INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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IUCR ACTIVITIES

Welcome to the IUCr's webinar programme



Our free-to-attend webinars from authors, editors and industry experts alike will position you in the very heart of the community, and further live question-and-answer sessions will put you directly in touch with experts where you'll be able to share their best practice to benefit your research.

Our webinar series will begin later in 2016 with an event from Professor Naomi Chayen of Imperial College, London, UK. Naomi will look at how the use of certain smart materials can improve the likelihood and quality of crystallising proteins.

The major problems in this area are usually the lack of crystals, low-quality crystals or, more frustratingly, large crystals that do not diffract at all. The webinar will present some practical solutions to these problems, and it will show some of the ideas and inspiration behind them and the rationale for conducting the experiments in the first place. Importantly, the event will present some valuable examples of successful results that may help attendees improve their skills in crystallising proteins.

The webinar will end with a fascinating look into how innovative research tools such as those discussed during the presentation can be developed into commercial products and, in this particular case, are now being sold to users and/or licensed to commercial entities.

Our second webinar, which will take place two to three weeks after Naomi's, will present a new theory for X-ray diffraction and will be presented by the former Head of Research at PANalytical, Paul F. Fewster.

The webinar will describe the concept behind a new theory for X-ray diffraction [Fewster (2014). *Acta Cryst.* A**70**, 257-282; doi: 10.1107/S205327331400117X] and its impact on the interpretation and collection of data. This presentation will use diagrams to explain how the intensity in a diffraction pattern is built and how intensity exists at the Bragg angle when the Bragg condition is not satisfied. This leads to a more complete diffraction pattern from a single crystal and polycrystalline powders than presently assumed. This theory has an impact on measuring the structure factors used in molecular structure determination and will modify the interpretation of the crystal microstructure. The webinar will be of interest to all crystallographers and those interested in structure determination.

New webinars will be launched at regular intervals with the goal of producing a significant body of knowledge, thus allowing attendees a unique insight into leading researchers in the field who are improving techniques, theory and best practice for us all.

Supplementary to this new educational webinar content is a growing volume of video material on our YouTube channel (www.youtube.com/user/theIUCr), amongst which are many leading names in the field, providing snapshots of their research endeavours and current thinking in their specialist fields.

As an example, recently published is a lecture given by Richard Henderson, MRC Laboratory of Molecular Biology, Cambridge, UK, on the *Potential for further improvements in single-particle electron cryomicroscopy*, a lecture he gave during the British Biophysical Society meeting (BBS2016) in Liverpool, UK, earlier in 2016 (https://youtu.be/jLxKf-lUGf0). Subsequent presentations within this series will include talks from Sir Tom Blundell on *Fighting drug resistance in cancer and infectious disease*, Sriram Subramaniam on *Cryo-EM has come of age* and finally Greg Petsko on *New therapeutics for Alzheimer's and Parkinson's diseases using structure-guided approaches*.

Visit the IUCr homepage and events pages regularly to keep informed of key dates and activities.

Jonathan Agbenyega, IUCr Business Development Manager (ja@iucr.org)

IUCR JOURNALS NEWS

2015 IUCr Journals impact factor results



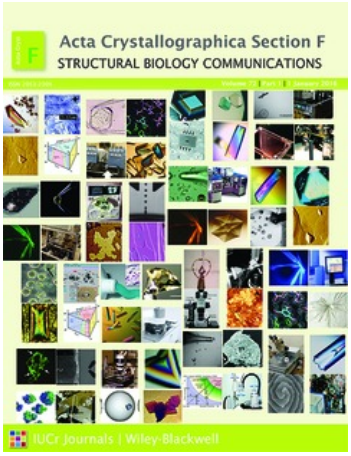
The IUCr is pleased to announce that its new open-access journal, IUCrJ, has received its first impact factor of 5.3 in the 2015 Thomson Reuters Journal Citation Reports, making it the top crystallography journal.

Other highlights from the 2015 Impact Factor results are as follows:

- Over half of the IUCr journals increased their impact factor
- *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials* (http://journals.iucr.org/b/) saw a 32% increase in impact factor
- *Acta Crystallographica Section C: Structural Chemistry* (http://journals.iucr.org/c/) saw a 46% increase in impact factor
- *Acta Crystallographica Section F: Structural Biology Communications* (http://journals.iucr.org/f/) saw a 24% increase in impact factor
- *Acta Crystallographica Section E: Crystallographic Communications* (http://journals.iucr.org/e/) remains one of the first journals to be listed in the Emerging Sources Citation Index.

IUCR JOURNALS NEWS

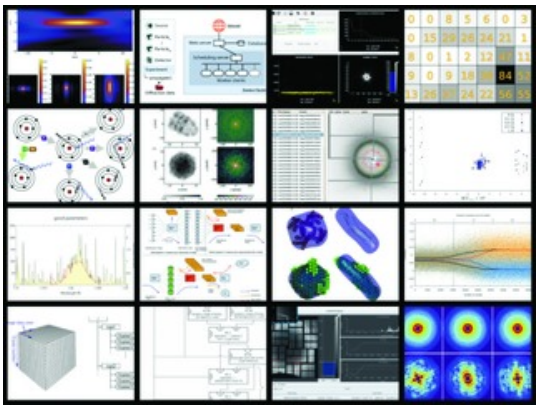
Special issues



IYCr Crystallization Series



Crystal structure prediction



CCP-FEL: a collection of computer programs for free-electron laser research

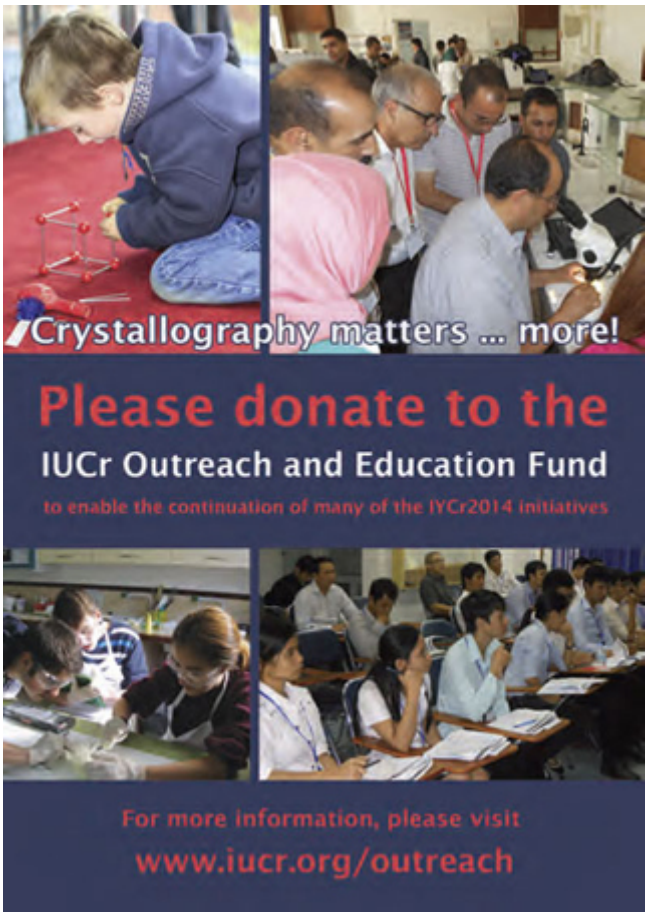
All 20 articles in *Acta Cryst. F*'s IYCr Crystallization Series are now available as a virtual issue (http://journals.iucr.org/special_issues/2016/crystallization/). **Protein crystallization - state of the art** is guest-edited by Howard Einspahr, and contains everything you need to know about the crystallization of biological macromolecules.

The August 2016 issue of *Acta Cryst. B* gives a flavour of progress and current research in the area of **crystal structure prediction** (http://journals.iucr.org/b/issues/2016/04/00/). Developments continue to be made in computational approaches for calculating the stabilities of molecular crystals, as well as for exploring crystal packing possibilities. As exemplified in the sixth blind test of crystal structure prediction, these methods are becoming applicable to complex target structures. The Guest Editors, Graeme M. Day and Carl Henrik Görbitz, hope that this varied and high-quality issue will stimulate interest and new research in this area, as well as the publication of future research in the journal.

The latest virtual special issue of the *Journal of Applied Crystallography* presents tools for a range of topics in free-electron laser (FEL) research such as simulation of experiments, online monitoring of data collection, selection of hits, diagnostics of data quality, data management, data analysis and structure determination for both nanocrystallography and single-particle diffractive imaging. **CCP-FEL: a collection of computer programs for free-electron laser research** (http://journals.iucr.org/special_issues/2016/ccpfel/) is guest-edited by Filipe R. N. C. Maia, Thomas A. White, N. Duane Loh and Janos Hajdu, and brings together a series of specially commissioned articles published in the journal between April and August 2016.

IYCR LEGACY

IUCr Outreach and Education Fund



IYCr2014 was amazingly successful in its aim to raise awareness about the importance of crystallography in the modern world. An incredible variety of activities worldwide brought the science to life for thousands of schoolchildren, university students and the general public. Many events were sponsored by UNESCO and the IUCr, supported by industrial and academic sponsors, and made real by a host of willing volunteers. They ranged from Science Fairs for schoolchildren, to professional-level OpenLab workshops and training sessions, to international summit meetings to shape future policy. They have ignited a fire in the new generation, most especially in parts of the developing world where structural science is still an infant science.

To build on these successes, the IUCr has embarked on an ambitious set of new initiatives to ensure that this newly kindled flame does not go out. More OpenLabs will be commissioned; more sustained efforts will be made in capacity building; more effort will go into public outreach activities. To this end, the IUCr Outreach and Education Fund (previously known as the IYCr Legacy Fund) has been established (www.iucr.org/iucr/sponsorship/iucr-outreach-fund).

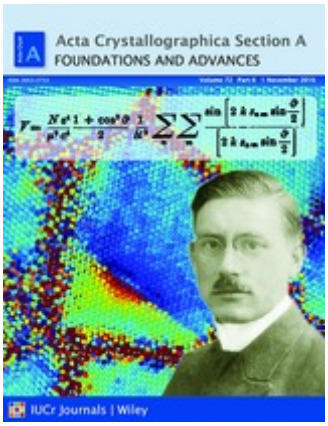
To enable the continuation of many of the IYCr2014 initiatives, please donate to the Fund at www.iucr.org/outreach.

NOTICE

100 years of the X-ray powder diffraction method



(Left) Peter Debye (photo credit: www.museumboerhaave.nl/contact/pers2a.html via Wikipedia Commons). (Right) Paul Scherrer (photo credit via Wikipedia Commons, https://en.wikipedia.org/wiki/Paul_Scherrer).



The 100th anniversary of powder diffraction is being celebrated in a blog by André Authier, Professor Emeritus at U. P. et M. Curie, Paris, France, and former president of the IUCr. The blog, at http://blog.oup.com/2016/09/x-ray-powder-diffraction-method/, describes the role of Paul Scherrer and Peter Debye in Göttingen, Germany, and Albert Hull in Schenectady, NY, USA, in discovering - independently - one of the most powerful and widely used methods for analysing matter. This centenary - along with the 50-year jubilee of the introduction of the Rietveld method - was recently commemorated at a Debye and Rietveld symposium in Amsterdam, The Netherlands (https://debye-rietveld.nl/). And it is 80 years since the Nobel Prize in Chemistry was awarded to Debye 'for his contributions to our knowledge of molecular structure through his investigations on dipole moments and on the diffraction of X-rays and electrons in gases'.

Furthermore, the November 2016 issue of Acta Cryst. A features selected papers from DSE2015: 100 years of the Debye scattering equation, a workshop held at Cavalese, Italy in June 2015. Please go to http://journals.iucr.org/a/issues/2016/06/00/.

AWARDS AND PRIZES

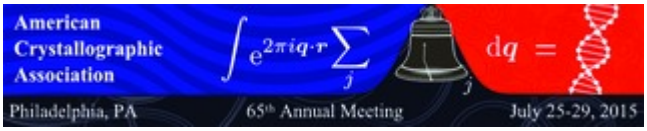
2016 Science Nobel Prizes

The Nobel Prizes in Physiology or Medicine, Physics and Chemistry were announced in early October. The Nobel Prize in Physiology or Medicine was awarded to Yoshinori Ohsumi 'for his discoveries of mechanisms for autophagy'. The Nobel Prize in Physics was divided, one half awarded to David J. Thouless, the other half jointly to F. Duncan M. Haldane and J. Michael Kosterlitz 'for theoretical discoveries of topological phase transitions and topological phases of matter'. The Nobel Prize in Chemistry was awarded jointly to Jean-Pierre Sauvage, Sir J. Fraser Stoddart and Bernard L. Feringa 'for the design and synthesis of molecular machines'.

Three of the Nobel Prize winners, Yoshinori Ohsumi of the Tokyo Institute of Technology, Tokyo, Japan; Sir J. Fraser Stoddart of Northwestern U., Evanston, USA; and Bernard L. Feringa of Groningen U., The Netherlands, have published in IUCr Journals (search for their articles at http://scripts.iucr.org/cgi-bin/full_search).

MEETING REPORT

ACA 2015



Philadelphia, PA, July 2015
www.amercrystalassn.org/

Excerpted from ACA *RefleXions*, Fall 2015, continued from Volume 24, Number 1

2.1.5: Structural dynamics

The session had a mixture of technique and application talks, and included work on metals, materials, small molecules and proteins. M. Schmidt (USA) gave a full kinetic description of the photocycle of photoactive yellow protein, including movies of transitions around the cycle. P. Coppens (USA) showed how to scale diffraction data properly to reveal transient electronic structure. G. Phillips (USA) described the work of his student Jonathan Clinger on a new photo-signaling system for time-resolved studies. M. Trigo (USA) discussed phonon dispersion as measured in real time with a pump-probe examination of Brillouin zone coverage between Bragg spots. T. Gallagher (USA) spoke about designed flexibility in antibodies. The construction of a special chamber that allows compounds to be exchanged in frameworks (MOFs) and viewed clearly was presented by J. Cox (USA). A. Dashti (USA) described the use of manifold embedding methods to reveal conformational landscapes of ribosomes and the ryanodine receptor.

George Phillips

2.2.1: Advances in multi-crystal approaches and serial crystallography



Advances in multi-crystal approaches and serial crystallography session speakers (l-r): back row: Danny Axford, Cornelius Gati, Nadia Zatsepin, Qun Liu; front row: John Spence, Jennifer Wierman, Gleb Bourenkov, James Holton.

Due to the design of novel X-ray light sources, X-ray beams with unique properties, femtosecond pulse duration and full spatial coherence, new techniques for data collection are needed. The session included

topics ranging from merging data from a handful of incomplete data sets collected at a synchrotron to serial femtosecond crystallography (SFX) at hard X-ray free-electron lasers, where a single crystal only withstands the X-ray pulse for fractions of a second before it is completely destroyed. J. Spence (USA) introduced the broad spectrum of exciting SFX experiments, as well as methodological developments and limitations of the technique. J. Holton (USA) covered the problem of anisomorphism in multi-crystal data merging and its utilization to overcome the crystallographic phase problem. J. Wierman (USA) introduced a novel algorithm to overcome the problem of indexing diffraction patterns with extremely low photon counts. G. Bourenkov (Germany) and D. Axford (UK) described novel data-collection schemes for micron-sized crystals with the major advantage of using easily accessible synchrotron light sources. Q. Liu (USA) described experimental phasing using multi-crystal approaches at synchrotron light sources, and obtaining phase information from SFX data sets using native S-SAD.

Nadia Zatsepin and Cornelius Gati

2.2.2: Materials discovery and crystal growth



Materials discovery and crystal growth session speakers (l-r): Paul Forster, Jared Allred, Efrain Rodriguez, Patrick Woodward, Jennifer Aitken, Kirill Kovnir, Susan Latturner, Joshua Goldberger.

This session brought together some of the top materials and solid-state chemists in the field to demonstrate how crystallography is key towards promoting materials discovery. The focus of the session was on inorganic solids such as transition metal oxides, chalcogenides, and some new main group compounds as well. P. Woodward (USA) revealed how cation ordering in layered perovskite oxides can influence the octahedral tilting and change their functionality. K. Kovnir (USA) illustrated how heavy alkaline earth metals (such as Sr and Ba) 'rattling' around inside clathrate cages produce specific thermal conductivity properties that make them potential next-generation thermoelectrics. J. Goldberger (USA) has prepared Group IV analogues to graphane, such as germanane, an interesting semiconductor with a direct band gap. J. Aitken (USA) showed that compounds such as $CdGeP_2$ that have the diamond structure are semiconductors with photovoltaic and luminescent properties. S. Latturner (USA) is investigating magnetic ordering in a series of intermetallic phases prepared through exploratory synthesis. J. Allred (USA) reported on a new ternary iron chalcogenide with unconventional magnetic behaviour at higher temperatures. J. M. Mangan (USA) discussed the synthesis and crystal chemistry of a series of pnictides in which electronic structure calculations and ion size effects were key to understanding their properties and their non-stoichiometry.

Efrain Rodriguez and Paul Forster

2.2.3: How I spent my summer vacation: experiences derived from small-molecule summer schools

This session featured presentations from past ACA summer school students, including academic faculty, postdoctoral researchers and graduate students. Presentations covered small-molecule crystallography, crystal engineering, mineralogy and the diagnosis of a new disease, 'Adult Onset Crystallography' (AOC). S. Hurst (USA) discussed her efforts to secure funding for the purchase of a single-crystal X-ray diffractometer to serve a host of schools in the Colorado Plateau area and collaborative studies using the ALS Synchrotron. L. Mitchell, postdoctoral researcher at US Naval Academy, discussed work that she

performed while a graduate student at U. Texas at Austin solving structures for 10 different synthetic groups, including luminescent iridium complexes to be utilized in OLEDs. C. Durr (USA) discussed utilizing crystallography to develop a new project within his research group. D. Johnston (USA) discussed the incorporation of his benchtop diffractometer into his department's undergraduate curriculum, research with undergraduates and collaborations with other institutions. J. Lee (USA) discussed his application of knowledge gained at the summer school to undergraduate research. As a new faculty member with no prior formal X-ray crystallography training, he used the ACA summer school experience to start an undergraduate research program in synthetic inorganic and organometallic chemistry using his department's benchtop diffractometer. N. Valdez (USA) is using X-ray crystallography to characterize minerals. Nichole showed several examples including how *Olex2* could be used to observe both extended structures and polyhedra.

John Lee and Amy Sarjeant

2.2.4: SAS with membranes and membrane proteins



SAS with membranes and membrane proteins session speakers (l-r): Marc Lensink, Frederick Heberle, Drew Marquardt, Volker Urban, Shuo Qian, Ryan Oliver.

V. Urban (USA) showed how a biocontinuous microemulsion system was used in a SANS study of the incorporated antimicrobial peptide melittin; the results were comparable to other studies of melittin in liposomes. R. Oliver (USA) presented his work on determining micelle and bicelle structure with SAS. Ryan's systematic studies on detergents and lipid-detergent mixtures provide important references to optimize membrane protein folding in solution for SAS experiments. M. Lensink (France) presented the latest developments in probing membrane protein structure with SAS and molecular modeling. Their strategy of combining explicit atomic detergent modeling with SANS measurements has significant potential for structural studies of other detergent-solubilized membrane proteins. D. Marquardt (Austria) focused on the methods and structures of asymmetric liposomes. The effort of developing well controlled asymmetric liposome bilayers constituted a significant step toward a more realistic model membrane system for biophysical and membrane protein studies. S. Qian (USA) reported that a membrane structure determined from SANS data is consistent with the previously determined X-ray structure and clearly revealed the water distribution in a membrane fusion intermediate structure.

Shuo Qian

2.2.5: Mechanistic and spectroscopic structural enzymology

The session focused on X-ray crystallographic studies of large complex enzyme families augmented by neutron diffraction, NMR and mutational analysis. The targets of the studies were a carbonic anhydrase surface variant that is a drug target for several aggressive cancers (B. Mahon, USA); mutation and cofactor analysis of a flavin trafficking protein from the syphilis spirochete (D. Tomchick, USA); the role of *S*-adenosyl-l-methionine (AdoMet)-dependent methyltransferases in metabolism and signal transduction (R. Trievel, USA); and GTPase and redox enzymes (F. Meilleur, USA).

Mohammed Taha

2.3.1: Professional development: communicating your science



Professional development: communicating your science session speakers (l-r): back row: Jarrod French, Joseph Gindhart, Darcy Gentleman, Celeste MacElrevey, Andrew Torelli; front row: Amalia Issa, Katherine Sippel. (Photo courtesy of Andy Torelli.)

In this session, organized by the Young Scientists Special Interest Group, speakers offered advice on how to effectively communicate to specific audiences. D. Gentleman (Manager of Science Communications at the American Chemical Society) challenged the audience to describe their research in a simple way to diverse audiences including government officers and policymakers. A. Issa (Chair of the Dept. of Health Policy and Public Health at U. of the Sciences in Philadelphia) outlined the design of presentations for policymakers and the general public. Pharmacokineticist C. MacElrevey (Nuventra Pharma Sciences) discussed the challenges of maintaining good laboratory practices while working within the guidelines set by the FDA and EPA. J. Gindhart, a program director in the Division of Cell Biology and Biophysics at NIH, discussed the importance of communicating with your program officer throughout the NIH grant cycle. K. Sippel, a contract science writer and editor from BioScience Writers, offered specific tips to clarify writing, such as removing redundant and unnecessary text, choosing appropriate power words, and balancing adjectives and prepositions. Copies of the presentations have been posted in the Young Scientists Zone on the ACA website.

Jarrod French and Andy Torelli

General interest posters

Three posters concerning solid-state reactions and two posters using data from small-molecule studies to inform protein crystallography fascinated poster session reviewer, C. Schwalbe (UK). The topics and authors of the posters were 'Doping effects on thymine monohydrate crystals' (E. Koch, USA); 'Dynamic reaction pathways in the single-crystal-to-single-crystal solid-state Diels-Alder reaction of *N*,*N*'-bis(cyclobutylimino)-1,4-dithiin with 9-vianyanthracene' (S. Khorasani, South Africa); 'Probing halogen photoelimination - how can photocrystallography help?' (S. L. Zheng, USA); 'Non-canonical hydrogen bonding to AdoMet is a common feature of AdoMet-dependent methyltransferases' (R. Fick, USA); and 'Protonation changes geometry of histidine rings' (Z. Dauter, USA). Carl's own poster concerned 'H...H clashes in published carboxylic acid structures'.

Carl Schwalbe

3.1.1: Etter Early Career symposium



Jessie Zhang

In her Etter Award Lecture, J. Zhang (USA) described her studies of the phosphorylation state of the C-terminal domain of RNA polymerase and its effect upon transcription. Eight other student and postdoctoral talks were selected for presentation in the symposium. M. Whitley (USA) combined small-angle X-ray scattering and NMR analysis of a mutant of human γD-crystallin. D. Mast (USA) described a powder diffraction study of technetium metal at high pressure and variable temperature. J. Gadient (USA) presented *in situ* high-pressure measurements for a number of negative thermal expansion materials. A. McGrath (USA) presented structural insights into ligand entry, malleable binding and induced helical movement in P-glycoprotein drug targets. K. Handing (USA) revealed how the binding of zinc to serum albumin sheds light on metal transport and distribution in mammals. L. Mueller (USA) discussed the structure and catalytic mechanism of a member of the acetoacetate decarboxylase-like superfamily. P. Janowski (USA) discussed how molecular dynamics can be utilized to improve the analysis of crystallographic data. P. Krotee (USA) described the use of electron diffraction to obtain crystal structures of Type II diabetes-related peptides from very small crystals.

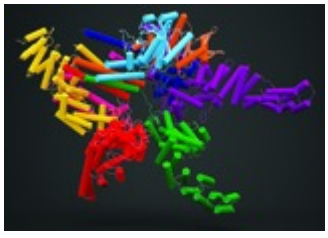
George Lountos and Andrey Yakovenko

3.1.2: Local structure and complex materials

O. Borkiewicz (USA) showcased *in situ* studies of energy storage materials found in batteries. Hard X-rays have elucidated failure and operational modes in new candidate materials. K. Jensen (USA) presented a relatively new experimental method: computed tomography pair distribution function (ctPDF) analysis. Jensen demonstrated the power of this technique for the spatial mapping of the internal crystalline and amorphous phases in a traditional AAA battery without even having to open up its case. She reported that ctPDF analysis was used to identify sources of sulfuric acid that are decomposing the hull of the Mary Rose, Henry VIII's warship that was sunk in 1545 and recovered in 1982. I. Levin (USA) discussed advances in reverse Monte Carlo modeling using multiple data types simultaneously, fitting one model to X-ray and neutron PDF, EXAFS and diffuse electron diffraction data. K. Page (USA) described recent advances in data reduction on the total scattering instruments at the Spallation Neutron Source. M. Donakowski (USA) presented data on a family of RuO_2-derived nanostructured composites that are enabling the development of ultracapacitor technology.

Graham King and James Neilson

3.1.3: Hot structures I - intracellular protein regulons





(Left) The human COP9 signalosome (CSN) is a master regulator of intracellular protein degradation. CSN regulates the largest class of ubiquitin ligases of which humans have several hundred. Ubiquitin ligases confer substrate specificity to ubiquitination. Ubiquitinated proteins include crucial regulators of DNA repair, growth and development. (Photo courtesy of Richard Bunker.) (Right) *Hot structures I - intracellular protein regulons* session speakers (l-r): Christopher Colbert, Huanchen Wang, Kristina Djinovic-Carugo, Hyun-Joo Nam, Richard Bunker, Chelsy Prince, Oluwatoyin Asojo. (Photo courtesy of Hyun-Joo Nam.)

R. Bunker (Switzerland) described his studies of an elaborate ~350 kD eight-protein hetero-complex that is a master regulator of intracellular protein degradation. Richard analyzed crystallographic and electron microscopic data and discussed the functions of each subunit based on the mutational studies. C. Colbert (USA) described the cytoplasmic domain of PupR, a TonB-dependent transporter. K. Djinovic-Carugo (Austria) reported on the high-resolution structure of the 200 kDa α-actinin-2 dimer from striated muscles. O. Asojo (USA) described the high-resolution structure of an 11 kD protein from sand fly salivary gland homogenate, part of an effort to develop a vaccine to combat leishmaniasis, which is transmitted by the sand fly. H. Wang (USA) presented structural studies of two kinases involved in cellular signal transductions. C. Prince (Canada) presented the structure of LapB, a key regulator of lipopolysaccharide synthesis pathways in *E. coli*.

Hyun-Joo Nam

3.1.4 and 3.2.4: Standard practices in crystallography I and II: data-collection strategies and data reduction



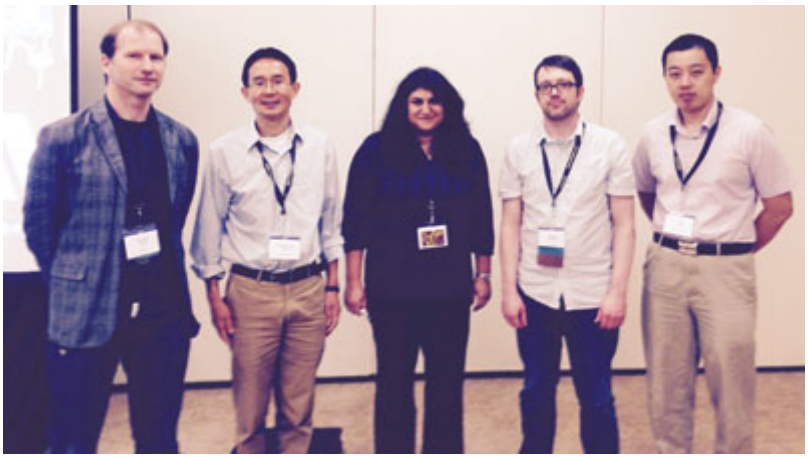


(Left) *Standard practices in crystallography I* session speakers (l-r): back row: George Sheldrick, Dorothee Liebschner, Gerard Bricogne, Tobias Weinert, Mitchell Miller, Dominika Borek; front: Peter Müller. (Photo courtesy of Peter Müller.) (Right) *Standard practices in crystallography II* session speakers (l-r): back row: George Sheldrick, Zbigniew Dauter, Bruce Noll, Leo Straver; front row: Peter Müller, Dominika Borek, Chelsy Prince, Dorothee Liebschner. (Photo courtesy of Peter Müller.)

The session began with three talks on SAD phasing. D. Liebschner (Japan), T. Weinert (Switzerland) and C. Prince (Canada) spoke on 'The challenges of soft X-rays: data collection above 3 Å wavelength', 'Fast native SAD phasing for routine macromolecular structure determination', and 'Tricks for success using zinc SAD phasing', respectively. D. Borek (USA) discussed 'Theory and practice in X-ray diffraction data processing'. Data-collection strategies were addressed by M. Miller (USA), G. Bricogne (UK) and Z. Dauter (USA). B. Noll (USA) and L. Straver (Netherlands) gave examples of how the data-collection strategy influences the outcome of a diffraction experiment. G. Sheldrick (Germany) described how modern absorption correction and scaling are performed on the software level. Bruker AXS provided financial support for the session.

Peter Müller

3.1.5: Structural modeling for SAS



Structural modeling for SAS session speakers (l-r): Thomas Weiss, Xiaolin Cheng, Farzaneh Tondnevis, Frederick Heberle, He Song. (Photo courtesy of Xiaolin Cheng.)

This session described combining solution small-angle scattering (SAS) data with computational modelling to uncover structure. X. Cheng (USA) combined molecular dynamics simulations with neutron contrast variation data to elucidate the lateral organization of lipid membranes. H. Zhang (USA) runs Monte Carlo calculations on highly parallel GPU architectures interfaced with a web-based GUI front end to interpret SAS data. F. Heberle (USA) focused on the spatial organization and raft formation in asymmetric lipid vesicles. H. Song (USA) described the solution structure of the full-length *Saccharomyces cerevisiae* RNase III with and without RNA. F. Tondnevis (USA) described her work in elucidating the structure of the *E. coli* clamp loader clamp complex with SAXS, in which the solution structure shows an opening of the sliding clamp sufficiently large for DNA loading not found in the crystal structure.

Thomas Weiss and Xiaolin Cheng

3.2.1 and 4.1.4: Important science from small-molecule structures



Important science from small-molecule structures session speakers (l-r): front row: Bruce Foxman, Marilyn Olmstead, Javier Campo, Matthew Wander, Larry Dahl, Larry Falvello; back row: Christine Beavers, Xiaoping Wang, Garry McIntyre, Feliu Maseras, Alberto Albinati.

The session combined physics and chemistry, theory and experimentation, graduate students and established scientists. Topics addressed included neutron diffraction studies of magnetic chirality (J. Campo, Spain), aperiodic crystals (G. McIntyre, Australia) and a single-crystal-to-single-crystal transformation relevant to catalysis in H_2 fuel cells (X. Wang, USA). Xiaoping showed a periodic table weighted by relative abundance at the earth's surface which explained why iron-based catalysts are particularly desirable. C. Beavers (USA) described a single-crystal-to-single-crystal transformation in a spin-crossover system, and B. Foxman (USA) discussed mother-daughter orientation relationships in phase transitions. Theory was addressed in talks on the bond-valence model (M. Wander, USA) and application of the AIM (atoms in molecules) approach to computational homogeneous catalysis (F. Maseras, Spain). M. Olmstead (USA) described ordered co-crystals of C_{70} with bromobenzene derivatives. K. Knope (USA) focused on actinide-organic interactions, and S. Bart (USA) discussed the

impact of size and reducing capability on the organometallic chemistry of uranium. In his lecture on the theme of multiferroics, with switchable electric and magnetic ordering, P. Stephens (USA) provided cautionary comments on the pitfalls of structure refinement using powder diffraction data. I. Đilović (Croatia) gave a talk on remarkable supramolecular chemistry involving host-guest complexes and a polyamine host that takes part in dynamic molecular recognition. The Cambridge Structural Database (CSD), now 50 years old, was the subject of two talks. C. Brock (USA) discussed the results of CSD-based studies of high-*Z*' organic structures, including translational modulation, an abnormal distribution of space group frequencies, and the common appearance of layered structures and polytypes. C. Groom (UK) gave a comprehensive review of science derived from the 787,912 structures in the CSD. An introduction to the philosophy and origins of the database led into a description of frontier knowledge-based studies, including an example of how the solubility of a compound can be improved by understanding its crystal structure. L. Dahl (USA) described Pd-based hetero- and homometallic clusters stabilized by CO and PR_3 that can be formed by up to 165 metal atoms.

Paulina Gonzalez, Alberto Albinati and Larry Falvello

3.2.2: Powder pair distribution function and pharmaceuticals

The session highlighted the use of the atomic pair distribution function (PDF) to study amorphous and nanocrystalline pharmaceutical drugs. X-ray powder patterns are used as fingerprints to characterize the presence of drugs in specific solid forms because the efficacy of the drug depends on its solid form. When some drug components are amorphous, or nanocrystalline, this approach breaks down and approaches such as PDF analysis are needed. Using synchrotron radiation, S. Billinge (USA) showed how extremely small signals from dilute nanocrystalline drug products in aqueous suspension could be extracted from solvent backgrounds, allowing the structure of an inhaler drug compound to be studied in dosage form. E. Cheung (USA) showed how small signals could yield critical information about recrystallization in the amorphous form of an excipient (packaging material). Understanding how drugs recrystallize from the amorphous state is a critical safety issue if drugs are brought to the market in the metastable amorphous form. Cheung highlighted the importance of gathering complementary experimental information such as NMR data, for a proper understanding of these complex problems. A. Sheikh (USA) showed that PDF could tell whether or not milling modified the structure of a drug. V. Petkov (USA) showed that rather high-quality PDFs useful for many applications might be obtained from in-house devices. P. Juhas (USA) described ab initio determination from PDF data of structures previously determined by conventional methods. This opens up the possibility of solving structures of nano-sized drug clusters that cannot be solved crystallographically. J. Kaduk (USA) used traditional powder diffraction to resolve troublesome issues with supposedly known structures of pharmaceuticals.

Simon Billinge

3.2.3: Hot structures from membrane systems



Hot structures from membrane systems session speakers (l-r): Jessica Thomaston, Elisabeth Lowe, Jason Moore, Elise Blankenship, David Lodowski, Yu-Chung Chang, Bil Clemons. Not shown: Martin Caffrey. (Photo courtesy of David Lodowski.)

Membrane protein structures reveal the mechanisms of transmembrane signaling, transport and secretion that are critical to understanding human health and disease and identifying key therapeutic

targets. E. Lowe (UK) discussed the sensor domains from the *Bacteroides* hybrid two-component systems, which regulate expression of genes involved in polysaccharide breakdown. B. Clemons (USA) discussed the differences between tail-anchored membrane proteins in fungi and humans. M. Caffrey (Ireland) described using his lipidic cubic phase technique to determine the structure of an outer membrane porin that is involved in the transport of a component of biofilms produced by *Pseudomonas aeruginosa* - a pathogen that contributes to the death of cystic fibrosis patients. J. Thomaston (USA) highlighted a continuous network of ordered solvent extending from the gating histidine to the N-terminus of the influenza M2 proton channel. E. Blankenship (USA) presented the structure of native-source rhodopsin stabilized in an active-state conformation competent for G-protein binding. A water-mediated hydrogen-bonding network, not seen in the ground state, directly links the chromophore binding site to the site of G-protein binding over 30 Å away. J. Moore (USA) reported on the crystal structure, mutational experiments, dimerization characteristics and signaling of the membrane proximal domain of a family of tyrosine kinases that play a role in angiogenesis.

David Lodowski

3.2.5: Evolving techniques for SAS



Evolving techniques for SAS session speakers (l-r): Hiroshi Okuda, David Green, Wim Bras (at rear), Kamila Wiaderek, Daniel Sunday (at rear), Brian Collins, Peter Mario Worsch (at rear), Tobias Madl (at rear), Cheng Wang. (Photo courtesy of Cheng Wang.)

Since the early attempts in the late 1930s, small-angle scattering (SAS) has evolved as a widely used high-resolution nondestructive structure probe for a broad range of applications in materials science, structural biology and environmental research. Over the past decade, with the development of third-generation synchrotron sources, spallation neutron sources and free-electron lasers, as well as advanced detectors, there have been many exciting new developments; for example, the application of resonant X-rays to provide both chemical and spatial information on materials, the development of advanced in situ sample environment techniques, and of high-pressure applications, as well as the use of coherent X-rays to capture the temporal correlation for kinetics and dynamics, such as fluctuation scattering. These developments have been accompanied by further improvement of high-performance computation tools for scattering modeling and data analysis.

This session aimed to bring experts in the forefront of SAS development to discuss recent advances and to foster novel ideas and solutions to the increasing challenges of complex structures in modern materials science. Researchers from Austria, France, Germany, Japan and the USA presented their advanced projects. Topics covered the latest trends in instrumentation development, from state-of-the-art laboratory SAXS equipment to synchrotron-based SAS systems, which use both hard and soft, as well as intermediate energy, X-rays. The research topics included a broad range of structural results for nanocomposite materials, organic electronic materials and biological complexes.

The session was well attended and the talks were followed by lively discussions, indicating a significant interest in modern SAS techniques.

Michal Sabat and Cheng Wang

3.3.1 Evening session on diversity and inclusion

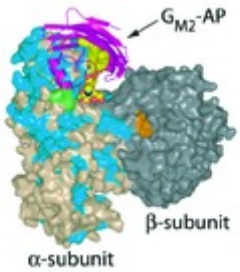


Evening session on diversity and inclusion speakers (l-r): Catherine Drennan, Krystle McLaughlin, Stephanie Wortel.

C. Drennan (USA), in her talk 'Does diversity training work?', described stereotype threat training that was developed in her lab and is now being used to train teaching assistants at MIT. Stereotype threat is the perceived risk of confirming a negative stereotype. S. Wortel (USA) described an after-school STEM Mentoring Program she has directed at NYAS for the past five years that connected elementary and middle school students with professional scientists and how professional scientists can reach young community members by leveraging existing community structures.

Krystle McLaughlin

4.1.1: Structural glycobiology



A model of β-hexosaminidase A and the G_{M2} activator protein with bound substrate G_{M2}.

A new form of β-hexosaminidase A, an enzyme mutated in some forms of lysosomal storage disease, has been patented by B. Mark (Canada). HexA normally forms a heterodimer of α and β subunits. Brian has engineered a homodimer, HexM, that may rescue the phenotype when either HexA or B is knocked out. P. Emsley (UK) addressed the characterization of N-glycans on protein structures. Paul has developed a builder/refinement routine within the *Coot* software for fitting N-glycan structures to electron-density maps in realistic conformations. P. Zaloba (Canada) is studying a glycosidase family from Salmonella. H. Blanchard (Australia) described the design of the first high-affinity selective gal-3 inhibitors, potential anti-leukemic agents, based on her crystal structures of galectins. M. Saper (USA) used a combination of crystallographic, binding and computational methods to understand how LpoA can span a periplasmic space of variable width in *H. influenzae* bacteria. M. Chaudet (Canada) has been testing the hypothesis that enzymes from the gut microbe play a role in digesting starch products that are resistant to the action of the human starch digestion system. K. Wangkanont (USA) presented the first structures of X-type lectins including human intelectin-1, and is attempting to identify the physiological substrate of the human lectin.

Michael James and David Rose

4.1.5: (Bio)Chemistry in the X-ray beam



(Bio)Chemistry in the X-ray beam session speakers (l-r): Sean McSweeney, Yasufumi Umena, Robert Thorne, Nigel Moriarty (back), Carrie Wilmot, Garth Simpson, Elspeth Garman. (Photo courtesy of Elspeth Garman.)

The session addressed kinetic processes that may be occurring intentionally or unintentionally in the X-ray beam. C. Wilmot (USA) used specific examples to highlight the importance of understanding oxidation state during a reaction. Y. Umena (Japan) discussed the determination of the valence states of the Mn atoms in photosystem-II. He demonstrated that high-resolution structures and anomalous dispersion techniques can help elucidate the water-splitting reaction of this system. G. Simpson (USA) discussed imaging of the electrical field developed through photo-electron escape and showed that it is possible to visualize the local changes to crystalline structure. N. Moriarty (USA) discussed the methods employed to provide appropriate chemical restraints in *Phenix* that allow for correct modeling of the species present in a crystal structure.

Sean McSweeney and Elspeth Garman

4.2.1: General interest III

I. Guzei (USA) entertained and inspired with his description of the Crystal-Growing Competition that he organized for high-school students in Wisconsin. A. Sarjeant (USA) used the CSD to track the top 61 journals reporting crystal structures between 1997 and 2012 and found that there was no correlation between the *R* factor of reported crystal structures and the impact factor of the journal. She found some other interesting trends in the popularity of certain structures/materials over time, revealing that culinary and crystallography fads are not so different. P. Forster (USA) described how his crystallographic studies are guiding synthetic efforts to produce new novel T_C compounds. L. Falvello (Spain) described analyses of samples that can only be formed and studied *in situ* by carefully controlling experimental conditions. T. Ramadhar (USA) discussed the crystalline sponge method, in which highly porous framework materials are used to incorporate and thereby 'crystallize' compounds that otherwise cannot be crystallized. Timothy emphasized the importance of having a well characterized framework material with the right pore sizes for the target molecule. J. Rose (USA) reported on the increasing success of the native SAD method due to advances in hardware and software that enable better data collection. B. Chakoumakos (USA) described the fascinating microstructure of sturgeon ear bones and how careful powder XRD analyses are providing a new level of understanding about the habitat and growth of these fish. A. Mesbah (France) discussed synchrotron powder diffraction experiments that led to a new monoclinic structure for hydrated rhabdophane in which the water molecules could be located.

Stacey Smith

4.2.2: Cool structures



Cool structures session speakers (l-r): Allen Oliver, Soorya Kabbekodu, Karina Heffernan, Yulia Sevryugina, Craig Bridges (at rear), Elinor Spencer, Patrick Carroll (at rear), Christopher Durr.

The *Cool structures* session commenced with an engaging talk on high-pressure crystallography by E. Spencer (USA). She described the challenges of high-pressure experiments and fundamentals of this field. She concluded with a discussion of how structural changes in lanthanide complexes over a range of pressures alter their luminescent properties. Etter Student Lecturer, K. Heffernan (USA), described how variation of pressure can alter topological characterization of rare earth phosphates. Y. Sevryugina (USA) presented a series of borate structures and described how borate topology is developed. S. Kabbekodu (USA) described the internal structure of the Powder Diffraction File and how inorganic materials are classified within the database. C. Bridges (USA) presented the mechanism of charge transport in Li-ion batteries and discussed modified battery materials designed to carry a higher charge and ultimately reduce reliance on fossil fuels. P. Carroll (USA) gave a talk on some 'un-cool structures'. He described in-depth analysis of four challenging studies undertaken during the past year.

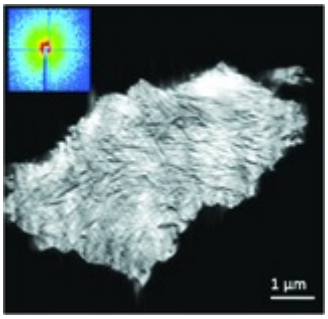
Christopher Durr and Allen Oliver

4.2.3: Structured nucleic acids

The session featured talks on reverse transcriptase bound to a DNA template (S. Martinez, USA), a transcriptional regulator bound to a cognate DNA promoter (S. Wang, USA) and a catalytic RNA with an unusual 2',5'-phosphodiester linkage (N. Toor, USA). H. Zheng (USA) presented a new online tool called Mg-RNA Server (www.csgid.org/metalnas) to assist in the identification/validation of bound magnesium ions in crystal structures, which can be particularly difficult to assign properly. B. Mooers (USA) discussed challenges that can arise during structure determination of long duplex nucleic acids that harbor intramolecular pseudo-translational symmetry. M. Wahl (Germany) presented work on the structure and function of protein-RNA sub-complexes belonging to the spliceosome, including the structure of an ATP-dependent RNA helicase, which is located near to the spliceosome's catalytic core.

Eric Montemayor and Manal Swairjo

4.2.4: Imaging with X-rays and electrons



Winner of the Etter Student Lecturer Award, Mariana Verezhak, showed a three-dimensional reconstruction of human dentine samples visualized with a voxel size of 28 nm, the highest attainable resolution reported so far.
The session included a report on a new discovery, in addition to reports on imaging techniques using photons and particles, and the complementarity of synchrotrons and electron microscopes. A wide range of applications in medical, biological, chemical, physical, materials and engineering sciences were discussed. D. Chapman (Canada) discussed diffraction-enhanced imaging and explained that, using multiple X-ray energies, it is possible to differentiate soft from hard tissues, improving and expanding the study of living subjects. V. Stanic (Brazil) and K. Evans-Lutherodt (USA) discovered an intermediate structure of hair between the cuticle and cortex. The structure is composed of β-keratin, which has toughness and elasticity and is usually associated with reptiles and birds. Further study may help explain why humans in different parts of the world have different hair types. B. Raghothamachar (USA) correlated electronic/optoelectronic device performance and defect distribution in nanomaterials and protein crystals. G. Calero (USA) is using transmission electron microscopy (TEM), bright-field microscopy and ultraviolet fluorescence microscopy to characterize the growth and quality of submicron-sized macromolecular crystals. He can distinguish nanocrystals from granular precipitates, vizulize crystal lattices and use electron diffraction patterns to identify crystal forms with higher order X-ray diffraction. A. Fluerasu (USA) described the use of X-ray photon correlation spectroscopy to analyze the speckle patterns of colloidal particles. A change of the speckle pattern reveals the dynamic behavior of the sample near the colloidal glass transition. M. Verezhak (France) showed the first three-dimensional reconstruction of human dentine samples visualized with coherent X-ray diffraction imaging. She used bone and dentine samples as models for heterogeneous composite materials. The three-dimensional dentine nanoporosity is believed to have a biological role in cell communication and mechano-sensing. C. Jacobsen (USA) presented the current status of soft X-ray cryomicroscopy to image cells and tissues using ionizing radiation with maximum preservation of structure and chemistry. Jacobsen argued that electrons excel for high-resolution imaging of samples thinner than a micrometre, while X-rays offer a path to image thicker samples such as whole eukaryotic cells and thin tissue samples. He also highlighted the role of cryo sample-preparation methods, along with the combination of fluorescence studies with ptychography to obtain thousand-fold increases in sensitivity for elemental and spectroscopic imaging compared to electron microscopes.

Vivian Stojanoff and Dean Chapman

4.2.5: Play it cool? Ambient and cryogenic approaches

This session focused on the effects of X-ray data collection at ambient and cryogenic temperatures upon macromolecular crystals and molecules. R. Thorne (USA) presented an overview of crystal cooling and a discussion of the effects of cooling rates on ice formation and crystal damage. T. Kumasaka (Japan) showed a novel technique of encasing crystals in a hydrogel for data collection that allows for robust ambient-temperature data collection without an additional cryoprotection step. D. Juers (USA) uses a flow of humid air over the crystal-viewing microscope that limits deleterious effects from dehydration during crystal handling, cryosoaking and cryomounting, and a new approach for cryoprotection using vapor diffusion to deliver volatile alcohols to loop-mounted crystals. A. Gonzalez (USA) compared radiation damage at ambient and low temperature (100 K) in crystals of thaumatin, lysozyme and cyclophilin A. At cryogenic temperature, greater doses yielded greater conformational variability. This was not the case at room temperature. Increased conformational heterogeneity in room-temperature crystal structures is not a result of radiation damage. D. Axford (UK) discussed data collection on beamline I24 at Diamond at both cryogenic and ambient temperature. Axford showed remarkable successes using *in situ* diffraction on virus crystals. D. Keedy (USA) described multi-temperature experiments on the diabetes therapeutic target PTP1B. The relative population of two conformations of an important loop was found to depend on temperature, and the impact of this conformational change on a distant ligand-binding site was explored.

Doug Juers

The full report on the meeting can be found on the ACA website at www.amercrystalassn.org.

MEETING REPORT

2nd Crystallography Olympiad

Wrocław, Poland, June 2016



Wojciech Jankowski (left) receives special prize (B. Rupp's textbook with author's dedication) for the youngest finalist. Photo courtesy of R. Paszkowski.



The Laureates, Organizers and some sponsors of the 2nd Crystallography Olympiad in Wrocław. The 1st Prize winner (*ex aequo* with A. Gotner), A. Truchlewski, is holding his air ticket to Japan. The Chair of the Organizing Committee, E. Michalski, is third from the right. Photo courtesy of R. Paszkowski.

On 22 June, 2016, the Finals of the 2nd Crystallography Olympiad were held in Wrocław, Poland. There were 38 finalists from Universities and 4 high-school pupils. The final 2-hour tournament consisted of 60 test questions and 5 open problems. The Olympiad Committee, chaired by Edward Michalski, selected questions and problems covering all aspects of crystallography of materials, chemistry and biology. Two first-place prize winners tied with a score of 70.25/80: Aleksandra Gotner (Marie Curie-Skłodowska U.) and Adam Truchlewski (Łódź U. of Technology). A MacBook computer went to Aleksandra, and Adam will go for a one-week trip to Japan sponsored by Testchem-Rigaku. The Committee named nine additional Laureates (www.komkryst.pan.pl/index.php/en/olimpiada-2016), whose results were outstanding. They received computers and computer accessories, sponsored by PANalytical, Rigaku Oxford Diffraction, Bruker and Devmatech-Stoe.

We hope that the annual Crystallography Olympiad in Poland will inspire an International Crystallography Olympiad.

Mariusz Jaskolski

MEETING REPORT

International School of Crystallography 49th Course: High-pressure crystallography: status artis and emerging opportunities

International School of Crystallography
49th Course:
High-pressure crystallography: *status artis* and emerging opportunities

Erice, Italy, May 2016, www.crystalerice.org

70 students from 20 nations were enrolled in The International School of Crystallography in Erice at the Ettore Majorana Foundation and Centre for Scientific Culture. Participants were largely from university (PhD students, postdoctoral and young researchers), with some attendees coming from commercial companies.

A typical day included a morning session, with four 45-minute lectures, and an afternoon session with two lectures, followed by different workshops and tutorials.



From left to right, Charlie McMonagle, Charles Pepin, Fabio Montisci, Rajikrishna Dutta, Anna Pakhomova, Eleanor Berryman, Dongzhou Zhang, Jerdjzei Marciniak, Paola Spadon and Annalisa Guerri.



Participants at the International School of Crystallography 49th Course, *High-pressure crystallography: status artis and emerging opportunities* in Erice, Italy.

The program focused on core experimental and theoretical high-pressure techniques in the first two days, introducing more specialized topics as the week progressed. Lectures were grouped according to research themes (basics of high-pressure research from experimental and theoretical perspectives, phase transitions, inelastic scattering and other complementary techniques to diffraction, techniques,

molecular crystals, materials). The last two days were dedicated to state-of-the-art techniques and instrumentation, setting the scene for the highly interactive combined round table/panel discussion session, where emerging challenges and opportunities in high-pressure research were discussed in greater detail. Fundamental topics covered in the course included experimental techniques for pressure generation (diamond anvil cells, large-volume presses), the basics of X-ray and neutron diffraction on single-crystal and powder materials, and comparative structural studies. These were demonstrated through examples of different chemical and structural complexity, from minerals to ices and biomolecules. Specialized high-pressure research topics included computational crystallography, dynamic compression, characterization of liquids and glasses and pair distribution function analysis. The course was rounded out by illustrating the use of high pressure as a means to study and access new materials for industrial applications such as pharmaceuticals, energy storage, magnetic and ultra-hard materials.

The program contained 31 lectures given by 21 invited speakers and 12 15-minute oral presentations by young participants (selected from the submitted abstracts). The young researchers selected were Davide Comboni (Italy), Piotr Guka (Poland), Lauren Evelyn Connor (UK), Andrew Cairns (France), Hannah Shelton (USA), Xenia Ritter (Germany), Christopher Woodall (UK), Sulgiye Park (USA), Dominique Laniel (France), Christian Childs (USA), Ramesh Devarapalli (India) and Kirsten Schultze (Germany).

Two software tutorials and ten workshops, each repeated at least twice over the course of the week, were open to all participants. Workshops were bundled in up to four parallel sessions to allow student rotation. An electronic sign-up program was developed for the course, the most workshop-intensive in recent years.

The participants presented 52 posters in two evening poster sessions. The 'poster preview during lunch' session was appreciated by poster presenters and participants alike. Equally successful were the two-minute 'come see my poster' précis immediately prior to each poster session. Several general events were organized during the day and in the evenings to further facilitate networking opportunities and scientific exchange among all participants. The last day featured a very lively and highly interactive 'Future Challenges' panel discussion and round table session.

Awards and participant feedback

Third place awards were presented to F. Montisci (Switzerland) and R. Dutta (USA), second place awards to E. Berryman (Germany) and A. Pakhomova (Germany), and first place awards to C. Pepin (Switzerland) and C. McMonagle (UK).

The Lodovico Prize recognizing the most active student inside and outside the lecture hall was awarded to J. Marciniak (Poland), with special mention made to E. Berryman (Germany) and D. Zhang (USA).

The Course survey indicated a high level of satisfaction with the content and practical organization of the course. Participants praised the lectures and workshops, the breadth of topics covered by 'passionate presenters', the 'pedagogical effort of the lecturers' and the 'energizing atmosphere that promoted learning' and 'intercultural exchange'. The high rating can in large part be attributed to the quality and teaching skills of the speakers, who were chosen among the world leaders in the field of high-pressure crystallography.

Annalisa Guerri

OBITUARY

Theo Hahn (1928-2016)

excerpted from *Acta Cryst.* (2016), 72, 294-295
doi: 10.1107/S2053273316004770



The mineralogist and crystallographer Theo Hahn died in Aachen on 12 February, 2016, six weeks after his 88th birthday. He was born in Duisburg, Germany, in 1928. He experienced the end of World War II at the age of 17 and started studying mineralogy and crystallography at the Universities of Marburg (as a student of Carl Hermann) and Frankfurt/Main in 1946. There he obtained a doctoral degree (Dr. rer. nat.) at the age of 24. The title of his dissertation was *Fluoberyllates as Model Compounds of Silicates*. This formed the basis for one of his early research fields, the study of 'stuffed' tetrahedral-framework structures, which he considered as models for silicates.

Theo worked as a postdoc for Martin J. Buerger at the Massachusetts Institute of Technology (MIT) in Cambridge, Massachusetts. There, and at the neighbouring Harvard U., he came into contact with Sydney C. Abrahams, Norio Kato, Andrew R. Lang and Charles T. Prewitt. In Buerger's laboratory he learned single-crystal structure determination by X-ray diffraction and developed his love for symmetry in crystallography and art, and its group-theoretical treatment.

Returning to Germany (1956), Theo became an assistant to Herbert O'Daniel at the Mineralogical Inst. of the U. Frankfurt/Main. He devoted his attention to the application of computers and the development of programs for single-crystal structure determination. Theo worked on this topic for his Habilitation (*Methods and Results of the Exact Crystal-Structure Research, Treated on Specific Examples*), obtaining the *Venia legendi* for Crystallography and Mineralogy in 1960.

At the age of 35, Theo was appointed full Professor and Chair for Crystallography of the Technical U. of Aachen (RWTH). He was director of this 'Institut für Kristallographie' until his retirement in 1993. He was also Dean of the Faculty of Mining, Metallurgy and Geosciences of RWTH Aachen, Chair of the German Mineralogical Society, and consultant and reviewer for the German Research Foundation.

Theo received several honours for his scientific work, including the Abraham Gottlob Werner Medal in Silver of the German Mineralogical Society (1997) and, with Hans Wondratschek, the Carl Hermann Medal of the German Association for Crystallography (2001). He was also an Honorary Member (from 1997) of the German Association for Crystallography.

Theo used X-ray and neutron diffraction methods for crystal powders and single crystals. Under his management a very effective neutron research group (U. Triple-Axes Spectrometer UNIDAS for Inelastic Neutron Scattering), affiliated to the Institut für Kristallographie, RWTH Aachen, and led by Götz Eckold, was established at the Nuclear Research Centre Jülich. Recently, his research concerned polymorphism, phase transformations and domain formation. He and I were invited to write a review article *Twinning of Crystals* for Volume D (*Physical Properties of Crystals*, 2004) of *International Tables for Crystallography*.

Hahn's greatest achievements for the worldwide crystallographic community started during the 1963 IUCr Congress in Rome, when a new Commission on *International Tables* was established with the aim of preparing and publishing a Pilot Issue in preparation for a future new edition of the first volume of

International Tables for X-ray Crystallography. During the 1972 IUCr Congress in Kyoto, Theo was appointed as Chair of the revised Commission on *International Tables* with the task of editing a revised Volume A (*Space-Group Symmetry*) of *International Tables for Crystallography* (hereafter abbreviated as *IT* A). Theo was the author of several parts of *IT* A. It was more than ten years until, in 1983, the first edition of the volume went to press. He introduced numerous amendments and supplements in the following four editions. Five years after the appearance of the fifth edition of *IT* A in 2002 and after more than 35 years in the role, Theo retired as Editor of the volume at the age of 79. However, until the end of 2015 he was engaged with the revision and update of Chapter 3.2 of the Sixth Edition of *IT* A, which is edited by his successor Mois I. Aroyo and will appear soon.

Theo served the International Union of Crystallography for 40 years (since 1963) as Chair of the Commission on *International Tables*, as editor of *IT* A (five editions), as author of various contributions to *IT* A and *IT* D, as a member of the IUCr Executive Committee and as President of the IUCr (1984-1987). His long service for the crystallographic community, in particular the editions of the new *International Tables* Volume A, forms a major part of his lifetime achievements.

Theo organized, usually with his close friend Hans Wondratschek, about 15 international summer schools on crystal symmetries and space groups. A school in Sofia led to the publication of the book *Symmetry of Crystals* by Th. Hahn and H. Wondratschek (1994).

Theo Hahn was a creative scientist of high international reputation, and his obliging and charming nature made him a fascinating partner for discussion and conversation. The community of crystallographers worldwide will miss him as an inspiring teacher and a wonderful person. Theo is survived by his wife Jane, one son and three grandchildren. Our sincere condolences are with them.

Helmut Klapper

OBITUARY

Hugo Rietveld (1932-2016)

excerpted from *J. Appl. Cryst.* (2016). 49, 1394-1395
doi:10.1107/S1600576716012061



Hugo Rietveld (left) receiving the Gregori Aminoff Prize from King Carl Gustaf of Sweden in Stockholm in 1995. (More detail given at http://home.wxs.nl/~rietv025/.)

Hugo Rietveld has died at the age of 84 after a short illness. He leaves behind his wife, a son and two daughters, to whom we extend our heartfelt sympathy on behalf of the more than one thousand members of the Rietveld Mailing List.

Hugo was born on 7 March, 1932, in The Hague and migrated to Western Australia, where in 1957 he enrolled at the U. of Western Australia at the same time as Brian O'Connor and Syd Hall. He obtained his PhD under the supervision of Ted Maslen. Hugo pioneered single-crystal neutron diffraction at Lucas Heights Sydney with Terry Sabine, and their first paper was published in *Nature* in 1961.

Hugo's experience with manual data collection and refinement convinced him of the need to computerize such tasks. He programmed two of the first IBM 1620 mainframes in Fortran II. After obtaining his PhD in 1964, he joined the neutron diffraction group of the Reactor Centrum Nederland in Petten and his interest turned to powder diffraction because large single crystals were not available for the inorganic materials of interest.

The group at Petten, including Bert Loopstra, Bob van Laar and Hugo Rietveld, first addressed the problem of overlapping powder reflections by using a relatively long neutron wavelength (2.6 Å) with a pyrolytic graphite filter. This spread out the long *d*-spacing peaks, allowing more of them to be resolved. However, for structure refinement many peaks were still unresolved, and the shorter *d* spacings needed for high atomic resolution could not even be seen.

In a 1966 paper (*Acta Cryst.* **20**, 508-513) Hugo had already used intensities from overlapping Bragg peaks. Along with others with the same problem, he then tried to fit multiple peaks to overlapping regions, but with limited success. A neutron powder pattern took a whole week to collect, and the local Electrologica X1 computer was less powerful than the IBM 1620 and programmed in Algol. It was in 1967 that the brilliantly simple but profound idea arose of refining the crystal structure together with the parameters describing the peak positions and profiles all together, as published in the famous 1969 paper (*J. Appl. Cryst.* **2**, 65-71). Hugo distributed his Algol refinement program widely, but few papers were initially published using the method. One of us (AH), at Harwell, encountered the same problems with neutron diffraction for structural transitions. On the advice of George Bacon, AH visited Hugo in 1971 and brought back Hugo's new Fortran II version of the profile refinement program. A Harwell version, modified to model the anisotropic vibrations preceding structural transitions, was very successful, both at Harwell and with Brian Fender's students at Oxford, in particular Tony Cheetham and Bob von Dreele.

In 1973, when the UK joined the EEC and AH moved to ILL in Grenoble, another Oxford student (WIFD) performed his first neutron powder experiments on AH's new D1A high-resolution diffractometer, where a powder pattern took only one day to collect, and later only one hour. Again this work was very successful, and the number of papers using what Terry Sabine, in 1978, christened the 'Rietveld method' exploded, supported by new computer programs including those of Bob von Dreele and Juan Rodriguez-Carvajal. Yet it was not until 1977 that R. A. Young and colleagues applied the method to X-ray powder diffraction, leading to further rapid growth in the number of publications. Thousands of X-ray publications using Rietveld refinement are now published every year.

Perhaps the greatest acknowledgement of Hugo's work was his receipt of the 1995 Aminoff Prize, awarded by the Royal Swedish Academy of Sciences. And in December 2012 Hugo was thrilled to receive an e-mail from David Blake of the CheMin team of the Mars Science Laboratory rover Curiosity. David wrote that he did not think they could have convinced NASA to send an X-ray powder diffractometer to Mars without the Rietveld method.

After almost 50 years, the Rietveld method has returned to its origins in the Netherlands, with the third of us (LvE) completing a fast new high-resolution neutron powder diffractometer (*J. Appl. Cryst.* **49**, 1398-1401) on the Delft reactor. Last year Hugo Rietveld was the guest of honor at the opening of this new diffractometer. He, who had been honored throughout the world for his achievement, was honored in his own country by a new generation working with neutron powder diffraction and Rietveld refinement.

Having achieved all of that, and with a loving family and friends, he will surely rest in peace.

Alan Hewat, William I. F. David and Lambert van Eijck

OBITUARY

Kazimierz Łukaszewicz (1927-2016)



Kazimierz Łukaszewicz, one of the founders of Polish Crystallography, died on 23 May in Wrocław (Poland). He was the corresponding member of the Polish Academy of Sciences (PAS), Chairman of the Committee on Crystallography, PAS, and Prof. and emeritus Prof. in the Inst. of Low Temperature and Structure Research, PAS, Wrocław.

K. Łukaszewicz was born in 1927 in Duboja, Polesie region. He settled in Toru after World War II where he attended Nicolaus Copernicus U. He continued his education in the Faculty of Mathematics, Physics and Chemistry at the U. of Wrocław. With an undergraduate degree in Chemistry, he went on to receive his PhD degree at Wrocław Technical U. in 1959 for his work on the crystal structures of strontium and barium titanates. After postdoctoral work at the Cavendish Laboratory, Cambridge U., with H. Megaw he earned his DSc in Crystallography at the Inst. of Physical Chemistry, PAS, in Warsaw.

Łukaszewicz's main research interests were structural studies of functional materials, phase transitions and order-disorder phenomena. He developed a method of high-precision measurements of the lattice parameters to detect extremely subtle phase transitions. In the 70s he undertook studies of modulated structures and devoted his last years of active research to work on crystals with correlated disorder. He is the author of many scientific papers and the first Polish textbook on X-ray structure analysis (together with Wodzimierz Trzebiatowski). His last paper was published in 2008.

Łukaszewicz persistently sought to modernize facilities and methodology and to broaden research topics. We owe the first Polish computer programs for crystallographic calculations to his efforts. Poland's first semi-automatic single-crystal diffractometer was launched in his department in 1968. In subsequent years, Łukaszewicz designed and implemented the first Bond-type diffractometers used for precise measurements of lattice parameters of single crystals. He actively supported the innovative work of colleagues on the first Polish four-circle diffractometer. Much of the credit for making Poland the world's leading manufacturer of such complex research equipment goes to Łukaszewicz.

In 1972 Łukaszewicz became the Chairman of the Committee on Crystallography of the PAS and led it until 2003, when he became Honorary Chairman. He was a member of the Executive Committee of the IUCr (1972-1978), and Vice President (1981-1983) and President (1983-1986) of the European Crystallographic Association. Thanks to his activities in the organizational field, Poland was chosen as the host of the XI Congress and General Assembly of IUCr in Warsaw (1978) and the 10th and 20th European Crystallographic Meetings in Wrocaw (1986) and Kraków (2001).

Prof. Łukaszewicz never ceased to promote crystallography. He believed that crystallography is an independent science bridging physics, chemistry, mathematics, mineralogy, materials science and biology. He was fascinated by the history and the philosophy of science. We will remember him as a passionate, ever curious, active, optimistic and enthusiastic man.

Marek Wocyrz

OBITUARY

Professor Yoshihiko Saito (1920-2014)



A global leader in structural chemistry, known for his studies of atomic arrangement, absolute configuration and electron density using X-ray diffraction, Yoshihiko Saito, Professor Emeritus at the University of Tokyo, died on 12 May 2014 of cerebral infarction at the age of 93.

Saito was born in Osaka on 3 November 1920. He graduated from Osaka U. in 1942 and was a Research Associate there until 1945, when he moved to Osaka City U. as Assistant Professor in 1949. He joined the Institute for Solid State Physics (ISSP) of the U. of Tokyo in 1960 as Professor in Crystallography.

His first years in the ISSP coincided with the vibrant period of rapid advances and innovations in computers and diffractometers to which Saito contributed. He trained young researchers from many universities in the methods and techniques of X-ray diffraction.

After retiring from the U. of Tokyo in March 1981, Saito served as Senior Professor in the Dept. of Chemistry of the newly organized Faculty of Science and Technology of Keio U.

The most important of Saito's achievements include the determination of absolute configuration and studies of electron-density distribution of metal complexes. His determination of the absolute configuration of a six-coordinate cobalt complex using X-ray anomalous scattering at Osaka City U. in 1955 was the world's first successful determination of the absolute configuration of a metal complex molecule. He continued his work in this field at the ISSP. His studies were instrumental in the establishment of empirical laws on the optical rotatory power and absolute configuration of metal complexes.

Saito began investigations of electron density within transition metal complex molecules around 1970. He introduced the automatic single-crystal diffractometer for precise intensity determination, which made it possible to obtain highly detailed data on electron distribution within a crystal. He determined electron configurations in the *d* orbital from the anisotropy in the three-dimensional distribution of the electrons localized in the vicinity of metal atoms.

Saito recieved the CSJ Award of the Chemical Society of Japan (1967), the Asahi Prize (1976), the Medal with Purple Ribbon (1981), the Second Class Order of the Sacred Treasure (1990) and the Japan Academy Prize (1991). He was president of the Crystallographic Society of Japan (1974-1975), on the editorial board of *Acta Crystallographica* and editor-in-chief of the *Bulletin of the Chemical Society of Japan*.

Several years after retiring from Keio U., Alzheimer's disease impaired Saito's walking ability and memory. His long struggle with the affliction sadly ended in confinement to bed. Prof. Saito fulfilled himself as a productive researcher and influential teacher at the right time, with an eventful and successful career. May his soul rest in peace.

OBITUARY

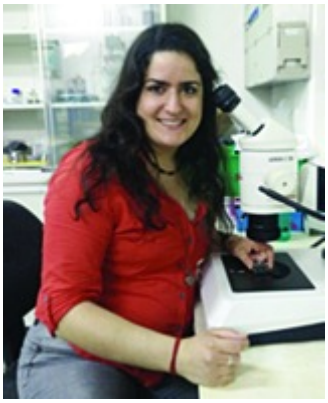
David Hoare (1966-2016)



David Hoare, a key member of the IUCr research and development group in the Chester office, died after a prolonged illness on 9 August 2016. David had worked with us for nearly 20 years, and had particular expertise in database and web programming. Many in the worldwide community of crystallographers got to know him through his prompt, courteous and careful responses to software support queries - typical of the way in which he always supported his in-house colleagues. Many more are unknowingly indebted to him each time they use the *World Directory of Crystallographers*, purchase goods or services directly through the IUCr website, submit articles, or search or navigate through the beautifully designed new journals website. He is survived by his wife and three children.

AWARDS AND PRIZES

Arianna Lanza wins fourth PANalytical Award



Arianna Lanza, winner of the fourth PANalytical Award.

The annual award recognizes innovative X-ray analytical research by young scientists. The PANalytical Award 2015 has been won by Arianna Lanza. She is affiliated to the Dept. of Chemistry and Biochemistry of the U. of Bern (Switzerland) and to the Swiss Light Source, Paul Scherrer Institute, in Villigen (Switzerland) and is currently finalizing her PhD. Her article about the dynamic behavior of a flexible and porous metal-organic framework was highly rated by all six members of the selection committee. They were impressed by the convincing and original results, which open the way to even more exciting possibilities in designing metal-organic frameworks. Ms Lanza's high competence and confidence in X-ray analysis and her scientific leadership were emphasized by the jurors, all leading experts in their fields. The winning article was selected from a record number of more than 90 contributions.

Arianna Lanza, and her co-authors Luzia S. Germann, Martin Fisch, Nicola Casati and Piero Macchi, were delighted by the good news. Arianna received the PANalytical Award at this year's Meeting of the European Crystallographic Association (ECM30) in Basel at the end of August where she presented her work to the professional community. More details about the award-winning article and its author can be found at www.panalytical.com/News/Winner-of-the-fourth-PANalytical-Award-Arianna-Lanza.htm.

PANalytical, a supplier of analytical X-ray instrumentation and software, seeks to reward early-career scientists who have demonstrated innovative thought to their research when using an X-ray analytical technique with a €5,000 prize. There are no restrictions on the manufacturer of the laboratory X-ray equipment that was used.

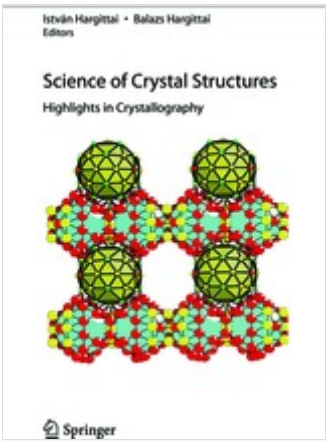
The PANalytical Award 2016 is now open for submissions. Applicants must publish a paper in print during the period 1 January 2015 until 1 December 2016 that demonstrates groundbreaking thinking in a topical field and required the use of a laboratory X-ray diffraction, X-ray fluorescence or X-ray scattering instrument as the primary analytical technique. The prize will be decided by a selection committee that includes established research scientists unaffiliated to PANalytical.

Applying for the award is easy via www.panalytical.com/award, with a closing date of 1 December 2016. Correspondence or questions about the award can be addressed to award@panalytical.com.

BOOK REVIEW

Science of Crystal Structures - Highlights in Crystallography

ISBN 978-3-319-19826-2
Springer International Publishing (2015), 335 pp.
Editors: István Hargittai and Balazs Hargittai



This anthology contains a selection of 33 articles by leaders in the field of crystallography that appeared in *Structural Chemistry* from 1990 to 2015. They are collected under the general headings of Direct Methods, Beyond the Classical System, Structural and Materials Properties, and Data Mining and Management. That the authors of the 33 articles come from 14 countries is testament to the international character of the field.

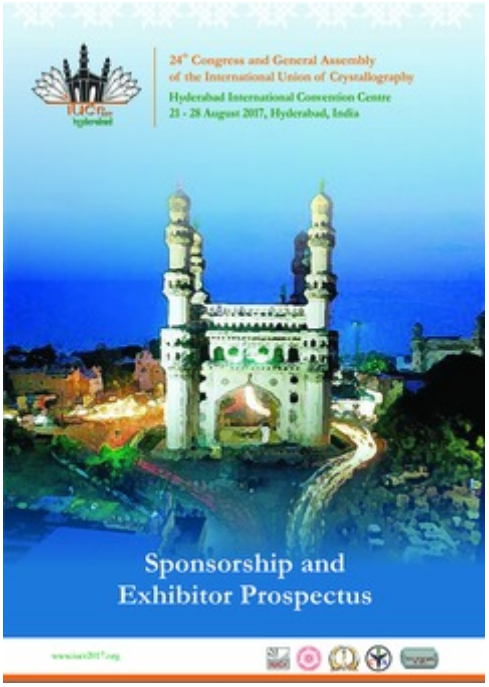
Quoting from the Preface:

From the start, there has been a characteristic direction in this periodical to bring out reports related to generalized crystallography, quasicrystals, icosahedral packing, other packing considerations, extended structures, data treatment and data mining, and what we would call 'living history'.

Several of the contributions came from the schools of such trend-setting crystallographers as J. Desmond Bernal and Aleksandr I. Kitaigorodskii. Internationally renowned scientists have figured as authors, among them Tom L. Blundell, Johann Jacob Burckhardt, John L. Finney, Jenny P. Glusker, Nobel laureate Herbert A. Hauptman, the 2014 Ewald Prize winner A. Janner, Aminoff Prize winner Isabella Karle, Nobel laureate Jerome Karle, the late doyen of Chinese crystallography K. H. Kuo, Buckley Prize winner Alan L. Mackay, Ewald Prize winner David Sayre, Vladimir Shevchenko and King Faisal Prize winner (and recent Nobel laureate) J. Fraser Stoddart.

IUCR ACTIVITIES

IUCr2017 Congress Sponsorship and Exhibitor Prospectus now available

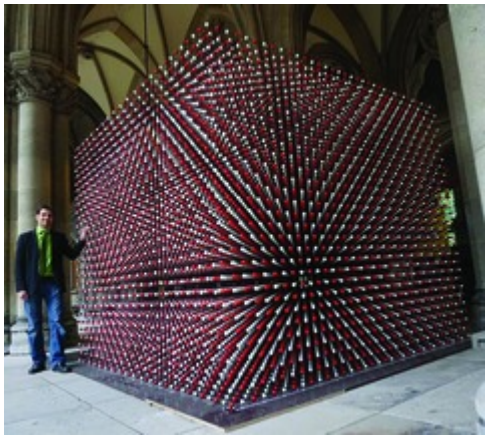


As the first IUCr Congress to take place after IYCr2014, IUCr2017 (www.iucr2017.org/) will reflect the greater awareness of the importance of crystallography and its applications, not only in an expanded scientific scope but also in an increased number of delegates from fast-emerging countries.

Companies are invited to participate and support the Congress by selecting one or more of the many sponsorship opportunities. In addition to the regular options, companies also have the chance to sponsor some exciting and unique activities, such as the display of the world's largest crystal structure model, a live Dragons' Den show, a Meet the Professor session and the e-Poster area.

The exhibition area within the Hyderabad International Convention Centre is large, modern and functional, and positioned stategically to ensure maximum engagement with delegates. All lunches, coffee breaks and poster sessions will be held in the exhibition area. Footfall will be boosted with a Best Stand Competition and Scavenger Hunt. The exhibition will open on the evening of Monday, 21 August, to coincide with the Welcome Reception in the adjacent hall, and close on the afternoon of Saturday, 26 August.

Full details are given in the Prospectus at www.iucr2017.org/prospectus/. For queries relating to the exhibition and sponsorship, please contact sponsorships@iucr2017.org. To stay up to date with the latest news, follow IUCr2017 on Facebook (www.facebook.com/IUCr2017/).



Krickl model, the world's largest crystal structure model.



Exterior view of the Hyderabad International Convention Centre.

REGIONAL NEWS

International School of Crystallography

Erice, Italy, 2-11 June 2017
http://crystalerice.org/2017/

Over the past decades, crystallography has developed from a method capable of determining the structures of isolated soluble proteins to one able to provide detailed information on the mechanisms of action of integral membrane proteins, whole viruses and the complex nano-machines that are central to cellular function. To discover how biology works, researchers are now combining the power of crystallography with a multiplicity of other methods, spanning from the atomic to the cellular scale, and including revolutionary developments in electron cryo-microscopy and tomography. This Course will celebrate its milestone as the 50th in the crystallography series started by Dorothy Hodgkin by focusing on integration: 1) of different techniques, 2) of molecular and cellular approaches and 3) of the crystallographic community, including diversity.

The aim is to provide young researchers with a review of the fundamental approaches and latest developments in the application of crystallography and hybrid methods to the structure and function of biological macromolecules and complexes. Lectures will exemplify the use of integrated approaches to analyse molecular mechanisms in human and pathogen biology. There will be hands-on workshops to provide practical experience and in-depth discussion of topics ranging from sample preparation to data analysis software. To commemorate the achievements of the Erice Crystallography School over the past 50 years, the course will feature several sessions that reflect on the past and look to the future to highlight the factors that create an inclusive discipline.

The program will include a session about the history of the School illustrated by preeminent scientists that attended the course in these years.

Annalisa Guerri