of **Rosalind Franklin**. The poster sessions which ran all through the conference featured a display of outstanding research in the field and fostered a dynamic system of feedback that promoted scientific discussion. The absolutely one of a kind Bragg exhibition brought together a fascinating and inspiring collection of artifacts, art and correspondence never before seen in one exhibition. The final lecture and the highlight of the conference was the plenary lecture given by Noble Laureate Prof. **Dan Shechtman**, a renowned crystallographer, which was aimed at motivating young scientists.

ECM28 brought together the beautiful, simple yet complex and scientific contributions of X-ray crystallography to science. It brought together scientists from over a 100 countries with varied experiences and knowledge. It gave me a feeling of belonging, to this huge and diverse community of crystallographers who work towards understanding everything at the atomic range.

I would like to thank University of Bath and the British Crystallographic Association for their sponsorship to enable me to attend this meeting.

Sneha Ramaswamy
University of Bath

Bi-annual International Conference on Structural Genomics (ICSG2013-SLS)
August 2013, Sapporo, Japan

THANKS in part to the generous support of the British Crystallographic Association (BCA), I was able to attend the bi-annual International Conference on Structural Genomics (ICSG2013-SLS) in Sapporo Japan in early August 2013. As a 3rd year PhD student from the University of Glasgow, whose project focuses on the use of crystallography and complementary biochemical and biophysical techniques to determine the mechanism of action of novel protein antibiotics, attendance of this conference provided an excellent opportunity to learn about the wider application of these techniques and see what cutting edge and innovative technology is being developed in the field.

Large scale structural genomics initiatives were launched around 12 years ago and the ICSG2013-SLS provided an

opportunity to reflect on the achievements of structural genomics (>90,000 PDB submissions and counting), and how the technology and software developed has revolutionized how labs of any size do structural biology. The conference also provided an opportunity to look to the future of structural life science (the new title for the evolving structural genomics initiative), with an increased focus on in depth analysis of structure/function relationships using complementary techniques.

The conference also provided excellent networking opportunities, through interactive poster sessions and conference dinners (the food was of an exceptional standard); many international leaders of structural biology (including professors **David Stuart**, **So Iwata** and **Thomas Terwilliger**) were in attendance, along with world class researchers from Japan and abroad. The quality of research was truly outstanding and I found it extremely useful and interesting to get a feel for the kind of structural research which is undertaken in Japan.

Research highlights included the stunning methodological developments in the United States and Germany on utilization of x-ray free-electron lasers (XFEL) to solve protein structures, presented by Professors **Petra Fromme** and **Ilme Schlichting**. The development of this technology seems sure to push the boundaries of what is currently possible with x-ray crystallography. The collection of diffraction images from nanocrystals consisting of as little as 100 protein molecules, with femto-second pulses of coherent x-rays 10^{12} times brighter than a 3rd generation synchrotron, overcomes two of the most serious limitations in modern protein crystallography; the inability to grow crystals of sufficient size for a synchrotron source and crystal degradation due to radiation damage. Both speakers presented data validating the technique with a number of soluble and membrane proteins. However, it seems to me that current limitations, including, volume of material required (at least 100 mgs of soluble protein) and required homogeneity of crystal size mean that, at least in the near future, XFEL will become a significant tool in our structural solution arsenal, rather than the solution to every protein crystallographic problem.

The presentation on the architecture of the eukaryotic nuclear pore complex by Professor **Michael Rout** was an impressive illustration of how multiple biochemical and structural approaches can be united to create a model of extremely large (>600 kDa) and intricate protein complexes.

The presentation of a model of the essential Nup84 complex to a precision of 1.5 nm, required the utilization of a diverse set of structural techniques (x-ray crystallography, SAXs, electron microscopy) to determine the structure of subunits along with the overall structure of the complex. Protein mapping, biological and biophysical data was then used to provide modeling and spatial restraints, to create a beautiful and very informative model of one of the key gate keepers of the eukaryotic cell.

On a computational front, Professor **Thomas Terwilliger** presented developments which expand the ability of molecular replacement (MR) to find a solution with more distantly related homology models. This talk was of particular interest to me (as I'm sure it is to most crystallographers), as I recalled past instances where MR has failed to find a solution with a model that (as it turned out) was very similar, but not quite similar enough. The approach relies on refinement and rebuilding of the homology model, using Rosetta and phenix.autobuild, using electron density from the initial MR-run. Iteration of this process, if the model is nearly good enough, pushes the model in the right direction and produces a solution. These stepwise improvements in MR promise to make the phase problem less of a problem in the future.

The research presented and the hospitality of the Japanese people made the ICSG2013-SLS, the most enjoyable meeting I have attended in my career thus far. It takes some organization and planning for a PhD student to independently attend an international meeting, but I would highly recommend making the effort.

Rhys Grinter
University of Glasgow

19th International Conference on ADP-ribosylation (PARP2013) Quebec, Canada

THIS year I was given an excellent opportunity to present the results of my PhD project entitled "Structure and Catalytic Mechanism of Poly(ADP-ribose) Glycohydrolases (PARGs)" at the annual International Conference on ADP-ribosylation. My attendance to this conference was kindly sponsored by the Biochemical Society and the British Crystallographic Association. This conference was held at the Centre Hospitalier Universitaire de Quebec, in the stunning Quebec City in Canada.

This meeting marked the 50th anniversary of the discovery of the poly(ADP-ribose) polymerase 1 (PARP1), the key producer of the ADP-ribose post-translational modification in the cell. This conference thus was filled with expert speakers from all over the globe, working on different aspects of this vital post-translational modification, such as further elucidation of the less studied components of this pathway, the therapeutic significance of targeting this pathway, the implication and progress of inhibiting ADP-ribose metabolizing enzymes. It was humbling to present my work among such renowned world-class researchers as Prof. **Masanao Miwa**, who first discovered the Poly(ADP-ribose) glycohydrolase (PARG), the protein which I was working on during my PhD. I was involved in the structural characterization of PARG, and we published the first PARG structure since its discovery in 1971.

Due to the specialized nature of the meeting every talk and poster presented was highly relevant. On a whole the meeting primarily focused on understanding the biochemistry of modification by mono-ADP-ribose and novel techniques to detect the sites of such modifications. However, the data presented by the keynote speakers (Prof. **Nicola Curtin** (Newcastle University) and Dr. **Mark O'Connor** (AstraZeneca)) also described the latest progress in targeting PARPs in cancer treatment, with several compounds having just entered Phase III clinical trials. Of particular importance to me was the structural work presented by several speakers, such as Dr. **J. M. Pascal**, Dr. **T. Karlberg**, Dr. **S. Guetller**, Dr. **L. Lehtio** and Prof. **W. Xu**, which focused on the latest PARP1, PARP3 and tankyrase structures.

I had an excellent opportunity not only to hear the latest unpublished data in the field, but also make new relevant contacts. In addition, I also had a chance to meet our collaborators from Prof. **P. J. Hergenrother**'s group at the University of Illinois, with whom we recently published our work. During our close collaboration they kindly provided us with their novel PARG inhibitors, however, due to the distance I never had a chance to personally meet the group, and this meeting has allowed me to discuss the future of our collaboration.

Last, but not least, I had an opportunity to visit an area of outstanding beauty. The Quebec province boasts its French heritage and Quebec City is one of the most popular tourist destinations. It was a great pleasure to walk around the historic Quebec old town in the evenings and reflect on the latest developments in the ADP-ribosylation field.

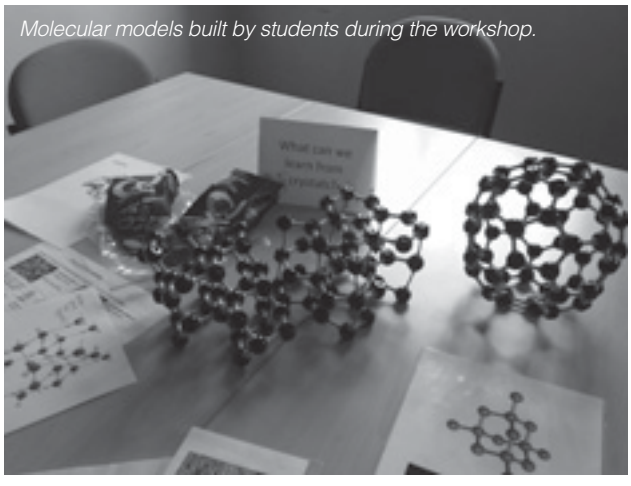
Eva Barkauskaite
Cancer Research UK

Outreach Report

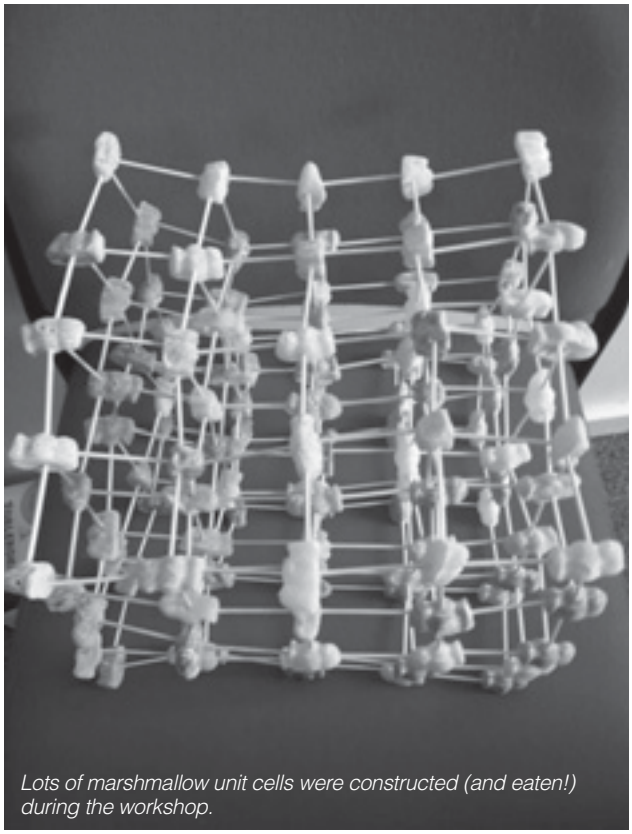
THE BCA Outreach coordinators have been busy running and organising a number of activities building on the Bragg Centenary year with a keen eye towards the International Year of Crystallography next year. In September we ran a series of workshops for the over 16s over 4 days at the British Science Festival run by the British Science Association in Newcastle. This was the first time that we had run the "structure of stuff is sweet" activity in workshop format but the enthusiasm of both the volunteers and the participants meant that we received some really good feedback. We had chocolate polymorphism, lasers with diffraction gratings, and more sweets that you could imagine – we even made a massive jelly baby crystal! This event wouldn't have been possible without our volunteers and we can't thank them enough for giving up their time to run this event (thanks to Hayleigh Lloyd, Alice Taylor, Liana Vella-Zarb and Mike Probert).

Next year will see the return of the Big Bang Fair. This will be running over four days (13-16 March 2014) at the NEC in Birmingham and is being funded by STFC again. We want to make sure we are well represented so we will requesting as much help as possible for manning the stand as ours is one of the most popular there! There will be over 70,000 people visiting and wanting to learn all about crystallography. Thanks to support from the BCA, STFC, Diamond and ISIS, we have some funding available towards travel and accommodation expenses. Please email (education@crystallography.org.uk) to register your interest. Training will be provided and if you have any questions do not hesitate to contact us. More than 30 eager crystallographers kindly gave up their time last year and they all had great fun using marshmallows to describe unit cells. Even if you have never done this before, we highly recommend giving it a go.

We've also been coordinating a program of activities for the IYCr with a kick-off meeting for interested parties taking place in December. We know that a number of you will already be planning events yourselves – we'd love to hear about what you are up to so that we can update the IYCr on the diverse range of things that we are doing within the UK and so that we can help to advertise your events through our website and social media.



Molecular models built by students during the workshop.



Lots of marshmallow unit cells were constructed (and eaten!) during the workshop.

There will be a number of additional activities occurring throughout the year (watch this space!), and we are always looking for volunteers so please email us if you would like to be added to the outreach mailing list. Also keep an eye on the website which our new vice president is helping us to redevelop as well as our twitter account (@Whatsinacrystal) and our facebook page (https://www.facebook.com/britishcrystallography). We are looking for ideas for tweets and blogs for these (tweets are short messages in 140 characters or less) to describe interesting facts about crystallography and crystals. This is an important way of highlighting crystallography to the general public (who may know nothing about crystallography!), so if you have any suggestions or would like to write a short blog post for the website please email Claire: caa.murray@gmail.com . Our twitter account is @Whatsinacrystal – follow us if you are on twitter for exciting crystal facts!

Anna Warren, Claire Murray and **Lynne Thomas**

New Honorary Membership

Moreton Moore – New Honorary Member of the BCA

PROFESSOR Moore studied mathematics and physics (MA) at Peterhouse, Cambridge, hoping to become an astronomer. Instead he became a postgraduate student of solid-state physics at the University of Bristol, studying the physics of materials (MSc) and defects in diamonds (PhD). He was appointed Lecturer in Physics at Royal Holloway College (RHC, University of London) in 1969; and his first research job was to ascertain whether there were any tiny diamonds in the Apollo 11 and 12 Moon samples, but sadly there was not enough carbon on the Moon's surface for meteoric impact to create any. Among a variety of subjects, for four decades he taught crystallography to physics, chemistry and biochemistry students. He was promoted in turn to Senior Lecturer, to Reader in Crystallography and to Professor of Physics; and his many research publications on X-ray topography of industrial crystals, especially diamonds, were recognized in the award of the higher doctorate: Doctor of Science (DSc).

Moreton was the first editor of the *BCA Newsletter* or *Crystallography News* (1982-87) and its predecessors for the Institute of Physics (IoP) Crystallography Group and for the combined IoP and Royal Society of Chemistry Crystallography Groups. He launched the international journal *Crystallography Reviews* in 1984, initially published by Gordon & Breach but now by Taylor & Francis. He designed the BCA logo; and he helped in the design of the BCA tie.

He has participated in every BCA Spring Meeting, except one. He organized the 1983 BCA meeting at RHC at which the Biological Structures Group and the Industrial Crystallography Group were inaugurated. He was Secretary of the Bragg Lecture Fund Committee (1980-87) and organized six Bragg lectures in England [at the Royal Institution (2), Cambridge, Leeds (2) and Manchester] and two in Australia [Adelaide and Perth]. He served on the BCA Council (1982-87) and also he was Secretary of the BCA (1995-97).

Jerome Karle (1918-2013): European Link

ALTHOUGH born in the USA, Karle's parents were from Eastern Europe (he extracted the funk out of his original name of Karfunkle), as were those of his wife, Isabella nee Lugoski, a brilliant student with a PhD at age 21. Karle and Isabella maintained a significant crystallographic link with Poland, especially through the triennial series of Organic Crystal Chemistry International Symposia of which Jerome became an active Honorary Chairman. These residential meetings, somewhat Gordon-like, organized by the Dept of Crystal Chemistry, Adam Mickiewicz University, Poznan, were held in the attractive Rydzyna Castle, between Poznan and Wroclaw.

Karle's papers contributed to the 9th (1994, a satellite of the 15th ECM at Dresden), 10th (1997), and 11th (2001) OCCIS, which are published in the Symposium issues of *Journal of Molecular Structure* **374**, 7 (1996), **474**, 9 (1999) and **647**, 9 (2003) respectively. Papers from the preceding 7th and 8th Symposia were published in the OUP/IUCr Book Series as Cryst Symp **4** (1991) and **7** (1994). I co-edited them all. Over a meal with Jerome and Isabella, I recall Karle remarking that, unlike most UK institutions, the ONR allowed one to hold an appointment as late in life as one wished (into the 80s and 90s, as it turned out). But he *was* a Nobel prizewinner and she received many prestigious awards.

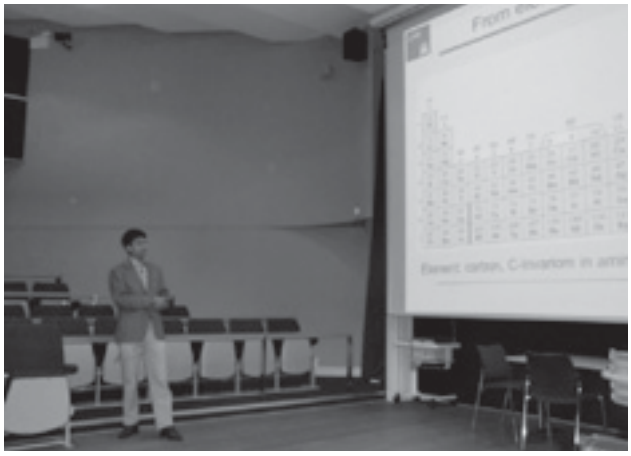
[Jerome may have participated in one of the York Direct Methods Courses, unless I'm thinking of Hauptman!]

Derry W Jones
University of Bradford

Young Crystallographers Group Update

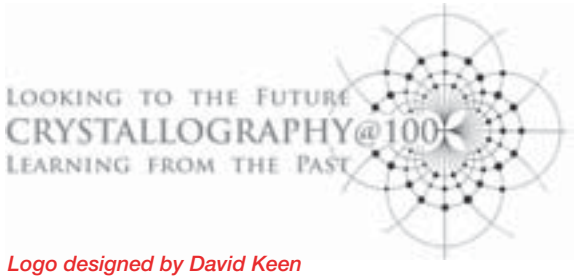
THE YCG were delighted to be co-organisers for the first European Young Crystallographers Satellite Meeting, held prior to ECM28, earlier this year. This was held in conjunction with the ECA General Interest Group – Young Crystallographers (ECA GIG-YC). The meeting was a huge success, with over 160 registered participants. The satellite took place during the day, finishing before the ECM opening ceremony in the evening.

The meeting kicked off with a plenary from Dr. **Birger Dittrich** from the University of Göttingen. He gave a great account of his refinement software *Invariom*; what was already available and the future directions. This was followed by a total of 13 talks from young crystallographers. There were a huge number of abstracts submitted for talks at the meeting and it was really difficult to select speakers. The chosen abstracts really covered a wide and varied number of topics, and the level of the talks was extremely high and really well received.



As a direct result of the meeting's success, it has been decided that a similar meeting will take place in Croatia prior to ECM29. This is a great outcome and our thanks go out to all the organisers. We are also grateful to the European Crystallographic Association and the International Union of Crystallography for their financial support; the meeting would not have been possible without their assistance.

We have started to put together a great programme for the next Young Crystallographers Satellite Meeting (YC2014) which will take place before the main BCA Spring Meeting between 1 pm on Monday 7 April and 11.15 am on Tuesday 8 April, at the University of Loughborough. We received a huge number of abstract submissions for our European meeting, and would like to keep this momentum going for our next satellite – so please continue to submit abstracts!



Logo designed by David Keen

At this year's AGM there were a number of new committee members appointed. **Claire Murray** stood down as vice-chair, being replaced by **Nick Funnell**. **Pascal Parois** took over from **Allan Pang** as our new Webmaster, and our BSG representative **Soshichiro Nagano** also retired, being replaced by **Anna Polyakova**. This year three positions were open for ordinary members, which were filled by **Lucy Saunders**, **Sarah Gurung** and **Sam Horrell**. The continuing members of the committee are **Anna Warren** and **Lauren Hatcher**, who remain as chair and secretary/treasurer, respectively. **Helen Mason**, **Kate Wittering** and **Anthony Phillips** are our respective CCG, IG and PCG representatives, and **Issy Kirby** remains as our fourth ordinary member.

If you are interested in keeping up to date with our activities please visit our website (**http://ycg.crystallography.org.uk/**), or alternatively join/follow our Facebook and Twitter pages (**http://www.facebook.com/YCG.BCA** and **https://twitter.com/YCG_BCA**). Alternatively you can contact us on ycg@crystallography.org.uk if you have any questions.

Anna Warren
(YCG Chair)

Physical Crystallography Group

ANNOUNCEMENTS

IoP Physical Crystallography Prize 2014

Call for Nominations

IOP | Institute of Physics
Structural Condensed Matter Group

THIS year the Physical Crystallography Prize is being sponsored by the Institute of Physics. The Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field. The award is traditionally presented at the BCA Spring Meeting and the winner gives a Prize Lecture at that meeting.

Nominations for the prize must be submitted to the Chair of the Physical Crystallography Group, Dr. **Ivana Evans** (**ivana.radosavljevic@durham.ac.uk**), by 31 January 2014 and the Prize will be awarded at the 2014 BCA Spring Meeting at University of Loughborough, 7-10 April 2014.

PANalytical Thesis Prize 2014

Call for Nominations

PANalytical

THE Physical Crystallography Group is pleased to invite entries for the PANalytical Thesis Prize in Physical Crystallography. The prize will be awarded for the best use of techniques or methods of Physical Crystallography in a successfully examined thesis submitted in the period from 1 September 2012 to 31 December 2013.

To be eligible for the prize, candidates must be a member of the Structural Condensed Matter Group of the IoP and/or the British Crystallographic Association (BCA). Non-members may enter the competition but will be required to join the BCA/PCG at the student rate to progress their nomination further (current rate £10 per annum or £35 for 4 years of the PhD degree).

To enter the competition, candidates must submit:

(a) a copy of the thesis in electronic format.

(b) a personal statement of not more than 500 words explaining why the thesis should be considered for the prize and including a clear description of the role of Physical Crystallography (as defined on the website **www.pcg-scmp.org** or otherwise) in the research.

(c) the names and contact details of two academic referees, one of whom may be the thesis supervisor, who will be able to comment on the thesis research of the candidate.

In order for a thesis to be eligible for the award, the Physical Crystallography element must be central to the work of the thesis, which must also demonstrate a context over and above structural work for its own sake.

Nominations for the prize must be submitted to the PCG-SCMP Chair, Dr. Ivana Evans (**ivana.radosavljevic@durham.ac.uk**), by 31 January 2014 and the Prize will be awarded at the 2014 BCA Spring Meeting at University of Loughborough, 8-10 April 2014.

Education

MANY of you will be aware of the fantastic work Professor **Mike Glazer** has been doing as part of his role as education officer. The superb "Two Braggs" exhibition that he organised with **Pam Thomas** to celebrate the centenary of the work of William Henry and William Lawrence Bragg was enjoyed by ~1040 visitors over 5 days at the Warwick Arts Centre during the ECM28 meeting in August. It was wonderful to be able to see some of the Braggs' equipment (including a number of their ionization spectrometers and crystal samples) as well as their Nobel prizes and lab notes all together. It was a privilege also to admire some of their paintings and other memorabilia lent by the Bragg family, to gain an insight into the lives of these remarkable men. Mike is grateful to many organisations for support and loans of scientific equipment (in particular the Royal Institution, the Cavendish Laboratory, the MRC Cambridge, the Science Museum London, the Diamond Light Source, and the Oxford Museum of History of Science) and for financial support (too numerous to mention here!!). I'd strongly encourage anyone who missed the exhibition to look out for the film being put together by the Diamond Light Source and some items from the exhibit to be displayed at the BCA 2014 Spring Meeting.

"The Two Braggs" exhibition organised by Mike Glazer and Pam Thomas which was enjoyed by ~1040 visitors; the photo must have been taken during one of the very few quiet moments!

On a related note, it was mentioned at the PCG-SCMP AGM that there may be some archive material relating to the Braggs' involvement in establishing the Physical Crystallography Group. If anyone can shed any light on this, please do get in touch (**e.e.mccabe@kent.ac.uk**).

Images from ECM28

An attentive group of crystallographers

Awarding the CCDC poster prize

Dave Allan informs us about facilities at Diamond

Invitation to ECM29 in Croatia

Puzzle Corner

GET your Periodic Table out and write down the symbols for the elements described by the following clues. The first letters will spell out a seasonal message.

___ The beginning of it all

___ Radioactive and chemically active – it's very much a non-metal.

___ Poisonous on its own but a vital part of our DNA

___ Keeps you safe if it stops your beam but could make you sick if it pipes your water

___ A relative of scandium which comes from the same part of Sweden as terbium

___ Giving bargain earrings with this metal in them may cause an angry reaction.

___ Named for a relatively brilliant scientist

___ Filament in old-style light bulbs

___ It also comes from the same part of Sweden as terbium.

___ UKIP would be glad it's a rare earth.

___ Filler in old-style light bulbs

___ Not Au or Ag, but it improves the appearance of metal onto which it's plated.

___ Without this, the Yule log would go out but you wouldn't notice.

___ You'll need this in your toothpaste after all those mince pies!

___ Must be present if it's organic

___ If you go to Cologne for a Christmas market, you'll see the river for which this is named.

___ That relative of scandium comes back for a second visit.

___ Substituted into methionine, it makes you SAD at the synchrotron.

___ Lightweight strong quadrivalent metal – good for Santa's sleigh?

Puzzle Corner Answers

June 2013

The winning answer has been supplied by **Jim Trotter**, as follows:

Pt words

Words beginning with "pter" derive from the Greek "pteron", meaning wing or feather (also used to refer to ferns, which I suppose are feather-like). Hence:

Pteridine = yellow base, constituent of various animal pigments (first found in butterfly wings).
pteridology = study of ferns.
pteridosperm = seed fern (cycadofilicales), extinct.
pterigold = sphenoid bone of the skull (shaped like a pair of wings).
pteropod = small gastropod mollusk, with a wing-shaped organ used for propulsion.
pterygium = wing-like triangular membrane in neck, eyes etc.
pterylosis = arrangement of feathers.
Also some others, e.g. **pterosaur** = flying lizard (pterodactyl).
Ptarmigan = bird (type of grouse). This derives from Scots Gaelic: tarmachan, which is part of a mountain group in Scotland (hill of the ptarmigan) – although I don't know where the Gaelic word comes from.
ptisan = nourishing decoction of barley and other ingredients.
ptomaine (Greek, to fall) = organic base formed by putrefaction (some are poisonous).
ptosis (Greek, to fall) = sagging of an organ, esp. eyelid.
ptyalin (Greek, saliva) = amylase in saliva, converts starch to sugar.

The word which led to all this, **"ptychography"**, is not to be found in my dictionaries, although I have not checked the latest OED. It is a form of scanning diffraction imaging, which can retrieve the phase of the diffracted beam (word derives from Greek, fold).

A sentence with more than one of these words would probably be gibberish, so a simpler one is:
"Pt is, of course, the chemical symbol for the element platinum".

September 2013

The answers suggested by the individual clues are:

Co-discoverer of insulin	B e s t
Isle frequented by yachtsmen	W i g h t
God of element 90	T h o r
Emit visible radiation	S h I n e
Big source of visible radiation	S u n
Most intense X-ray source (initials)	F E L
Point-and-click software access (initials)	G U I
Fe bridge across this river	S e v e r n

The quotation by W. H. Bragg is: **"Light brings us the news of the universe."**

Appropriately, the winning answer was given by **Jim Trotter**, who has pointed out several scientific connections between himself and the Braggs:

'I can consider myself a scientific grandson of **W. H. Bragg**, as I was a student with **J. Monteath Robertson**, who worked with W.H. Bragg at the Royal Institution – not as a student, but later in his career. I remember JM saying that people like **J. D. Bernal** and **Kathleen Lonsdale** were there, so he (as an organic chemist) had to learn crystallography quickly, as "those people did not suffer fools gladly"… My connections with **W. L. Bragg** are: (1) I almost went to work with him at the RI. We corresponded when I was in Ottawa in 1959, but something went missing in the mail, I think, so I never went to the RI. (2) My graduate students, Norman and Arthur Camerman, went as postdocs to work with W. L. Bragg in the 1960s; I guess that makes him the scientific step-father of my scientific sons.'

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.

1-6 December 2013
2013 MRS Fall Meeting and Exhibit, Boston, MA, USA.
http://www.mrs.org/fall2013/

2-6 December 2013
Thermec 2013: Neutron Scattering & X-Ray Studies for the Advancement of Materials, Las Vegas, NV, USA.
http://www.thermec.org/template3s/

16 December 2013
BCA Biological Structures Group Winter Meeting, King's College, London.
http://crystallography.org.uk/bsg-winter-meeting-2013/

18 December 2013
Biophysics and Synthetic Biology Symposium, University of Liverpool.
http://www.iucr.org/news/notices/meetings/meeting_2013_370

3-5 January 2014
CCP4 Study Weekend, University of Nottingham.
http://www.cse.scitech.ac.uk/events/CCP4_2014/

20-22 January 2014
1st International Symposium on Nanoparticles, Nanomaterials and Applications, Caparica, Portugal.
http://www.isn2a2014.com/

31 January – 4 February 2014
XVI. Annual Linz Winter Workshop. Advances in Single-Molecule Research for Biology & Nanoscience,. Linz, Austria.
http://www.nano-tm-agilent.com/index.php/linz-winter-workshop-2013

15-19 February 2014
Biophysical Society 58th Annual Meeting. Bridging the Sciences to Explore Biology, San Francisco, CA, USA.
http://www.biophysics.org/2014meeting/Main/tabid/4177/Default.aspx

16-20 February 2014
Neutron and X-ray Studies of Advanced Materials VII – Challenges of the Future World. 2014 TMS Annual Meeting & Exhibition, San Diego, CA, USA.
http://www.programmaster.org/PM/PM.nsf/Home?OpenForm&ParentUNID=CCEF4E8CAEF7CB7A85257839004F9CE3

19-21 February 2014
NIBB 2014. Neutrons in Biology and Biotechnology, Grenoble, France.
http://www.ill.eu/html/news-events/events

23 February – 26 March 2014
HERCULES. Neutrons & Synchrotron Radiation for Science, Grenoble & Paris, France, & Villingen, Switzerland.
http://hercules-school.eu/

25 February – 6 March 2014
ISIS Practical Neutron Training Course, ISIS, Didcot, Oxfordshire.
http://www.isis.stfc.ac.uk/learning/neutron-training-course/

3-7 March 2014
APS March 2014 Meeting, Denver, CO, USA.
http://www.aps.org/meetings/march/

13-21 March 2014
34th Berlin School on Neutron Scattering, Berlin, Germany.
http://www.helmholtz-berlin.de/events/neutronschool/index_de.html

16-20 March 2014
247th ACS National Meeting & Exposition, Dallas, TX, USA.
http://www.acs.org/content/acs/en/meetings/spring-2014.html

17-20 March 2014
22nd Annual Conference of the German Crystallographic Society (DGK) 2014, Berlin, Germany.
http://www.dgk-conference.de

24-27 March 2014
Studying Kinetics with Neutrons (SKIN 2014). Third International Workshop, Grenoble, France.
http://www.ill.eu/html/news-events/events/skin-2014/

30 March – 4 April 2014
G Protein-Coupled Receptors: Structural Dynamics and Functional Implications (Z1), Snowbird, UT, USA.
http://www.keystonesymposia.org/index.cfm?e=web.Meeting.Program&meetingid=1250

7-11 April 2014
Computational Structural Biology – from data to structure to function. EMBL-EBI Training Course, Cambridge.
http://www.ebi.ac.uk/training/course/structural-biology-2014

8-10 April 2014
BCA Annual Spring Meeting, University of Loughborough.
http://crystallography.org.uk/spring-meeting-2014/

14-16 April 2014
The Physics of Soft and Biological Matter, Cambridge.
http://softbio.iopconfs.org/home

17 April 2014
Ion Beam Analysis Techniques in Materials Science (from eV to MeV), London.
http://www.iop.org/events/scientific/conferences/calendar/index.html

21-25 April 2014
2014 MRS Spring Meeting and Exhibit, San Francisco, CA, USA.
http://www.mrs.org/spring2014/

24 April 2014
The Physics of Self-Assembling Biopolymers, London.
http://www.iop.org/events/scientific/conferences/calendar/index.html#/?i=1

28 April – 2 May 2014
41st ICMCTF. International Conference on Metallurgical Coatings and Thin Films, San Diego, CA, USA.
https://www2.avs.org/conferences/ICMCTF/

7-9 May 2014
Molecular Simulations and Visualization. Faraday Discussion 169, Nottingham.
http://www.rsc.org/FD169

11-16 May 2014
QENS 2014/WINS 2014, Autrans, France.
http://www.ill.eu/news-events/events/qens-2014-wins-2014/

18-21 May 2014
Molecular Machines: lessons from integrating structure, biophysics and chemistry. EMBO EMBL Symposium, Heidelberg, Germany.
http://www.embo-embl-symposia.org/symposia/2014/EES14-03/index.html

20-23 May 2014
META'14. 5th International Conference on Metamaterials, Photonic Crystals and Plasmonics. Singapore.
http://metaconferences.org/ocs/index.php/META14/META14#.Un-A9eL3yZR

21-23 May 2014
Mechanochemistry: From Functional Solids to Single Molecules – Faraday Discussion 170, Montreal, Canada.
http://www.rsc.org/ConferencesAndEvents/RSCConferences/

24-28 May 2014
2014 Annual Meeting of the ACA, Albuquerque, NM, USA.
http://www.amercrystalassn.org/content/pages/main-annual-meetings

27-29 May 2014
E-MRS 2014 Spring Meeting, Lille, France.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=691&Itemid=1619

30 May – 8 June 2014
Erice 2014 – Structural Basis of Pharmacology, Erice, Italy.
http://www.crystalerice.org/Erice2014/2014.htm

1-5 June 2014
2014 American Conference on Neutron Scattering (ACNS), Knoxville, TN, USA.
http://www.mrs.org/acns-2014/

1-6 June 2014
The 13th International Conference on Muon Spin Rotation, Relaxation and Resonance, Grindelwald, Switzerland.
http://indico.psi.ch/internalPage.py?pageId=0&confId=2039

7-11 July 2014
International Conference on Highly Frustrated Magnetism 2014, Cambridge.
http://hfm2014.tcm.phy.cam.ac.uk/

12-19 June 2014
Bombannes 2014.12th European School on Scattering Methods Applied to Soft Condensed Matter, Carcans-Maubuisson, France.
http://www.ill.eu/news-events/events/

15-19 June 2014
6th International Workshop on Crystal Growth Technology, Berlin, Germany.
http://iwcgt-6.ikz-berlin.de/

15-18 June 2014
EPDIC14. European Powder Diffraction Conference, Aarhus, Denmark.
http://epdic14.au.dk/

16-19 June 2014
16th International Workshop on Physical Characterization of Pharmaceutical Solids, Prague, Czech Republic.
http://www.assainternational.com/workshops/iwpcps-16/

22-27 June 2014
Hybrid Electronic & Photonic Materials and Phenomena. Gordon Research Conference, Hong Kong, China.
http://www.grc.org/programs.aspx?year=2014&program=hybridelec

7-11 July 2014
International Conference on Highly Frustrated Magnetism 2014, Cambridge.
http://hfm2014.tcm.phy.cam.ac.uk/

9-11 July 2014
Emerging Photon Technologies for Chemical Dynamics – Faraday Discussion 171, Sheffield.
http://www.rsc.org/conferencesandevents/rscconferences/

20-25 July 2014
Structural Nanomaterials. Gordon Research Conference, Hong Kong, China.
http://www.grc.org/programs.aspx?year=2014&program=strucnano

21-25 July 2014
ICSOS'11: 11th International Conference on the Structure of Surfaces, Coventry.
http://icsos11.iopconfs.org

3-8 August 2014
Conductivity & Magnetism in Molecular Materials: Understanding and Controlling Emergent Properties. Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=conduct

5-12 August 2014
IUCr2014. 23rd Congress and General Assembly, Montreal, Quebec, Canada.
http://www.iucr2014.org/

10-15 August 2014
DNA Topoisomerases in Biology & Medicine: from Molecular Structure to Drug Targeting. Gordon Research Conference, Newry, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=dnatop

10-15 August 2014
Multiferroic & Magnetoelectric Materials: Designing for Multifunctionality. Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=multiferr

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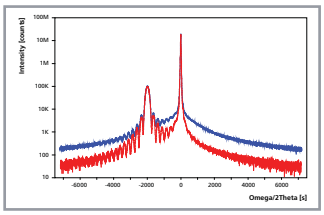

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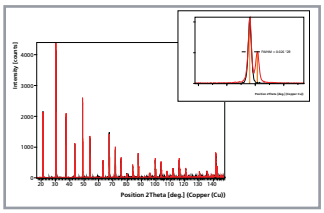

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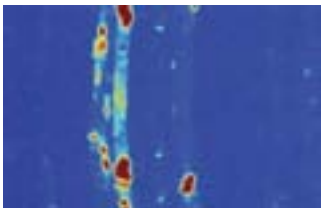

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