Crystallography News

British Crystallographic Association

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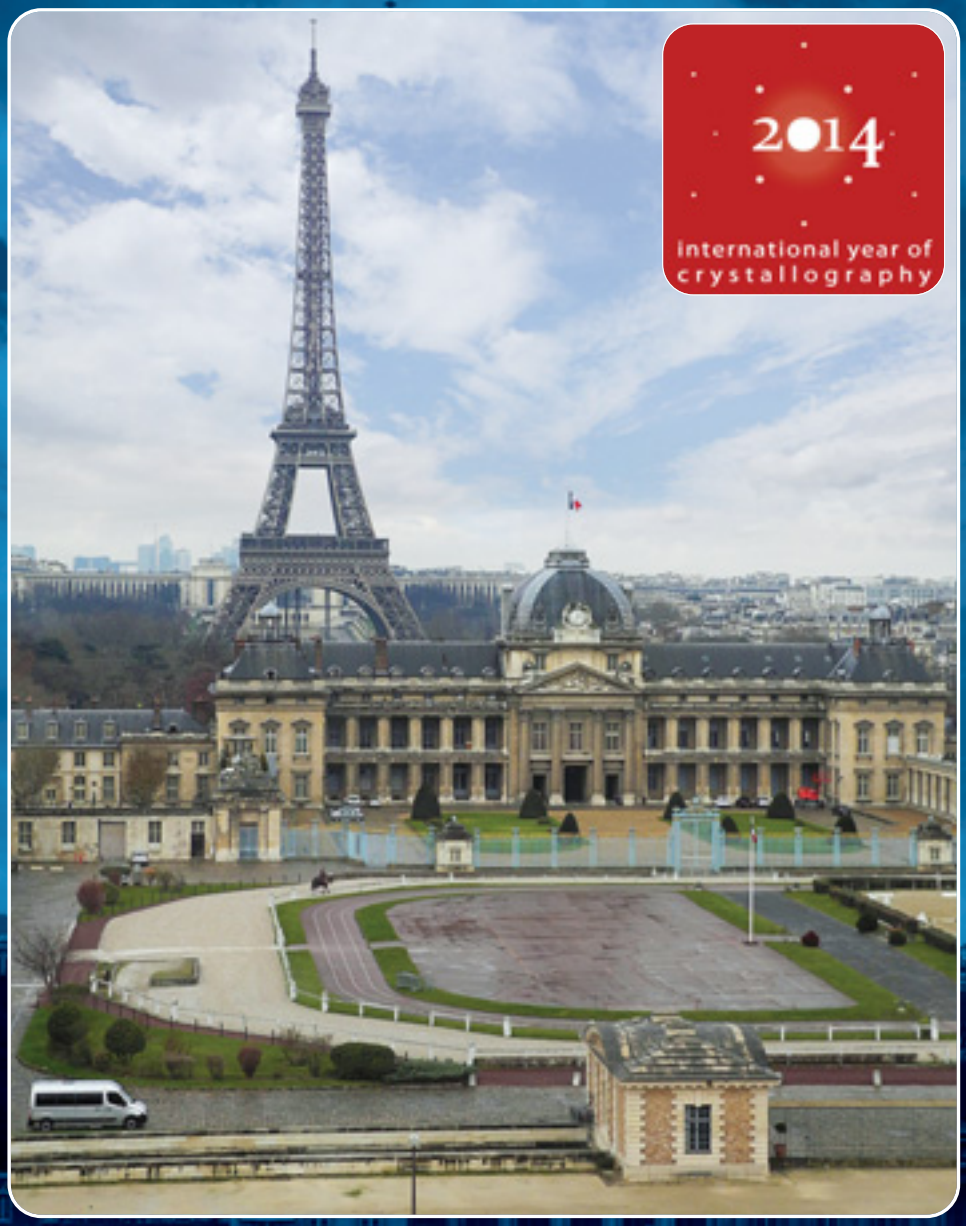
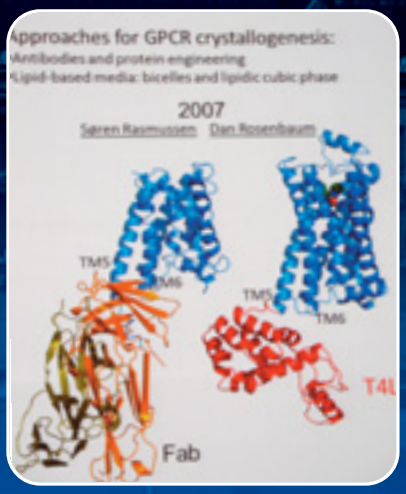


Bilingual Address by Irina Bokova

Lively Discussion of PSII

Nobel Laureate Brian Kobilka



Brian Kobilka's Breakthrough

Coming soon: BCA Spring Meeting

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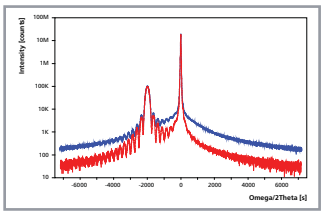
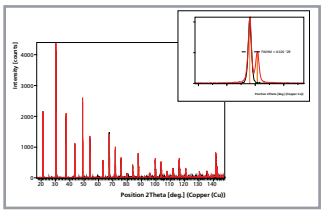
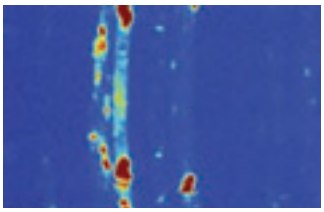
0D



1D



2D



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Crystallography

Innovation with Integrity

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

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This month's cover:

Opening Ceremony of IYCr at UNESCO House in Paris

From the President

THIS time last year Oxfordshire was carpeted with millions and millions of those pesky white winter crystals, blocking our roads, covering our drives and generally looking stunningly beautiful. This year we've witnessed a phase transition and instead the rivers are swollen with the liquid form and fields are flooded around the Thames; others around the country are faring far worse. What a difference a year makes (and the weather being a few degrees of warmer)! I have been doing some work on ice structures recently and it has amazed me how quickly people developed an understanding of the structure of everyday ice, namely the Ih phase. Indeed even as early as 1929 a reference is made to a review where over one hundred papers had been written on the subject [1], less than twenty years on from Lawrence Bragg's first paper on x-ray crystallography. In 1949 – very soon after the first demonstration of neutron diffraction by Wollan and Shull – Wollan and co-workers [2] were using neutrons to investigate the arrangement of the hydrogen (deuterium) positions using powdered samples. This was followed by a single crystal study in 1957 confirming the random 'ice-rules' model of hydrogen bonding and thus the disordered arrangement of the water molecules [3]. This molecule continues to fascinate crystallographers, whether it is the myriad of high-pressure phases of ice or the impact of water molecule orientations in their structures or the role of water molecules and their hydrogen bonds in protein structures. There is something for everyone and I have little doubt that H_2O will continue to be studied by crystallographers for many more years to come.

By the time that you are reading this column the Spring Meeting will be fast approaching. I am delighted with the way that the scientific programme has developed through the hard work of **Lee Brammer** and his team. We have an excellent array of plenary and invited speakers and I am confident that the standard will be maintained right through the meeting. We have also decided to allow Poster submissions beyond the published deadline – if you thought that you had missed your chance then there is still time! Please see details either on the BCA website or later in this issue for how to send in 'late submission' poster abstracts. As is usual, we will also be holding the Annual General Meeting of the British Crystallographic Association during the Spring Meeting. There are a number of vacant posts on BCA Council, including for a – now elected – Education and Outreach Coordinator. Please consider nominating someone for these positions; we like to have elections. Further details are available later in this issue with the formal announcement of the AGM.

Some of you will have been to Paris earlier in January for the Opening Ceremony of the International Year of Crystallography, IYCr2014, at the UNESCO building. This was a fairly grand affair with live translation of all the presentations and representation from all around the world. I was only able to attend for the first day of the two-day meeting, but I was particularly impressed by the contribution in the middle of the day by younger crystallographers taking part in a panel discussion. The enthusiasm for the subject is still out there…

Of course, as part of IYCr2014 we are continuing to communicate the 'celebrating crystallography' message through public engagement. As I mentioned in the last issue of Crystallography News we will be running a stand at this year's Big Bang Fair in a week or so's time and later in March the Oxfordshire crystal growing competition will be reaching its conclusion. Several BCA members are continuing to give public lectures on crystallography, including **Judith Howard**'s Bragg Lecture, *"A century of symmetry discovered: a crystallographer's tale"* given as a Friday Evening Discourse at the RI at the end of January. (Judith will also be giving the Bragg Lecture at the Spring Meeting this year.) Crystallography 'content' is also being rapidly produced online, with further contributions to the Ri Channel (**richannel.org/collections/2013/crystallography**); **Mike Glazer** has produced interesting pages around the Two Braggs exhibition in Warwick last year (see **www.amg122.com/twobraggs**) including video of interviews of Lonsdale, Ewald and others. Our Education and Outreach Coordinators, with assistance from our Web Team have also produced excellent web pages with a strong teaching bias (**learn.crystallography.org.uk/** – they are looking for volunteers to help with writing further content). All are definitely worth a look. Finally various science journals are commissioning and/or giving space to articles around a crystallographic theme and already too many have appeared to mention individually. I will nonetheless highlight the recent issue in Nature, including an interesting Comment by **Paolo Radaelli** about science funding and crystallography, see **http://www.nature.com/nature/journal/v505/n7485/index.html** .

I look forward to seeing you all at the Spring Meeting in April, I hope that many of you have been successful in getting abstracts accepted (and travel funds in place) for this summer's 23rd IUCr Congress in Montreal, and I commend this edition of Crystallography News to you.

[1] Barnes Proc Roy Soc A 125 (1929) 670.

[2] Wollan, Davidson and Shull Phys Rev B 75 (1949) 1348.

[3] Peterson and Levy Acta Cryst. 10 (1957) 70.

David Keen

BCA Council 2014

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

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

From the Editor

OUR cover story features the Opening Ceremony of the International Year of Crystallography, held at UNESCO Headquarters in Paris from 20-21 January. Among its many advantages was a fine view towards the Eiffel Tower from its 7th floor cafeteria. We were welcomed with a brief well-crafted address on video by UN Secretary-General Ban Ki-moon. A second welcome address followed, delivered in person in beautifully clear English and French by Irina Bokova, pictured on the cover, a Bulgarian diplomat who is the Director-General of UNESCO. A response on behalf of the International Union of Crystallography was given by Gautam Desiraju, setting out the beauty and usefulness of crystallography. The UNESCO connection was interesting. As expected, considerable attention was paid to the historical development of crystallography, the 100th anniversary of Laue's Nobel Prize being the hook on which to hang a centenary celebration. Recent towering achievements of crystallography were also presented. However, a great deal of emphasis was devoted to spreading the benefits of crystallography to the developing countries. Under UNESCO sponsorship, with donations from equipment manufacturers, a series of "open labs" are being established in Africa, south Asia and Latin America, so that researchers in the host country and neighbouring countries can do crystallographic research. We also heard a progress report about SESAME, a synchrotron being built in Jordan by a consortium of usually hostile countries with the aim of providing a modern facility for the Middle East and the hope that scientific collaboration will lead to better personal and political understanding.
A full report on this stimulating meeting appears in this issue. If you wish to view many more photos than we are able to provide here, see http://www.iycr2014.org/photos/iucrunesco-events/iycr2014-opening-ceremony .

Of course, the Big Event for the BCA is the forthcoming Spring Meeting at the University of Loughborough from April 8-10. We present updated information about the exciting programme for this meeting. **Lee Brammer** burned a lot of midnight oil to provide us with the very latest titles and times for lectures. Please note that the deadline for Early Bird registration is March 7. People who haven't already registered should just be able to meet this deadline if, immediately after receiving this issue of *Crystallography News*, they get their skates on. The website is http://www.hg3.co.uk/bca/bcaregistration.aspx .

A plenitude of interesting crystallographic material has appeared on the Web. In his "From the President" column **Dave Keen** has told us about the excellent "Two Braggs" website prepared by **Mike Glazer** as well as the special issue of Nature. The *Chemistry World* website also provides some perspective on the International Year of Crystallography at http://www.rsc.org/chemistryworld/2013/10/crystallography-international-year-2014-history-progress .

On the subject of websites, I can also direct readers' attention to http://www.iucrj.org/m/ , which takes you to the new IUCr Journal. Since this is an open access journal, it is possible for everyone not only to explore the range of crystallographic expertise represented in the issue but actually to delve into the full articles and appreciate their quality. As someone who had published the structures of some inositol derivatives in the 1990's, I took a particular interest in the article by **S. L. Bekö**, **E. Alig**, **M. U. Schmidt** and **J. van de Streek** reporting a systematic analysis of hydrogen bonding and melting points in the various stereoisomers of inositol. They made two important points: in these systems that are liable to polymorphism, any serious attempt to relate crystal structure to melting point must ensure that the appropriate polymorph has formed and the nature of any phase transition is understood; and a simple count of hydrogen bonds is only a start, which must be supplemented by more subtle analysis of symmetry.

Our December issue inadvertently demonstrated the importance of keeping up with the latest literature. One of the clues in the Puzzle Corner was "Radioactive and chemically active – it's very much a non-metal", which had the intended answer Astatine ("chemically active" to distinguish it from radon and "a non-metal" to distinguish it from uranium, radium, etc.). After I had gone to press with it, the next issue of *Chemistry World* carried an article describing theoretical calculations on solid astatine which indicated it would be metallic! Indeed, it had already appeared on the web pages of Chemistry World in September at http://www.rsc.org/chemistryworld/2013/09/astatine-metallic-superconductor-predictions, but my excuse for missing it there is that I was busy writing up all the exciting events at ECM28. Because of this uncertainty, I am holding over the answer to the December Puzzle Corner until our next issue.

Some readers may have wondered about my description of **Moreton Moore**, our newest Honorary Member, as a "diamond geezer". This is Cockney slang for somebody who is 'one of us', reliable, solid, trustworthy, according to no less an authority than Professor **David Crystal** OBE on the BBC, http://www.bbc.co.uk/worldservice/learningenglish/radio/specials/1453_uptodate3/page4.shtml . As someone based in the West Midlands, who doesn't get to London very often, I had to assume that Cockney slang is the conventional medium of discourse at Moreton's institution, the University of London; and these attributes certainly fit him, along with the brilliance and clarity of a diamond.

Carl Schwalbe

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- Influence on the development of crystallography and the BCA

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Puzzle Corner

OUR report on the Opening Ceremony of the International Year of Crystallography at UNESCO mentions the 9 countries that are members of the SESAME synchrotron consortium, along with the 5 countries that are hosting the first Open Laboratories.

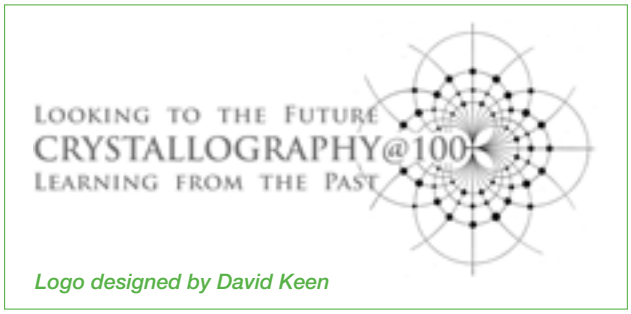
In the forwards, backwards, vertical and diagonal word search below, find these 14 countries and 9 of the countries with observer status for SESAME. Finally, find its postal town, which matches the name of a famous beamline scientist.

R	U	S	S	I	A	N	E	L	I	Z	A	R	B	Y
M	B	O	N	N	N	O	I	T	A	R	E	D	E	F
I	Y	S	J	I	S	R	A	E	L	N	S	W	O	G
N	A	O	T	V	R	A	L	L	A	N	K	A	P	F
A	N	C	U	O	W	A	B	I	E	P	S	C	N	L
L	I	C	R	R	C	N	N	A	T	S	I	K	A	P
A	T	O	K	Y	T	I	R	O	H	T	U	A	D	M
G	N	R	E	C	T	H	V	S	T	R	T	R	R	Y
U	E	O	Y	S	Y	C	P	C	U	W	A	M	O	N
T	G	M	E	T	T	I	J	G	O	R	A	I	J	A
R	R	L	V	N	J	K	U	A	S	A	P	Y	N	M
O	A	F	R	I	C	A	E	L	P	M	S	Y	H	R
P	X	U	E	G	Y	P	T	B	Y	A	A	T	C	E
E	C	N	A	R	F	S	W	E	D	E	N	I	T	G
F	U	N	I	T	E	D	K	I	N	G	D	O	M	A

BCA Annual Spring Meeting

University of Loughborough
8-10 April 2014

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



Logo designed by David Keen

Young Crystallographers Satellite Meeting

YC Chemical Plenary
Iain Oswald (University of Strathclyde)
High Pressure Studies of Illicit Materials

YC Biological Plenary
Elspeth Garman (University of Oxford)
Triumph over Adversity: Structure Solution of M. tuberculosis NAT, 'difficult' throughout

Parkin Lecture
Claire Murray (Diamond Light Source)

Debate: *Are Crystallographers Still Necessary?*
Simon Coles (University of Southampton): **Yes**
Graeme Winter (Diamond Light Source): **No**

Plenary and Award Lectures

Bragg Lecture
Judith Howard, FRS
(Durham University)
Exploring a Century of Reciprocal Space: Same Old Theory - Endless New Results

Chair: **David Keen** (ISIS Facility)

Lonsdale Lecture
Henry Chapman (Center for Free-Electron Laser Science, DESY, Hamburg)
Macromolecular Crystallography with X-ray Laser Pulses

Chair: **Elspeth Garman** (University of Oxford)

Early Career Prize Lectures and Awards Ceremony
CCDC-CCG Young Scientist Prize Lecture
IoP Physical Crystallography Prize Lecture
BSG Prize Lecture
YCG-IG Prize Lecture

PSG Plenary
Malcolm McMahon (University of Edinburgh)
Extreme Crystallography in a Flash

Chair: **Ivana R. Evans** (Durham University)

CCG Plenary
Paul Raithby (University of Bath)
Understanding the Solid-State into the Next 100 Years

Chair: **Simon Coles** (University of Southampton)

IG Plenary
Joel Bernstein (NYU Abu Dhabi)
Crystallography@100: Learning from the Past and Trying to Look into the Future

Chair: **Cheryl Doherty** (Pfizer)

BSG Plenary
Neil Isaacs (University of Glasgow)
How Times Have Changed

Chair: **Peter Moody** (University of Leicester)

Session Lectures

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)

Stephen Hull (STFC Rutherford Appleton Laboratory)
In situ Neutron Diffraction Studies of Battery and Fuel Cell Materials

Jorge Sotelo (University of Edinburgh)
In situ Gas Adsorption Single-Crystal X-ray Diffraction Study: Understanding the Uptake Properties of a Sc-Based Metal-Organic Frameworks

Iñigo Vitórica (University of Manchester)
Gas Sorption in Non-porous Crystalline Materials

Bill David (ISIS and University of Oxford)
In-operando Diffraction Studies of Reversible Hydrogen-Storage Systems

Andrzej Katrusiak (Adam Mickiewicz University, Poland)
Pressure-induced Changes in the Hierarchy of Intermolecular Interactions

Simon Parsons (University of Edinburgh)
Elucidating Structure-property Relationships with High-pressure Crystallography

Nicholas Funnell (University of Oxford)
Hydrogen Bond Order/Disorder in a Polar One-dimensional Confined Ice

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)

Colin Pulham (University of Edinburgh)
Crystal Engineering of Energetic Materials – a Step Change in the Design of Safer Explosives and Propellants?

Neil Champness (University of Nottingham)
From Frameworks to Spheres – Exploiting the Co-ordination Bond

Kate Wittering (University of Bath)
Continuous-flow Crystallisation of Multi-component Systems of Pyrazine Carboxamide: A World Health Organisation (WHO) Essential Medicinal Compound for Tuberculosis Treatment

Andrew Maloney (University of Edinburgh)
Competition between Hydrogen Bonding and Dispersion Interactions in the Crystal Structures of the Primary Amines

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)
Just a Spoonful of Neutrons helps the Chemistry move on...

Dominic Fortes (University College London)
Analogue Materials for High-pressure Studies of Planetary Ices

Matthew Cliffe (University of Oxford)
Frustration and Disorder in Simple Molecular Frameworks

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)
Magnetic Structures – Representations, Space Groups and other Relatives

Alex Gibbs (University of Tokyo)
Phase Diagrams of $Ba_2M^{2+}Te^{6+}O_6$: Insight into an Intriguing Interplay between Crystal and Magnetic Dimensionalities

Paul Saines (University of Oxford)
Anisotropic Negative Thermal Expansion driven by Magnetoelastic Coupling in a Cobalt Adipate Antiferromagnet

Paolo Radaelli (University of Oxford)
Can Complex Magnetic Structures be used to Store and Retrieve Information?

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)
X-Ray Powder Diffraction in Context – Case Studies in Pharmaceutical Solid Form Selection

Philippe Fernandes (SAFC, Cambridge)
Routine XRPD Investigations on Active Pharmaceutical Ingredients

Mark Eddleston (University of Cambridge)
Probing the Mechanism of Aspirin Degradation

Pushing the limits: Faster

Free-electron lasers and single-shot synchrotron experiments.

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

Gebhard Schertler (Paul Scherrer Institut, Villigen, Switzerland)
Fast Protein Crystallography at the Future Free Electron Laser in Switzerland: SwissFEL

Petra Fromme (Arizona State University, USA)
Femtosecond Nanocrystallography of Membrane Proteins

Leonard Chavas (Center for Free-Electron Laser Science, DESY, Hamburg
Structural Femtosecond Crystallography Objectives at the XFEL.EU

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** (University of Bath)

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

Mark Warren (Diamond Light Source)
Collecting Time-resolved Data on I19

Helena Shepherd (University of Bath)
Exploiting Volume Change in Dynamic Phase Transitions

Rudolph Winter (Aberystwyth University)
Dynamic Strain Measurements after Shock Impact in Minerals and Ceramics

Pushing the limits: Smaller

The session will investigate the theoretical and practical limits for the measurement of useful diffraction data from micro- and nano-sized protein crystals at synchrotrons and FEL sources. Some consideration will be given to the implications of current developments in micro and nanocrystallography for users of these sources.

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

Colin Nave (Diamond Light Source)
Theoretical Limits for Micro/Nano-Crystallography and Comparison with Experiments on Synchrotron and FEL Sources

Robin Owen (Diamond Light Source)
Reaching the Practical Limit in Micro-crystallography: Current Best Cases and Future Outlook

Cornelius Gati (Center for Free-Electron Laser Science, DESY, Hamburg)
Title: TBA

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)

Marc Payne (BP)

Andy Doré (Heptares Therapeutics)

Simon Coles (University of Southampton)

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)

Joke Hadermann (EMAT, University of Antwerp, Belgium)
Mapping of Chemical Order in Inorganic Compounds

Yaroslav Khimyak (University of East Anglia)
Probing Intermolecular Interactions and Dynamics in Porous Host-guest Systems using Solid-state NMR

Anthony Phillips (Queen Mary, University of London)
Comparing the Dynamics of Coordination Polyhedra in a Metal-cyanide Framework

Martin Dove (Queen Mary, London)
Reverse Monte Carlo Method: Coupling Scattering Data with Computer Simulation

Manolis Vasileiadis (Imperial College London)
Prediction of the Polymorphs of axitinib using the CrystalPredictor and CrystalOptimiser Algorithms

Jerome Wicker (University of Oxford)
Predicting Crystallisation Propensity of Small Molecules

Pushing the limits: Larger

Viruses, complexes, etc.

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

Gabriel Waksman (Birkbeck College, London)
Pilus Biogenesis at the Outer Membrane of Bacterial Pathogens

Russell Wallis (University of Leicester)
Unravelling the Mechanism of Complement Activation via the Classical Pathway

Leonid Sazanov (Mitocondrial Biology Unit, MRC Cambridge)
Structure and Mechanism of Respiratory Complex I, a Giant Molecular Proton Pump

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

LOOKING TO THE FUTURE
CRYSTALLOGRAPHY@100
LEARNING FROM THE PAST

Logo designed by David Keen

Late Breaking Abstract Invitation

Deadline 17.00, Friday 7 March 2014.

Although the abstract deadline has now closed for submissions for an oral presentation at the forthcoming **BCA Spring Meeting**, the organisers have agreed to keep the abstract submission form open for **poster presentations only** until 17.00, Friday 7 March.

Please go to **http://hg3.co.uk/bca/abstracts invited.aspx** if you wish to submit a late breaking abstract.

BCA Annual Spring Meeting Programme 2014

	DAY 0: Monday 7 April 2014		DAY 1: Tuesday 8 April 2014		
09:00			CC.00.21	Room CC.01.09	Edward Herbert Building
09:15			YC4	Olex2 workshop	
09:30			Parkin Lecture: **Claire Murray**		
09:45					Registration
10:00			Chair: **Kate Wittering**		
10:15					
10:30			YC5: Are Crystallographers Still *Necessary? (Panel)*		
10:45					
11:00			Chair: **Anthony Phillips**		
11:15			**James France Exhibition Area**		
11:30			Lunch & Registration/Exhibition		
11:45					
12:00			**Lecture Theatre CC.00.11**		
12:15			12.00-12.50 Lonsdale Lecture: **Henry Chapman**		
12:30			Chair: **Elspeth Garman**		
12:45					
13:00	**Lecture Theatre CC.00.21**	**Room CC.01.09**	12.50-13.30 Break		
13:15	YC1	Olex2 workshop			
13:30	YC Chemical Plenary:		**Lecture Theatre CC.00.11**		
13:45	**Ian Oswald**		13.30-14.20 PCG Plenary: **Malcolm McMahon**		
14:00			Chair: **Ivana R. Evans**		
14:15	Chair: **Lucy Saunders**		Break 10 mins		
14:30			Sessions 14.30-16.00		
14:45			**Lecture Theatre CC.00.11**	**Lecture Theatre CC.00.21**	
15:00	Coffee	Coffee	*Crystal engineering*	*Non-ambient diffraction (I)*	
15:15	15.00-15.30	15.00-15.30			
15:30	**Lecture Theatre CC.00.21**	**Room CC.01.09**	Chair: **Lynne Thomas**	Chairs: **Emma McCabe & Ivana R. Evans**	
15:45	YC2	Olex2 workshop			
16:00	YC Biological Plenary		Coffee 16.00-16.30		
16:15	**Elspeth Garman**				
16:30			Sessions 16.30-18.00		
16:45	Chair: **Anna Polyakova**		**Lecture Theatre CC.00.11**	**Lecture Theatre CC.00.21**	
17:00	Break	Break	*Application of neutron diffraction in chemical crystallography*	*Non-ambient diffraction (II)*	
17:15					
17:30	**Lecture Theatre CC.00.21**	**Room CC.01.09**	Chair: **Samantha Callear**	Chairs: **Emma McCabe & Ivana R. Evans**	
17:45	YC3	Olex2 workshop			
18:00	YCG AGM		Break 10 minutes		
18:15	Flash presentations		**Lecture Theatre CC.00.11**		
18:30	Chairs: **Sarah Gurung**		18.10-19.00 CCG Plenary: **Paul Raithby**		
18:45	**& Nick Funnell**		Chair: **Simon Coles**		
19:00	**James France Exhibition Area**		**James France Exhibition Area**		
19:15			Buffet Dinner, exhibition and posters		
19:30	Young Crystallographers' Buffet				
19:45	Dinner & Poster Session				
20:00					
20:15					
20:30					
20:45					
21:00					
21:15					
21:30					
21:45					
22:00					

BCA Annual Spring Meeting Programme 2014

DAY 2: Wednesday 9 April 2014

Lecture Theatre CC.00.11

9.00-9.50 IG Plenary: **Joel Bernstein**
Chair: **Cheryl Doherty**

Coffee 9.50-10.15

Session 10.15-12.15

Lecture Theatre CC.00.11

Early Career Researcher Prize Symposium

CCDC-CCG prize
BSG prize
IoP-PCG prize
IG -YCG prize

CC.00.11	CC.00.13	CC.00.21
12.15-12.45: ***PCG AGM***	12.15-12.45: ***BSG AGM***	12.15-12.45: ***IG AGM***
12.45-1.15: ***CCG AGM***	**James France Exhibition Area**	
	12.15-13.30 Lunch, Exhibition	

Sessions 13.30-15.00

CC.00.11	CC.00.13	CC.00.21
XRD in the pharma-ceutical industry Chairs: **Cheryl Doherty & Peter Wood**	*Pushing the limits: Faster* Chairs: **Henry Chapman & Peter Moody**	*Magnetic structure determination* Chair: **Emma McCabe**

Coffee 15.00-15.30

Sessions 15.30-17.00

CC.00.11	CC.00.13	CC.00.21
Dynamic processes and reactions Chair: **Paul Raithby**	*Pushing the limits: Smaller* Chair: **Gwyndaf Evans**	*Getting a job* Chairs: **Elizabeth Shotton & Anna Warren**

Break 10 minutes

Lecture Theatre CC.00.11

17.10-18.00 Bragg Lecture: **Judith Howard, FRS**
Chair: **David Keen**

Lecture Theatre CC.00.11

18.00-19.00: ***BCA AGM***

Comfort time

The Village Restaurant

Conference dinner 19.30 for 20.00

DAY 3: Thursday 10 April 2014

Lecture Theatre CC.00.11

9.00-9.50 BSG Plenary: **Neil Isaacs**
Chair: **Peter Moody**

Coffee 9.50-10.15

Sessions 10.15-11.45

CC.00.11	CC.00.21
Complementary non-diffraction techniques (I) Chairs: **Ivana R. Evans & Graeme Day**	*Pushing the limits: Larger* Chair: **John Schwabe**

Break 15 minutes

Sessions 12.00-13.30

CC.00.11	CC.00.21
Complementary non-diffraction techniques (II) Chairs: **Ivana R. Evans & Graeme Day**	*Pushing the limits: Slower - the X-ray limits* Chair: **John Helliwell**

Close 13.30

09:00 09:15 09:30 09:45 10:00 10:15 10:30 10:45 11:00 11:15 11:30 11:45 12:00 12:15 12:30 12:45 13:00 13:15 13:30 13:45 14:00 14:15 14:30 14:45 15:00 15:15 15:30 15:45 16:00 16:15 16:30 16:45 17:00 17:15 17:30 17:45 18:00 18:15 18:30 18:45 19:00 19:15 19:30 19:45 20:00 20:15 20:30 20:45 21:00 21:15 21:30 21:45 22:00

Opening Ceremony of the International Year of Crystallography

A century after Laue's Nobel Prize, the United Nations declared 2014 to be the International Year of Crystallography. I was lucky enough to attend the opening ceremony at the UNESCO building in Paris. My wife Joan was also present and has provided all the photographs on the cover and in the photo spread. The perceptive welcoming comments made us feel good about the way that crystallography underpins all the sciences and is still fresh at the age of 100. On behalf of the Organizing Committee of the International Year of Chemistry 2011 Nicole Moreau made a telling comment: many members of the public don't like chemicals but think crystals are magic! We also learned that ambassadors should be called "Excellency", and we pretended to be ambassadors ourselves as we listened to simultaneous translation on the headphones provided. Along with past achievements, the potential of crystallography particularly In the developing countries received emphasis. Examples include: to quantify the minerals present in an ore for efficient processing, to determine the structure(s) of the active chemical(s) in traditional medicines, and to identify the materials used in art works to guide conservation procedures. UNESCO and equipment manufacturers are setting up a series of "open laboratories. The first such labs have been made ready for use early in 2014 in Argentina, Ivory Coast, Morocco, South Africa and Uruguay. Scientists from these countries and their neighbours within these regions will be able to work with and learn from local staff and apply crystallography to their research.

Next we had an excursion into crystallographic history. **Jenny Glusker** told us that the Vikings may have been early crystallographers, using the birefringence of calcite to locate the sun from the polarisation of its light for purposes of navigation on cloudy days. She reminded us that already in 1665 **Robert Hooke** envisaged sphere packing in crystals. Turning to modern times, she showed how technical advances by **Patterson**, **Bijvoet** and the pioneers of neutron diffraction led to important results in structure determination.

Philip Ball introduced a different aspect of history. He displayed a photograph of the participants at the Solvay Conference held in Brussels in 1913 with "The Structure of Matter" as its theme, inevitably dominated by the new information arising from crystallography. Participants, including **Laue**, **W. H. Bragg**, **Einstein** and **Marie Curie**, sat or stood in groups of mixed nationality. This collegiality in search of knowledge was shattered by World War I, and most German scientists were excluded from the next conference in 1921. As a display of rebuilt consensus today, a panel of young crystallographers from around the world was introduced. Wisely, they all had prepared videos introducing themselves and their research. In the ensuing panel discussion they outlined their aspirations and the obstacles that might prevent their accomplishment. A recurring theme was that for young crystallographers to attack challenging problems, they need to be given patient long-term support and timely access to the required facilities.

The first of a set of lectures presenting splendid achievements of modern crystallography was given by **Brian Kobilka**, the winner of a 2012 Nobel Prize. Having trained and begun his career as a medical doctor, he came to the conclusion that crystallography was absolutely essential to the research he wanted to do. He described work on the structure of G-protein coupled receptors. These large complicated molecules transmit signals across cell membranes. They are involved in our senses of vision, smell and taste, and they are the targets for about half of the drugs in current medical use. Knowing their structure should make it possible to design more specific drugs with fewer side effects. To determine the structures in the inactive and activated states, numerous obstacles had to be overcome, starting with the need to make enough protein, extract and solubilize it. Even pure protein has a variety of conformations, making it difficult to obtain crystals of sufficient size and quality. Thanks to pooling of knowledge, even between "rival" groups, and the development of the microfocus beamline at ESRF, structure determination became possible.

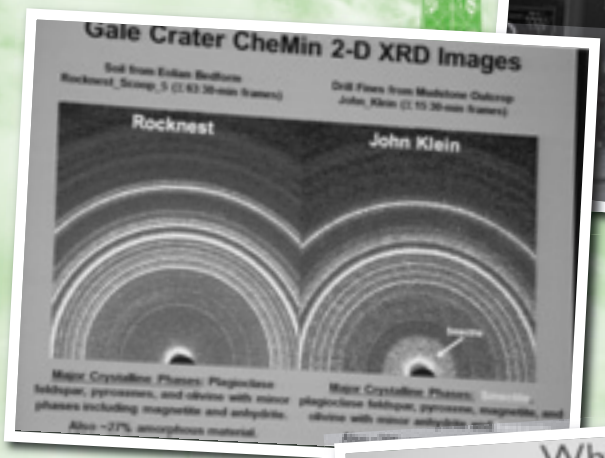
Presentations followed about crystallography in the BRICS countries (the usual Brazil, Russia, India, China plus South Africa). It was noteworthy that important funding for this meeting was being contributed by the governments of India, South Africa and Brazil. If such persuasion were still needed, these presentations certainly served to persuade those of us from the "First World" that these nations are emerging major powers in crystallography. It is hoped that their example will inspire other Third World countries.

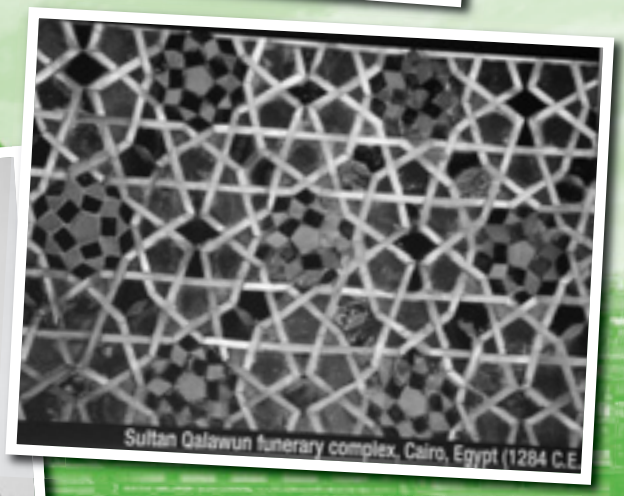
The next morning, **John Spence** told us the story of the X-ray free-electron laser (XFEL). This was initially seen as a very bold, even foolhardy idea: to spend $600 million on a device that, even if it worked, would blast your crystal to smithereens. The method began to look feasible after the discovery that with very brief pulses diffraction occurs before radiation damage spreads out, and the design of a submicron droplet injector ensuring a continuously refreshed sample of nanocrystals. Based on a repurposed linear accelerator at Stanford, the first XFEL became operational in 2009 and provided 10^{12} photons per pulse. It has now become possible to get data to 1.9 Å resolution, to do time-resolved crystallography on macromolecules involved in photosynthesis and to study large viruses like mimivirus.

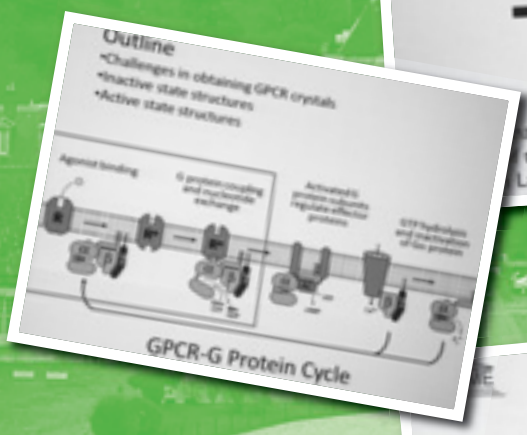
continued on page 14 ▼

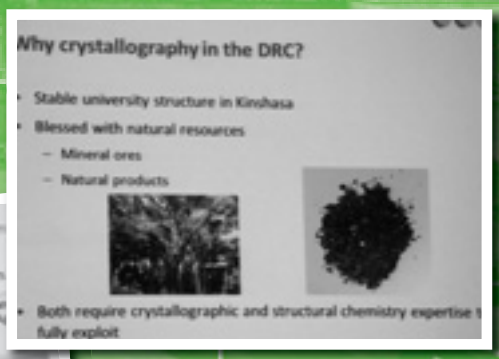
Images from the Opening Ceremony of the International Year of Crystallography

UNESCO Headquarters • Paris • 20-21 January 2014









Martijn Fransen grabbed our attention with a display of the enormous crystals in the Naica mine in Mexico. Then he presented a series of very practical applications. Iron ore bodies vary in their iron content and have traditionally been graded visually as "low-grade" or "high-grade". Powder X-ray diffraction gives more precise classification, leading to a consistent feed for efficient processing. Metal components in systems like aircraft where metal fatigue could be disastrous are often pre-loaded with compressive stress to prevent the growth of any micro-cracks that might form. This can be verified by X-ray techniques. In layered microelectronic devices the unit cells must be forced to match. Finally, polymorphism must be monitored and controlled if pharmaceuticals are to have consistent properties. Martijn made it very clear to the non-crystallographers in the audience that devices on which people in all parts of the world depend, such as mobile phones, would be impossible without crystallography.

Juliette Pradon from CCDC perfectly illustrated the main practical point of this meeting. We keep seeing depressing reports on our television news about war and atrocities in the Democratic Republic of Congo (DRC). It is much less well known that the University of Kinshasa has maintained a stable environment through the troubles. CCDC has formed a partnership with this university, providing the Cambridge Structural Database and other computational chemistry resources and supporting two postgraduate students. A research student was trained in Cambridge and then returned to Kinshasa, cascading the knowledge that had been obtained. Their research has developed valuable new information about the intermolecular interactions of selenium and tellurium. Scope also exists for sabbatical visits from the DRC to CCDC.

Next came two lectures about another great achievement of crystallography. We heard from **David Bish** and **David Blake** about the miniature X-ray laboratory aboard the Curiosity rover now on Mars. Starting from 1990-era X-ray equipment, about the size of a cooker and weighing about 550 kg, it was miniaturised until it would fit into a shoebox. A video showed the spectacular launch of Curiosity, followed by an artist's impression of the landing on Mars. A sample taken at the landing site, "Rocknest", contained only minerals of volcanic origin, resembling those found at Mauna Kea in Hawaii. However, after Curiosity had driven closer to the layered Mount Sharp, another sample, "John Klein", contained clay minerals. Since, as far as we know, clay can only form in water, there must have once been water on Mars.

Important equipment manufacturers have been generous not only to the "open labs" but also in support of this meeting. They were given opportunities to make general points about the development of crystallographic apparatus, inevitably illustrating them with their own offerings. One talk by **Frank Burgäzy** provoked widespread mirth. Three days after **Wilhelm Röntgen** discovered X-rays, he was visited by **Max Gebbert**, who thereafter joined Siemens to produce X-ray tubes. Röntgen wrote a letter trying to persuade them that if they lowered the price, they would sell many more units. Plus ça change…

The importance of crystallography to the understanding and conservation of art and architecture followed. **Philippe Walter** showed how crystallography gives useful insight into the preparation of pigments with four objectives: (1) to compile a list of pigments available in a given place and period, (2) to identify their sources from the impurities and thereby map the trade of pigments, (3) to define the physical properties of paint matter, and (4) to monitor chemical modification occurring over time.

Next, we were treated to a dazzling display of Islamic ornamental art: western Islamic art by **Abdelmalek Thalal** and eastern art by **Emil Makovicky**. An analysis in terms of modern mathematics by **Peter Lu** followed. The patterns went by too fast for my by now fatigued eyes and mind to follow the details of the symmetry, but the beauty was awe-inspiring and it was clear that the designers had been able to incorporate decagons into their patterns long before crystallographers had thought about quasicrystals.

As Editor-in-chief of the journals of the International Union of Crystallography, **Samar Hasnain** gave us the good news about the successful launch of IUCrJ, the fully open-access journal that is now publishing high-quality structural science papers.

A talk by **Chris Llewellyn Smith** was very inspiring. Data for the structure determination of complicated macromolecules should nowadays be obtained with a synchrotron. However, there is no synchrotron anywhere in the Middle East. The SESAME project to build one is run by a set of countries, some usually thought of as enemies. Currently it includes the following 9 members: Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority, and Turkey, but more countries are still welcome to join. Germany donated the useful bits of the obsolete BESSY synchrotron, a design team including Israeli and Iranian engineers defined what additional equipment would be needed, and various countries donated it. Jordan provided the building. It is hoped that professional scientific collaboration will lead to personal friendships and, eventually, better political understanding. This was the long-term objective when CERN was established in the aftermath of World War 2. As a former Director General of CERN, Chris could report that it has been triumphantly successful in both scientific and interpersonal terms. It serves as a model for SESAME.

The director of UNESCO's Division for Basic and Engineering Sciences, **Maciej Nalecz**, concluded by exhorting us to continue the enhanced emphasis on crystallography long beyond 2014. In particular, the open labs should create hubs for training a whole generation of crystallographers.

This upbeat meeting combined fascinating science with international good fellowship. There was just one downside: the atrocious timekeeping, with some sessions running hours late, not just minutes. The Excellencies did not help when they trooped into the first session 17 minutes late. If the main speakers exceeded their allotted time, I didn't notice because most of their talks were so interesting and so well presented. I attribute most of the blame to the session chairs, who felt impelled to present the research done in their own groups or countries at considerable length before getting on with the job of introducing the speakers or summarising their results. A shining counter-example was **Judith Howard**, who summarised **Brian Kobilka**'s talk briefly and to the point by just mentioning the extreme technical difficulties in studying such membrane proteins and the importance of collaboration in surmounting the difficulties.

Carl Schwalbe

Swiss Post commemorates the International Year of Crystallography

The two commemorative stamps (pictured) will become available and valid for postage on 6 March 2014.

Stamp collectors can order them at www.post.ch/philashop .

BCA 2104 AGM

THE 2014 Annual General Meeting of the British Crystallographic Association will be held in the James France building at the University of Loughborough at 18:00 on April 9th 2014.

Elections

Elections for several positions on Council will be held at the AGM: the Treasurer (**Pamela Williams** completes a 3-year term); one ordinary member (**Amber Thompson** completes a 3-year term); and the newly created post of Education and Outreach Coordinator will be elected for the first time.

Nominations for any of these vacancies may be made by any two members and should be accompanied by the written consent of the candidate to serve if elected. Nominations must be received by the Secretary (secretary@crystallography.org.uk) not less than 4 days before the AGM (i.e. by April 4th)

Pamela Williams has been nominated by **David Keen** and **Richard Cooper** for the post of Treasurer.

Education and Outreach Coordinator

The position of Education and Outreach Coordinator was created as an elected role at the last AGM with the required changes to the statutes. A description of the role follows the Agenda and is also available at http://crystallography.org.uk/education-and-outreach-coordinator-description

Draft Agenda

1) Approval of Agenda
2) Apologies for Absence
3) Minutes of last AGM
4) President's Report
5) Secretary's Report
6) HG3 Report
7) Report of the Treasurer to include Presentation of the Accounts for 2013 and the Examining Accountant's Report
8) Acceptance of the Accounts
9) Appointment of Examining Accountant for 2014
10) Elections to Council
11) Honorary Members
12) Any other business

British Crystallographic Association Education and Outreach Coordinator

THE elected position of Education and Outreach Coordinator was formally added to the BCA Statutes at the AGM in 2013. Previously the BCA President had appointed an Education Coordinator who was also co-opted onto Council.

At the same AGM, the BCA Bye-Laws were revised to outline the role of the Education and Outreach Coordinator: "The Education and Outreach Coordinator shall take primary responsibility for the coordination of the education activities of the Association and the promotion of Crystallography to the scientific community and the general public. The overall responsibility for crystallographic education and outreach shall rest with the Council collectively."

This purpose of this document is to further develop the above role description, to set out what the role entails and to explain how the Education and Outreach Coordinator will interact with counterparts from the individual BCA Groups.

The Role

The role of the Education and Outreach Coordinator is to coordinate activities that are aligned with of the educational remit of the BCA. Statute A.2 defines this remit very broadly: "The purpose of the Association is to advance the education of the public in the science of crystallography particularly within the British Isles."

The Education and Outreach Coordinator will coordinate activities with Education Representatives of each of the BCA Groups, and any other interested parties. The Education and Outreach Coordinator may convene and chair a working group of these representatives, outreach volunteers, and representatives of other organisations for the purposes of coordinating outreach and education projects.

Definitions:

public engagement	activities to increase awareness of crystallography and its impact to non-specialist audiences, which may include, amongst others: the general public; teachers; politicians.
education	activities or resources designed to teach aspects of crystallography, or to assist others to teach, within an existing educational curriculum at any level from pre-school to post graduate.
outreach	activities to encourage studying or work in crystallography and related sciences, aimed at people who may not otherwise consider this path of study or career.

Example of activities undertaken or coordinated by the BCA Education and Outreach Coordinator include, but are not limited to:

- organisation of public engagement events to increase awareness of crystallography
- development of resources for public engagement (e.g. posters, print, web, videos)
- highlighting of existing resources for public engagement (e.g. web sites and videos)
- organisation of outreach events and talks (schools)
- engagement with target groups through social media as appropriate
- liaison with national and international organisations for coordination of outreach and education projects (e.g. the Royal Institution, Cambridge Crystallographic Data Centre, Protein Data Bank, museums, funding agencies, etc.)
- preparation of grant proposals to support public engagement and outreach as appropriate

Responsibilities

The Education and Outreach Coordinator will submit a report to the biannual BCA Council meetings and will communicate closely with the President or another nominated officer during the rest of the year.

Commitment to undertake high profile projects should be given only with the agreement of the BCA Officers or Council, as appropriate.

Commitment to undertake projects that require financial support from or underwriting by the BCA should be given only with the agreement of the BCA Officers or Council, as appropriate.

Election of a candidate to this role at a BCA AGM will not mandate the BCA, Council or Officers to approve or fund any specific projects.

Related Roles

The primary purpose of the BCA, as set out in its statutes, is to advance the education of the public in the science of crystallography. To ensure that each Group has the opportunity to engage with the educational activities of the Association, an Education Representative will be nominated by each Group to liaise and work with the BCA Education and Outreach Coordinator. The range and scope of activities undertaken by each Education Representative may include: organisation and attendance at educational events; development of outreach or teaching resources; contribution of ideas to the BCA Education and Outreach Coordinator.

Biological Structures Group

BCA BSG Winter meeting 2013, Kings College London

THIS year's Biological Structures Group winter meeting was organised by Mark Sanderson and Yu Wai Chen, hosted at Kings College London, and focused on macromolecular structures in the Bragg Centenary Year. Structures of macromolecules have become essential for understanding biological processes as well as providing a platform for drug and vaccine design. Approximately 100 years since the publication of Bragg's Law, X-ray crystallography is one of the most widely recognised techniques for molecular biologists.

The day started off with a fantastic presentation from **Bonnie Wallace** of Birkbeck College London on the structure and function of voltage-gated sodium channels. Her work on these challenging membrane proteins spanned over a decade and included several spectroscopic techniques including high resolution synchrotron circular dichroism (CD). The results of the CD experiments tied in nicely with a series of crystal structures obtained many years later of the various states of the ion channel. These data, along with detailed molecular dynamics (MD) simulations, provided a complete picture of the action of the channels which are a key target in many human diseases as well as being the targets of many commonly used insecticides.

Dave Stuart of Oxford University and the Diamond Light Source spoke about his work on understanding picornavirus structure. The Picornaviruses include the causative agents of the common cold, foot-and-mouth disease and polio. The impressive use of 3D graphics instantly showed the lifecycle

of these viruses and highlighted where this work contributes and what stages might provide viable drug targets. We were also reminded of the massive advances in X-ray diffraction from virus crystals, from Dorothy Hodgkin's tobacco necrosis virus diffraction image that took a 90 hour exposure to more recent diffraction images taken at Diamond from a 0.1 second exposure. High resolution crystal structures of the virus particles allowed for the observation of a pocket which retains an amphipathic molecule that could possibly be replaced with a drug molecule that would stop the progression of the viral life cycle. *In silico* drug design was used and validated to show that designing drugs for viruses is viable.

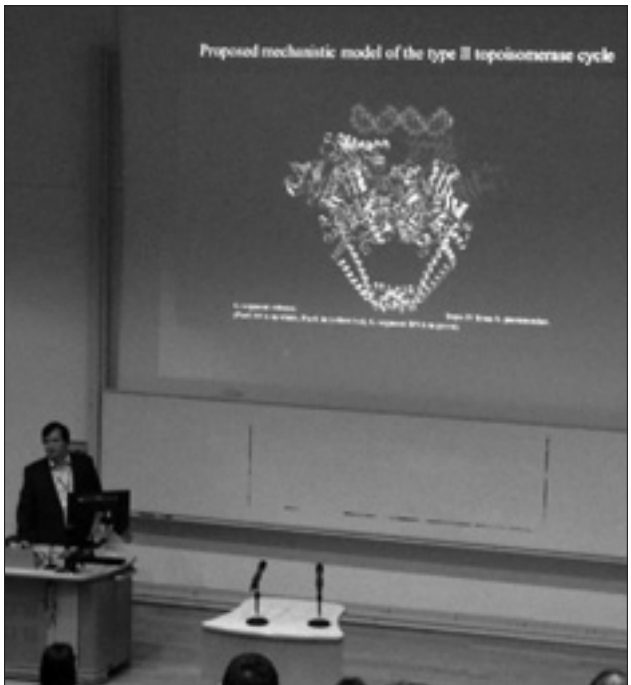
With a great increase in the interest of X-ray Free Electron Lasers (XFEL) for macromolecular crystallography, **James Naismith** from St. Andrews University told us about the UK's plans for XFEL access and instrumentation. The UK's prestigious and significant contribution to X-ray crystallography was highlighted, spanning many decades from **Max Perutz** and **Ian Kendrew** to **Venkatraman Ramakrishnan**, and encompassing projects such as CCP4 and Instruct. With the plan to set up a hub at Diamond to help people learn about the practical challenges of using the XFEL and the design of a UK beamline, the clear synergy between the two sites is clear. With the increasing desire of UK groups to collect XFEL data it was great to see that we are getting involved and there will be fantastic support for the biological community.

After lunch, **Ivan Laponogov** of Kings College London spoke about the structural studies of type II Topoisomerase, the enzyme responsible for controlling the DNA supercoil within cells. The structure and function of this enzyme is important as it is currently a target for the development of novel antibiotics. A series of crystal structures of the enzyme in complex with DNA, drug molecules and magnesium revealed how the DNA is cleaved together with the mode of action of bound drugs. An interesting experiment they performed was to soak the crystals in EDTA to remove the magnesium and reveal additional states of the reaction and distortion to the DNA. These complex structures not only revealed the detailed and complex mechanism of the enzyme but also provide a platform for rational drug design. The X-ray crystal structure of the complex including the ATPase domain was also presented which led to a model of how the T-gate DNA is clasped.

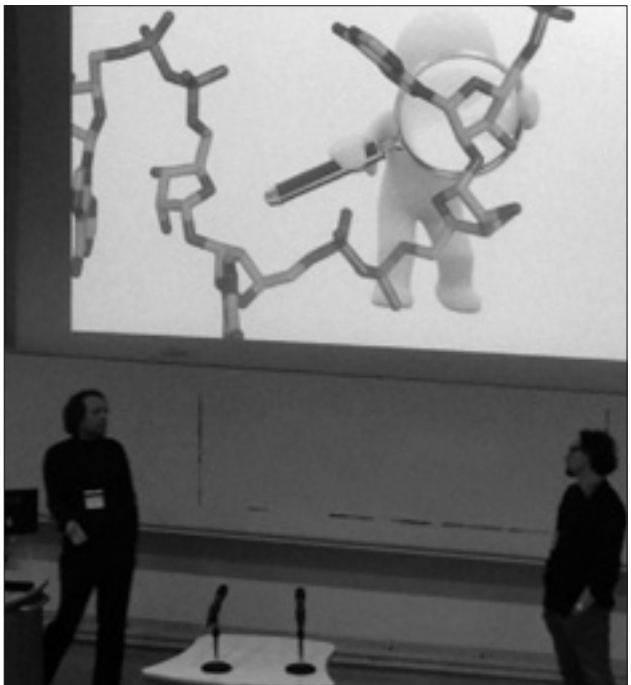
Continuing with nucleic acid complexes, **David Leys** from Manchester University presented his work on Poly-ADP-ribose glycoside hydrolase (PARG). This enzyme, along with PAR-polymerase (PARP), is involved in signalling DNA damage in eukaryotic cells and resulting in apoptosis of the cell. An extensive search for structural homologues of the human enzyme led to the discovery of bacterial proteins with similar action and structure. High resolution X-ray crystal structures showed the fold of the protein and where a single PAR molecule binds. When they finally received poly-PAR molecules there was only enough for 10 crystallisation trials which provided an interesting challenge for the team. Remarkably they succeeded in generating crystals of the complex and were able to reveal the action of the enzyme.

Stefano Pernigo from Kings College London shared his work on Kinesin-1. This protein is responsible for the traffic of anything from proteins up to whole organelles toward the cell membrane. An important factor for correct transport is the recognition of the cargo by the Kinesin. A common, W-acidic, motif was identified among multiple transported proteins and binding assays revealed that polypeptides containing the motif only bound with high affinity in low salt, a challenge for crystallography. However, crystals of the ligand bound TPR recognition domain were obtained and the structure showed the tight binding interface conformational change upon binding. Complementary work using mutatgenesis and in cell assays confirmed that this was indeed the binding site for the W-acidic motif.

Finishing off the day of talks was **Liz Carpenter** from the Structural Genomics Consortium (SGC) who shared her work on human membrane proteins and more specifically a membrane embedded zinc metalloprotease, ZMPSTE24. The statistics from membrane protein crystal structures were an



Ivan Laponogov


David Leys

eye-opener in terms of the amount that never make it through the pipeline: from 186 proteins forming 1800 constructs, only a handful now have structures. ZMPSTE24 has been implicated in premature ageing disease, such as progeria, as well as natural ageing through the build-up of membrane bound lamins. Normal, active ZMPSTE24 cleaves the farnesylated lamin producing a soluble protein which is no longer retained on the membrane. The structure of ZMPSTE24 revealed a huge 12,000 Å^3 cavity inside the protein where the active site resides. The future aims of the project were to obtain ligand bound crystals to understand the role of the cavity and the protein binding site and to map disease related mutations onto the structure with the aim of developing novel ageing therapeutics.

The day's talks highlighted what X-ray crystallography has contributed to the field of biology, what it will contribute in the future and the direction that this century old technique is heading with the constant advances in X-ray sources and capabilities. The common use of *in silico* drug design and MD demonstrated how macromolecular structures can be used to understand drug binding, enzymatic action and the nature of the large complexes in solution.

We would like to acknowledge **Mark Sanderson**, **Yu Wai Chen** and **Brian Sutton** together with the excellent support provided by HG3 and Kings Events.

Richard Martin, Ph.D student University of Portsmouth

Photos: **John McGeehan**

Stefano Pernigo

Liz Carpenter

The local organising committee at Kings College London with some of the speakers

Diamond MX User Meeting

THE Main CCP4 meeting was preceded as usual by the Diamond MX User Meeting. Chaired by David Lawson, Dave Hall opened proceedings with an overview of current and upcoming facilities at our UK synchrotron and pointed us in the direction of the website where all current information can be accessed (www.diamond.ac.uk/mx). The hardware has been under continual development and all beamlines now boast a Pilatus detector, with the 100Hz model already available on I24. The automated data collection and processing is now very stable and remote access is available on all beamlines at all times, with prior discussion being advised. This mode has become a very popular option and following user requests, there has now been implemented a process for shipping your dewars directly via the Diamond account. Many users are now embracing *in-situ* collection, and several novel structures have recently been solved using this method. This will be further enhanced with I24 undergoing an end-station upgrade to allow automated switching between pins and plates. New beamlines, such as the long-wavelength I23 project, are well underway. It has already achieved first-light in the hutch and will take first users later on in 2014, engaging the community with a workshop in October 2014. I04-1 will be adapted for HTP fragment screening while in the longer term, we look forward to the new VMX stations that will allow sub-micron variable focus capabilities and dedicated in-situ capabilities.

Ralf Flaig promoted the use of the mini-kappa device that is currently integrated on the I04-1 diffractometer and also available on I04. The instrument, that allows the re-orientation of the crystal while mounted on the beamline, has a number of advantages including: improved sample-sample comparison; improved data completeness for low symmetry space groups and the avoidance of overlaps with large unit cell parameters; utilisation of symmetry to reduce total exposure and therefore reduce radiation-induced damage; collection of a Bijvoet pair on the same image for improvement of weak anomalous signals. The system now benefits from a newly upgraded user interface within GDA.

Robin Owen presented the latest applications of the new breed of ultra-fast detectors with the 100Hz Pilatus 6M and tests on the 500Hz model. Robin reiterated that the rule of thumb for fine phi-slicing (XDS-determined mosaicity / 2) remains the best strategy for these detectors. He also recommended that the dose on the crystal should now be controlled by reduction in exposure time rather than the traditional attenuation of the X-ray beam, vastly reducing collection time without any impact on data quality. Robin also revealed the lag phase observed in radiation induced damage during room-temperature collection, opening up the possibility of significantly outrunning these damaging processes by employing high frame rates.

Martin Walsh gave us an update on the UK contribution to the billion-Euro European XFEL through participation in a user consortium which has successfully received funding to build a beamline for structural biology exploiting the intense pulsed x-ray source of the European XFEL. The SFX (Serial Femtosecond Crystallography) beamline that will be delivered by the user consortium is the only planned dedicated MX beamline at an XFEL facility. The UK has put up a 28% stake in financing the construction and commissioning via a 5 year grant from the RCUK and Wellcome Trust and will take the lead role in the project. The application of serial femtosecond crystallography is likely to make a huge impact on the field; and in order to support the UK involvement, a new UK Hub for the European XFEL will be based at Diamond. The UK HUB will in the first instance support users to access currently available facilities based at LCLS (USA) and at SACLA (Japan); since beamtime is limited, the Hub will facilitate the submission of highly competitive proposals by UK users and aid in data reduction and analysis and management of the high data volumes generated by user experiments. In addition to the user program, the Hub will contribute to the development of novel ways of presenting samples to the XFEL beam and sample environments at the SFX beamline as well as software development for data reduction and analysis of XFEL data. Martin encouraged the community to support this endeavour and consider how these new technologies may benefit your projects.

The second session was chaired by **John McGeehan** who introduced **Jun Aishima**. He presented an overview of the current automated processing utilising the fast-dp and xia2 pipelines and the advantages of utilising re-processing via the DAWN interface. A straw-poll of the audience suggested that most users perform re-processing of their data at home but a few take advantage of the multi-cluster processing power available at Diamond. The recommended route to this is via an NX client, and details are available on the website for how to install and access data remotely. The selection of portions of data together with adding *a priori* information was seen to produce significantly improved data in some cases, and this could be achieved using minor modifications to the current pipeline scripts.

James Doutch provided us with an overview of the SAXS facilities available at Diamond. Upgrades to I22 include a new Pilatus 3-2M detector, a newly designed beamstop and scatterless slits. Furthermore, the second SAXS beamline, B21, designed for routine biological use, has now been commissioned. The first user data collected by Dr **Andy Pickford** (University of Portsmouth) on radiation sensitive matrix-metalloproteinases was presented demonstrating the high quality beam and end-station design. Future upgrades this year include an automated camera distance setup and the possibility of both in-line HPLC and multi-angle laser light scattering.

In the final session, **Andrew Thompson** gave us an overview and update on the MX facilities available at Soleil. Their two MX beamlines, Proxima 1 and 2, run an enhanced version of MXCube (as used by the ESRF) and are both equipped with CATS robots. Andrew reports a high uptake of the use of their mini-kappa device for crystal re-orientation. Andrew also noted that the focus of the MX beamlines at Soleil is for the careful and considered experimental approach that can offer some advantages to some of the HTP approaches used on other beamlines. There is clear synergy between the two approaches and users were welcomed to the facility.

The meeting ended with a lively user discussion chaired by the Diamond MX User Representatives, **David Lawson** and **John McGeehan**, who both promoted and encouraged continued user feedback.

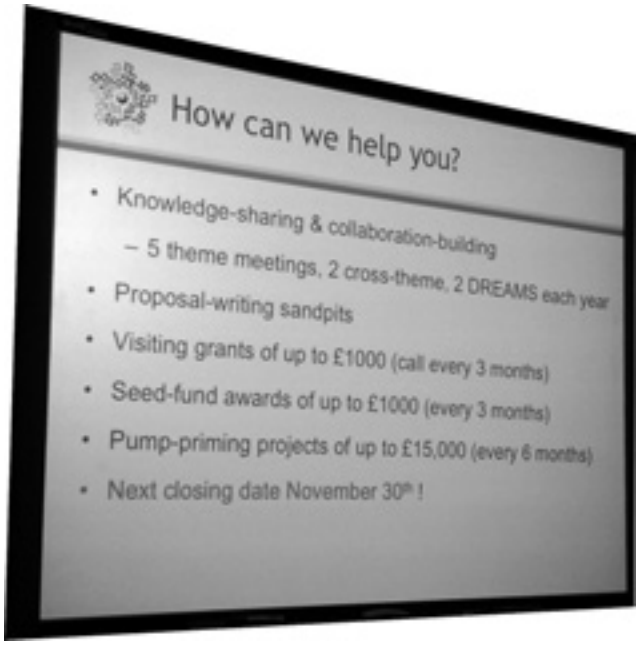
CCP4 Study Weekend, "Complementary Methods – a two way street"

Proceedings of this event with articles up to 6 pages in length contributed by the speakers will be published in a special issue of *Acta Crystallographica*, Section D.

Chemical Crystallography Group

Chemical Crystallography Group Autumn Meeting

THE CCG Autumn Meeting entitled 'Increasing Complexity in Crystal Engineering of Materials' was this year co-hosted with the Directed Assembly Grand Challenge and held at the Rose Bowl in Leeds Metropolitan University on 20th November, 2013. A stellar line-up of speakers drew on a broad range of scientific research to address various aspects of how we can begin to engineer highly complex materials via a number of strategies and how we can begin to predict this complexity. We are very grateful to Bruker AXS for their kind sponsorship of this meeting and also to Louise Male (CCG secretary) and Simon Coles (CCG chairman) for their efficient management and organization of such an interesting program. After Simon Coles and Jenny Woods (Directed Assembly Network coordinator) opened the meeting and gave a brief background to the Directed Assembly Grand Challenge and Network, the day's talks began with Harry Anderson (University of Oxford). He described the synthesis of large macrocyclic porphyrin assemblies via a number of templating stratagies ranging from large rigid template molecules through flexible cyclodextrin templates to 'vernier complexes'. These strategies allowed the production of massive rings containing up to 24 porphyrin units which can in turn be used as templates to produce structures mimicking the light harvesting structures in photosynthetic assemblies found in nature. Next up was Howard Colquhoun (University of Reading) who recounted his studies of infinite π stacks of alternating electron- rich and electron-poor rings and thus how guest molecules can cause a 'breathing' effect on interleaved complexes such as paraquat and diquat. This developed into searching for ways to exploit this via ring opening chemistry and through the use of molecular 'tweezer' moieties to join oligomers to form high molecular weight polymers.



Lunchtime presented a chance to meet new faces and catch up with old friends and was followed by a talk from **Euan Brechin** (University of Edinburgh) describing his work with single molecule magnets. He showed how the use of "dirty solvents" (a mixture of every miscible solvent available) can lead to serendipitous self-assembly as the "molecule picks its own complementary solvent". The remainder of the talk focussed on the variety of modifications his group had carried out on the triangular $[Mn^{III}_3]$ antiferromagnetic complex in an effort to turn it ferromagnetic including ligand modification and application of high pressure. The second talk of the afternoon was given by **Jonathan Nitschke** (University of Cambridge) who showed the use of stoichiometry of simple precursors to control the formation of desired final metal-organic cage products. This formation occurs because the left-over reactants are unable to form forbidden products. The product distributions of these systems can be modified with additional reagents or by adding different metals, and unstable molecules can be stabilized by confinement within these cages. Additionally there is some potential as a separating medium as large cubic cages are able to accommodate large guests such as fullerenes. After coffee the final session began with **James McKenzie** (University of Sheffield) explaining the difficulties of using intermolecular interactions to predict and thus manipulate properties in novel materials. He is looking to correlate two parameters, α (H-bond donor) and β (H-bond acceptor) with propensity of H-bond formation. His initial studies using the CSD calculated propensity value yielded no correlation and alternate methods of determining αβ are also problematic, but he is continuing to look for patterns using the CSD. The final speaker of the day was **Andy Cooper** (University of Liverpool) who talked about functional organic porous crystals and whether they are predictable and thus able to be designed or simply waiting to be discovered. His work has shown that subtle changes in ligands can have a large effect on the final cage structure, however collaborative work has shown that despite some problems it is possible to, *in-silico*, design a cage from starting reagents, compute its most stable geometry and compute how it will pack and from there compute its physical properties. **Paul Raithby** (Directed Assembly Grand Challenge PI) brought this highly successful meeting to a close by highlighting the inspirational and elegant chemistry presented here and emphasizing the 'future is exciting' and that the vision for directed assembly is a long term one. I would refer any readers interested in a more in-depth write-up of this meeting to **John Warren**'s excellent blog at http://blog.x-rayman.co.uk/2013/11/27/bca-ccg-autumn-meeting-increasing-complexity-in-crystal-engineering-of-materials/

Graham Tizzard and the NCS team

Industrial Group

IG Autumn Meeting 2013 at Diamond, Didcot

Mineralogy and Materials

Chairs: **Cheryl Haidon** & **Richard Morris**

All three presenters described their use of different beam lines available at the Diamond Light Source.

1. **XRD; the adjustable spanner in the material consultant's tool box, Andy Smith, CERAM.**

Andy presented an overview of Ceram, and described their core business interests; customer product development and innovation, problem solving and adding value to customer processes. The XRD services provided by Ceram include: phase identification e.g. quartz / cristobalite / tridymite for silica, phase quantification, % crystallinity, Rietveld Structure Refinement, Grazing Incidence XRD, measurement of layer thickness using X-Ray Reflectivity (XRR) and small area analysis and phase mapping by Micro X-ray Diffraction (μXRD).

One major area of expertise is in the analysis of brick raw materials and finished product for the construction industry. During the last forty years or so Ceram have created a database that allows them to predict the properties of any given brick formulation and the likely crystalline components that are produced during manufacture – "time temperature transformations". Their expertise in brick analysis helped forensic specialists and police detectives solve two murders!

2. **Keeping a greener world on the move in winter: controlling crystallization in fuels and bio-fuels, Ken Lewtas, Infineum UK Ltd.**

Ken introduced Infineum as collaboration between two major manufacturers from the global petrochemical industry. This was followed by an introduction to waxes, fuels and crystal modifying additives. Ken then proceeded to describe selected new research work and the analytical techniques being used to investigate them, such as;

Crystal nucleation: Small-Angle Scattering (SANS & SAXS)

Crystal growth: Wide-Angle Diffraction (XRD)

The Real-World: Filtration: X-Ray Tomography (XRT)

The reasons for such large investment are that wax crystallizes in diesel fuels in winter. If not effectively modified, the crystals can block fuel filters. There is also a global focus on emissions reduction which is driving major changes in both combustion engine technology and fuel composition. N-alkanes in fuels crystallise at low temperature in vehicle systems. Fuel additives are employed to modify the shape and size of fuel crystals, to allow low temperature vehicle operation. Bio-fuel changes the way waxes crystallise in vehicle systems and creates added complications. Ken discussed only a small part of the research into fuels. There is much still to do, e.g. what problems will the next generation of bio-fuels bring? Legislation creates unintended consequences!

3. **Evolution of primitive materials, Stephen Thompson, Senior Beamline Scientist for the I11 High Resolution Powder Diffraction Beamline.**

Stephen explained that his main area of interest is in the processing and evolution of solid phase materials in circumstellar, interstellar and planetary environments i.e. "primordial mineralogy". The synthesis of similar materials and the use of synchrotron structure-probing and spectroscopic techniques such as FTIR and Raman in their analysis, will lead to greater understanding of the physical properties and structural evolution of these primordial forms of solid matter in the universe. Measuring the formation of materials under non-ambient conditions is the key to understanding the arenas and processes that drive the creation and evolution of solid matter as it cycles between stellar and interstellar environments. The final part of the presentation described the evolution of solid matter and its journey into to the early solar nebula and its incorporation into planetary objects during the "birth" of our solar system, hence forming the precursors of Earth and the material origins of life.

Catalysis in action

Chair: **Elizabeth Shotton**

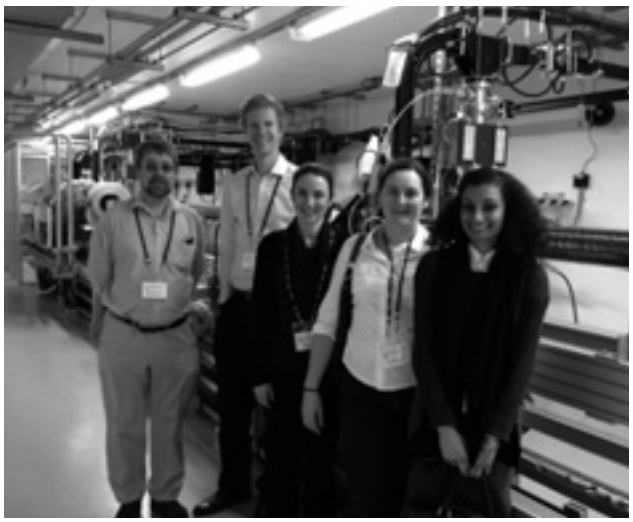
Following tours of Diamond, the second day kicked off with a session focusing on Catalysis in Action. **Tim Hyde** from Johnson Matthey, **John Brazier** from Imperial College and **Andy Beale** from UCL/Research Complex at Harwell, gave us an insight into how combining multiple techniques, both lab and synchrotron based, are helping with their research.

Tim explained how using a combination of techniques allows researchers at Johnson Matthey to explore their catalysts at varying length scales ranging from atomic to nano- and micrometre scale. He then proceeded to give a number of examples of where this approach has helped the business.

John gave us a presentation demonstrating how chemists and chemical engineers are combining their expertise to study flow reactions. His colleagues in the chemical engineering department are helping to design new reactors which can be used on spectroscopy beamlines, allowing for X-ray absorption measurements to be made throughout the reaction process. John and colleagues are now studying real-time changes in catalyst structure and reactivity.

Finally, Andy gave us a presentation highlighting some technique developments in tomography. He explained to us the benefits of absorption contrast CT, XRD-CT, PDF-CT and XRF-CT, novel methods for looking at catalytic processes. By using them in combination, new insight into the catalysis can be achieved.

The importance of *in situ* experimentation was a common theme throughout the presentations, with real understanding of the performance of the catalyst now obtainable rather than post mortem investigations. With technique developments both by users and central facilities, catalysis research promises some exciting discoveries in the coming years.



L-R: Dr Jeremy Karl Cockcroft (UCL), Dr Kevin Back (Pfizer), Dr Sophie Janbon (AstraZeneca), Dr Cheryl Doherty (Pfizer), Dr Spoorthi Dharmayat (LGC).

Pharmaceutical Materials 1

Chair: **Cheryl Doherty**

Our afternoon sessions focussed on Pharmaceutical Materials, and the first of these sessions was presented by **Sven Schroder** from the University of Manchester, **Kevin Back** from Pfizer and **Qendresa Osmani** from MSD. This session started with Sven who spoke on the use of soft X-ray spectroscopies in formulation research. He started by introducing XPS and talking about the advantages and caveats of XPS in relation to other commonly used techniques. This was followed by a study of salt and co-crystal systems by several of these techniques and showed the important differences observable in each between the two systems. The use of XPS in identifying the root of a problematic formulation and a PEG coating of two API were covered next. Sven finished by showing some applications for NEXAFS, including looking at some hydrated cluster systems.

Kevin Back then presented a case for the influence of molecular conformation in flexible pharmaceutical molecules leading to crystallisation difficulties. Kevin introduced two systems which have been seen to be extremely challenging to crystallise. He presented database studies and calculated conformational energies on these case studies to demonstrate that "unusual" or highly energetic conformations can detrimentally impact the ease of crystal growth.

Finally Qendresa introduced diffraction techniques as used in excipient compatibility testing, in order to ensure the development of stable pharmaceutical formulations. She introduced commonly used types of excipient in API formulations and discussed the features that make the excipient, and excipient-API interactions a crucial feature in drug product development. Qendresa then described the use of powder diffraction in conjunction with other characterisation techniques to assess the impact of storage conditions, drug loading and compaction on the physical and chemical stability of API-excipient blends. Qendresa finished by comparing powder diffraction with complementary Raman spectroscopy to provide key information for early stage formulation development.

Pharmaceutical Materials 2

Chair: **Brett Cooper**

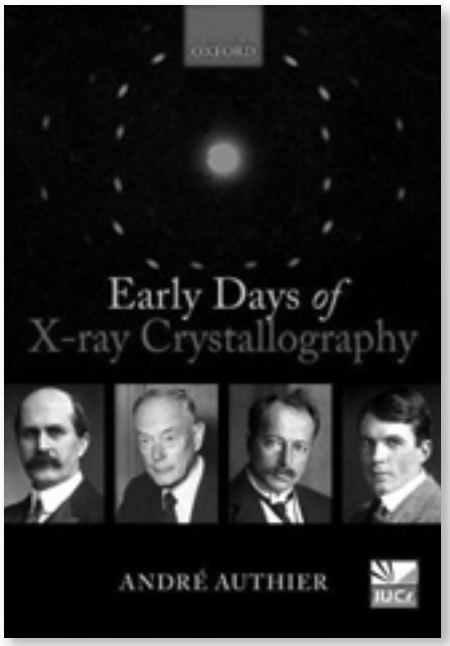
The first speaker in the final session of the day was **Graeme Day** from the University of Southampton, who presented on his work: Joining crystal structure prediction with solid state NMR for structure solution from powders. Graeme described the challenge: to go from a small molecule to predicting the crystal structure. This approach firstly involves the use of *in-silico* predictions by simulating millions of structures rapidly followed by attempting to get reliable lattice free energies to plot the energy landscape. From these the plan is to pick the most likely structures based on how deep they sit in the energy landscape. This however still leads to a multitude of potential structures. Next though, Graeme described how he could predict the solid state NMR of these structures and then attempt to match the measured NMR spectrum to attempt to validate the hits based on the accuracy of the match. Through some case study example Graeme described how the 1H NMR appeared to work more successfully than 13C and also that the more protons you had and if the peaks were assigned then the process had a better potential for success.

The final speaker of the day was **Sophie Janbon** from Astra Zeneca. Sophie was presenting: Counselling drug development using crystal structures. First Sophie described a case study investigating the relationship between two forms of API that appeared to show different relative stabilities in different solvent systems. By determining the crystal structures she was able to demonstrate that one form was actually a channel hydrate and that this form showed greater stability in solvent systems with higher water content. Later Sophie described, with the use of another case study, the AZ approach to determining the crystal structures of a compound, then comparing the key features of the crystal structure with those you would expect to see in the CCDC database. If the key structural features appeared to match those that would be expected in the majority of similar compounds, this could then give you confidence that the structure may be the most stable form. This should then allow you to prioritise when to run extensive polymorph screens as an urgent need, or whether to delay as a confirmatory screen.

Early Days of X-ray Crystallography

By André Authier

published for the International Union of Crystallography by Oxford University Press, 2013
441 pp
Price £45 (hardcover)
ISBN 978-0-19-965984-5.



READERS of *Crystallography News* will be well aware that we have recently been celebrating the centenaries of the discovery of X-ray diffraction (1912) and the determination of the crystal structures of some simple materials (1913); and that the General Assembly of the United Nations has declared 2014 as the International Year of Crystallography. **André Authier**'s latest book is therefore very timely, as we look back over the past hundred years to assess what has been achieved, and to look forward to ever more successful results in the next century, with wide application in various technologies. As can be expected from the title of this book, Authier introduces (on page 1, and in greater detail in Chapter 6) **Max Laue** (later Max von Laue) who conceived the X-ray diffraction experiment in Munich; and his two experimentalists, **Walter Friedrich** and **Paul Knipping**, who first directed X-rays on to a crystal of copper sulphate pentahydrate. In his Nobel Lecture, Laue said that, after several hours' exposure, and after development, the photographic plate 'betrayed the presence of a considerable number of deflected rays, together with a trace of the primary ray coming directly from the anticathode'. This key experiment elucidated the debate on whether X-rays were particles or electromagnetic waves; and it confirmed the space-lattice hypothesis for crystal structures.

The book is divided into twelve chapters: Significance of the discovery of X-ray diffraction (8 pages); The various approaches to the concept of space lattice (14 pp); The dual nature of light (29 pp); Röntgen and the discovery of X-rays (11 pp); The nature of X-rays – waves or corpuscles? (20 pp); 1912 – The discovery of X-ray diffraction and the birth of X-ray analysis (47 pp); 1913 – The first steps (40 pp); The route to crystal structure determination (43 pp); X-rays as a branch of optics (17 pp); Early applications of X-ray crystallography (40 pp); Unravelling the mystery of crystals – the forerunners (48 pp); The birth and rise of the space-lattice concept (83 pp).

André has created an *historical tour de force*: every page contains precious nuggets of much interest. Not only does he clearly describe the science, but he also gives the portraits and biographies of the major players in over fifty 'panels' and briefer life-sketches of a further 130 scientists in footnotes. They range from **Johannes Kepler** (1571-1630), **Rasmus Bartolin** (1625-1698) and **Christiaan Huygens** (1629-1695) to **John Desmond Bernal** (1901-1971), **Linus Pauling** (1901-1994) and Dame **Kathleen Lonsdale** (1903-1971). In thirty-two pages, André lists over a thousand references to books and journals – a rich mine of historical research. I hadn't realized that Röntgen was colour-blind and that his eyes had enhanced sensitivity in the dark – a very useful attribute for X-ray experiments! Nor had I known that four of the great scientists had had their lives terminated by traffic accidents: **Pierre Curie** (1906, aged 46); **Paul Knipping** (1935, aged 52); **Arnold Sommerfeld** (1951, aged 82); and **Max von Laue** himself (1960, aged 80).

The news in 1895 of the discovery of X-rays by Röntgen quickly spread around the world (Chapter 4); and so did the news of X-ray diffraction (Chapter 6). **Lars Vegard** played a key role in informing the father-and-son team of **W H Bragg** and **W L Bragg**; and their work is fully described in Chapter 7. In addition to photographic methods, WHB's specially invented X-ray ionization spectrometer was employed by them to find out the positions of atoms or ions in the unit cells of crystals; and thus the structures of some alkali halides (NaCl, KCl, KBr, KI), diamond (C) and zinc blende (ZnS) were quickly determined (1913), and many others soon followed. André writes (in Chapter 8) that 'by 1925, nearly 600 structures had been analysed: sixty elements (including many of their allotropes), 300 inorganic compounds, 160 organic compounds, and thirty alloys; these were all listed by

R W G Wyckoff'. For each of them, the lattice mode, structure type and lattice parameters were reported, as well as the space group, if known. An exhaustive survey of simple structures by **V M Goldschmidt** and his school established tables of atomic and ionic radii. As one of the first applications, the structure of beryl was determined by W L Bragg and **J West** using nothing else but space groups and known atomic radii. Bragg later remembered that they had worked out the structure in the record-breaking time of less than an hour!

Applications of X-ray crystallography (Chapter 10) include the understanding of chemical bonds in the crystal structures of inorganic and organic compounds; in metallurgy (solid solutions, phase diagrams, order-disorder transformations, intermetallic compounds, and crystal imperfections); in mineralogy and materials science; the structural interpretation of physical properties (such as piezoelectricity); in biological sciences (studies of fibres); and X-ray spectroscopy and the structure of the atom.

The final, and longest, chapter discusses the origins and history of the space-lattice concept, starting with **René-Just Haüy**'s *Theory of the structure of crystals* (1784) and ending with the 230 space groups of **Evgraf S Federov** (1891), **Arthur Schoenflies** (1891) and **William Barlow** (1894). Barlow, an amateur with no formal training, considered the geometry of packing spheres. He was the first to consider hexagonal close packing and he noted that binary compounds (AB) were usually cubic. In 1897, he proposed the structure for sodium chloride (NaCl), which was confirmed by X-ray diffraction by W L Bragg in 1913!

This fluently written, scholarly treatise, covers not only the early days of X-ray crystallography but also it sets the historical context in the centuries leading up to the discovery of X-ray diffraction, and what followed therefrom. Historians of science will enjoy reading it, as will students and researchers in crystallography, chemistry, biochemistry, solid-state physics, materials science, and mineralogy.

Moreton Moore
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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.

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

18-21 March 2014
Euro Bio-Inspired Materials. International School and Conference on Biological Materials Science. Potsdam, Germany.
http://www.dgm.de/dgm/bio-inspired/

20-21 March 2014
Scanning PhotoEmission Microscopy Workshop (SPEM2014) Diamond Light Source, Oxfordshire.
http://www.diamond.ac.uk/Home/Events/SPEM2014.html

23-28 March 2014
Ligand Recognition & Molecular Gating, Gordon Research Conference, Ventura, CA, USA.
http://www.grc.org/programs.aspx?&year=2014&program=ligand

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 – 3 April 2014
Powder Diffraction and Rietveld Refinement School, Durham.
http://community.dur.ac.uk/john.evans/webpages/pdrr_school_2014.htm

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

30 March – 4 April 2014
Spring meeting of the German Physical Society – Condensed Matter Section, Dresden, Germany.
http://dresden14.dpg-tagungen.de/index.html

7-10 April 2014
BCA Annual Spring Meeting, University of Loughborough.
http://crystallography.org.uk/spring-meeting-2014/

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

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.iopconferences.org

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

26-27 April 2014
Molecular & Ionic Clusters, Gordon Research Seminar, Lucca, Italy.
http://www.grc.org/programs.aspx?&year=2014&program=grs_molion

27 April – 2 May 2014
Molecular & Ionic Clusters Structure and Dynamics of Isolated Particles: From Small Clusters to Atmospheric Aerosols, Gordon Research Conference, Lucca, Italy.
http://www.grc.org/programs.aspx?year=2014&program=molionic

27 April – 2 May 2014
RapiData 2014 - Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-ray Diffraction Measurement, Brookhaven National Laboratory, Upton, NY, USA.
http://www.bnl.gov/RapiData/

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/

30 April – 9 May 2014
School of Neutron Scattering, Erice, Italy.
http://www.sonsfpricci.org/sons-school-2014

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

9-10 May 2014
MDANSE2014 School - Molecular Dynamics (and Lattice Dynamics) to Analyse Neutron Scattering Experiments, ILL, Grenoble, France.
http://www.ill.eu/mdanse2014/

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

11-17 May 2014
International Summer School of Crystallography at DESY, Hamburg, Germany.
http://conferences.cfel.de/issc14/

14-17 May 2014
5th Meeting X-ray and other techniques in investigations of the objects of cultural heritage, Krakow, Poland.
http://www.iycr2014.org/events/conferences/5th-meeting-x-ray-and-other-techniques-in-investigations-of-the-objects-of-cultural-heritage

17-21 May 2014
51st CMS Annual Meeting, College Station, TX, USA.
https://cms2014.tamu.edu/

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

31 May – 1 June 2014
Crystal Engineering: Mechanochemistry and Solid-state Reactivity: State of the Art, Gordon Research Seminar, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?year=2014&program=grs_cryst

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

1-6 June 2014
Crystal Engineering: Form Meets Function, Gordon Research Conference, Waterville Valley, NH, USA.
http://www.grc.org/programs.aspx?year=2014&program=crystal

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

1-6 June 2014
Biopolymers: Mechanisms of Biomolecular Interactions: From Physical Principles to Biological Insights, Gordon Research Conference, Newport, RI, USA.
http://www.grc.org/programs.aspx?year=2014&program=biopolym

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/

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

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

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/

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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/

18-22 June 2014
1st International Symposium on Halogen Bonding (ISXB-1), Porto Cesareo, Italy.
http://www.isxb-1.eu/

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

22-27 June 2014
Bioinspired Materials: Exploiting Biological Concepts and Strategies in Functional Synthetic Materials, Gordon Research Conference, Newry, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=bioinsp

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/

13-17 July 2014
Membrane Transport Proteins: Structure, Function, Physiology, and Targets in Disease, Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?year=2014&program=membtrans

20-25 July 2014
Colloidal Semiconductor Nanocrystals: From Fundamental Physics to Functional Materials, Gordon Research Conference, Smithfield, RI, USA.
http://www.grc.org/programs.aspx?year=2014&program=collsemi

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

26-27 July 2014
Diffraction Methods in Structural Biology, Gordon Research Seminar, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=grs_diff

27 July – 1 August 2014
Diffraction Methods in Structural Biology: Faster, Smaller, Better: Novel Technologies for Diffraction Experiments in Molecular Biology and Drug Discovery, Gordon Research Conference, Lewiston, ME, USA.
http://www.grc.org/programs.aspx?year=2014&program=diffrac

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/

9-15 August 2014
2014 PSI Summer School on Condensed Matter Research (13th edition) Exploring time, energy and length scales in condensed matter, Zug, Switzerland.
http://indico.psi.ch/conferenceDisplay.py?confId=2672

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

17-23 August 2014
Biomineralization: Where Geology Meets Biology: The Inorganic-Organic Interface, Gordon Research Conference, New London, NH, USA.
http://www.grc.org/programs.aspx?year=2014&program=biomin

25-29 August 2014
FEL2014. Free Electron Laser Conference, Basel, Switzerland.
http://www.fel2014.ch/

25 August – 3 September 2014
EMU School 2014 - Planetary Mineralogy, Glasgow.
http://eurominunion.org/?p=571

28 August - 6 September 2014
ECS1. First European Crystallography School, Pavia, Italy.
http://ecs1.azuleon.org/

1-5 September 2014
IMA 2014 - 21st General Meeting of the International Mineralogical Association, Gauteng, South Africa.
http://www.ima2014.co.za/

14-17 September 2014
2nd International Science at FELs Conference, PSI Villigen, Switzerland.
http://science-at-fels-2014.eurofel.eu/

14-17 September 2014
Annual Meeting of the German Biophysical Society, Luebeck, Germany.
http://www.biophysical-congress.de/

14-19 September 2014
XTOP 2014: The 12th Biennial Conference on High-Resolution X-Ray Diffraction and Imaging, Grenoble, France.
http://xtop2014.org/

14-20 September 2014
ICCBM15. 15th International Conference on the Crystallisation of Biological Macromolecules, Hamburg, Germany.
http://www.iccbm15.org/iccbm15.xhtml

16-19 September 2014
ISIC19. International Symposium on Industrial Crystallization, Toulouse, France.
http://www.isic19.fr/

16-19 September 2014
Mid-European Clay Conference 2014, Radebeul near Dresden, Germany.
http://www.mecc2014.de

17-19 September 2014
Physical Chemistry of Functionalised Biomedical Nanoparticles. Faraday Discussion 175, Bristol.
http://www.rsc.org/ConferencesAndEvents/RSCConferences/FD/FD175/index.asp

25-27 September 2014
17th Heart of Europe Bio-Crystallography meeting (HEC-17), Berlin, Germany.
http://www.helmholtz-berlin.de/events/hec/

29 September - 3 October 2014
ICANS XXI - 21st Meeting of the International Collaboration on Advanced Neutron Sources, Mito, Ibaraki, Japan.
http://j-parc.jp/researcher/MatLife/en/meetings/ICANS_XXI/index.html

5-8 October 2014
Summer School: Theory and Practice of Modern Powder Diffraction, Ellwangen, Germany.
http://www.kofo.mpg.de/iycr/index.html

16-17 October 2014
Crystal (cl-)Year, Turin, Italy.
http://www.nettab.org/2014/CCY/

19-23 October 2014
JCNS Workshop on neutron instrumentation, Munich-Tutzing, Germany.
http://fisica.cab.cnea.gov.ar/hacesra10/index.php/9-novedades/51-first-circular-jcns-workshop-on-neutron-instrumentation-2

26-28 October 2014
2014 Pittsburgh Diffraction Conference, Athens, GA, USA.
http://www.pittdifsoc.org/

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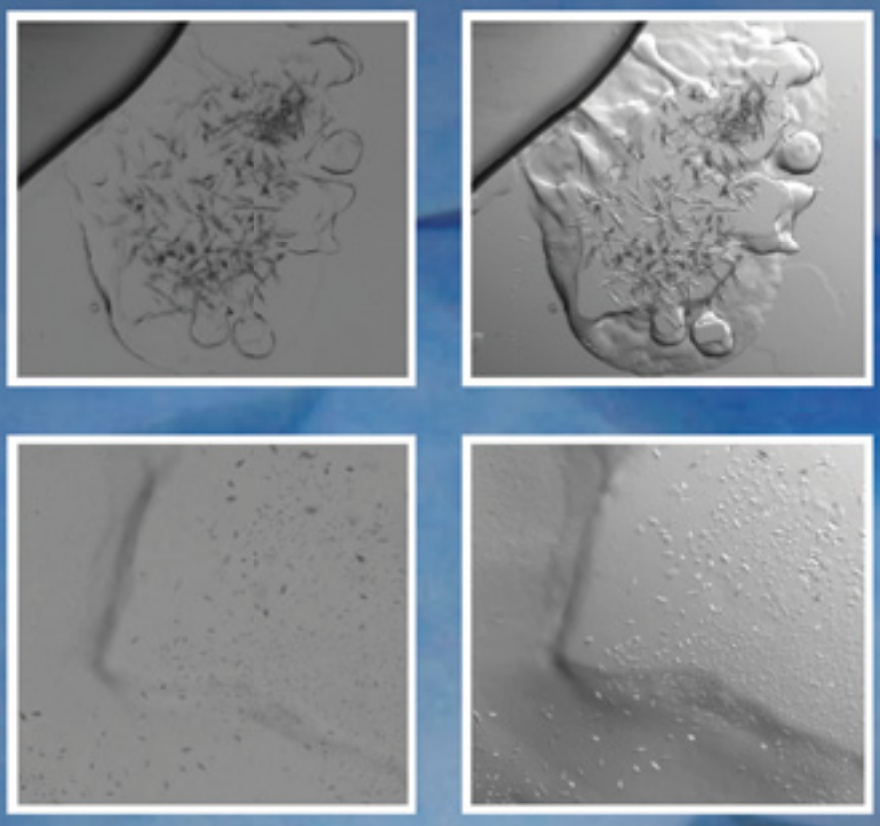

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