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Contents

> Extraction incomplete: missing article positions 1, 5.

IUCr journals news

2017 Nobel Prize for Chemistry 3

IYCr legacy

A double event to launch LAAMP 4

São Paulo School on Scattering: Diffraction and Imaging using Light, Neutrons and X-rays 6

IUCr activities

New developments of the symmetry database 10

News from the IUCr Executive Committee 11

Meeting report

XXIV Congress and General Assembly 13

AsCA 2016 21

Obituary

Philip Coppens (1930-2017) 29

Davide Viterbo (1939-2017) 31

Awards and prizes

The W. H. & W. L. Bragg Prize 33

Yue Deng wins fifth PANalytical Award 34

Aminoff Prize awarded to Piet Gros 35

Advertising feature

EIGER2 X detectors for the brightest X-ray sources 36

Choosing a diffractometer - navigating a minefield of technology and jargon 38

Benefits of hard X-ray radiation 41

Innovations in powder XRD - fast measurements in Debye-Scherrer geometry 44

Emily ensures your screens are perfect every time 46

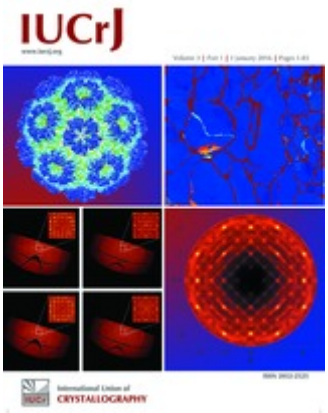
IUCR JOURNALS NEWS

2017 Nobel Prize for Chemistry



Richard Henderson (right) with Gautam Desiraju, LOC Chair, at IUCr2017.

Richard Henderson, IUCrJ Editorial Board member and winner of the 2017 Gjønnes Medal in Electron Crystallography with Nigel Unwin, has been awarded the 2017 Nobel Prize in Chemistry with Jacques Dubochet and Joachim Frank 'for developing cryo-electron microscopy (cryoEM) for the high-resolution structure determination of biomolecules in solution'.



In 1995, Henderson published a rigorous theoretical analysis of the potential of cryoEM of single particles to determine atomic resolution structures of randomly oriented macromolecules. He identified key barriers to progress, particularly the need to develop better electron detectors and improved computer programs for single-particle image analysis. These methods, particularly the development of new direct electron detectors with higher detection efficiency, have revolutionized cryoEM as a mainstream structural biology tool, exemplified by the IUCr's decision to launch a cryoEM section in its premier journal, IUCrJ (https://dx.doi.org/10.1107/S2052252515023738).

Samar Hasnain, Editor-in-Chief of IUCr Journals, commented, 'Henderson continues to lead in the development of cryoEM by helping to solve remaining barriers, namely (a) the need for higher detector detective quantum efficiency, (b) the need to reduce beam-induced specimen charging and motion, and (c) the deleterious effect of interaction of biological macromolecules with the air-water interface during plunge freezing'.

Professor Hasnain went on to say, 'Henderson's vision and ability to identify and solve key problems while focusing on an important biological problem has transformed cryoEM, which has been adopted by X-ray-based structural biologists around the world'.

In August 2017 Richard delivered his Gjønnes Medal lecture at the 24th Congress and General Assembly of the IUCr in Hyderabad, India. A video of his talk entitled 'From electron crystallography to single particle cryoEM' can be viewed at http://www.youtube.com/watch?v=TR9kalpc6FY.

IYCR LEGACY

A double event to launch LAAMP

Both the IUCr and IUPAP celebrated the start of their joint project *LAAMP* (Lightsources for Africa, the Americas and Middle East Project), funded by the 2016-2019 ICSU Grants Programme, by hosting a kick-off event during the 24th Congress and General Assembly of the IUCr (Hyderabad, India, 21-28 August, 2017) and the 29th IUPAP General Assembly (São Paulo, Brazil, 11-13 October, 2017), respectively.



Marvin L. Hackert announcing *LAAMP* at the 24th IUCr Congress opening ceremony.



Speakers at the *LAAMP* kick-off event at Hyderabad. l-r: Sandro Scandolo, Michele Zema, Andrea Lausi, Gihan Kamel, Aldo Craievich, Daniel Nyanganyura, Jean-Paul Ngome Abiaga, Richard Garratt and Andreas Roodt.

The *LAAMP* kick-off meeting at the 24th IUCr Congress was held as part of the Parallel Programme, a semi-formal programme running in parallel with the scientific sessions and focused on education, outreach and capacity building as well as general interest topics. The 150-min *LAAMP* session was chaired by *LAAMP* EC members Michele Zema (IUCr) and Sandro Scandolo (IUPAP), with over 40 in attendance. IUCr President Marvin L. Hackert (now Immediate Past President) welcomed the participants and emphasised the importance of joining efforts for such big, important projects. Daniel Nyanganyura, Director of ICSU Regional Office for Africa, presented the ICSU Grants Programme 2016-2019 and showed the many actions that ICSU is implementing for supporting science in Africa. The full framework of outreach and capacity-building initiatives run by the main international scientific and educational organisations was completed by Jean-Paul Ngome Abiaga, Deputy Executive Secretary of UNESCO-IBSP, who explained the importance of *LAAMP* also within the context of the UN Sustainable Development Goals. A general introduction to *LAAMP* was given by Michele Zema and Sandro Scandolo, whereas Andrea Lausi (Elettra synchrotron) explained the role of partnering Advanced Light Sources (AdLSs) and informed the audience about the progress of the preparation work for the brochure '*Advanced Light*

Sources and Crystallography: Tools of Discovery and Innovation', one of the tasks of *LAAMP*. The rest of the session featured contributions about the importance of AdLSs for sustaining socio-economic development, by using three case studies at three different stages of development: Aldo Craievich and Richard Garratt gave a thorough analysis of how a nowadays highly recognised scientific community was born thanks to the implementation of the Laboratório Nacional de Luz Síncrotron (LNLS) facility in Brazil, and how in relatively few years, the usage requests are so high that a new fourth-generation facility, SIRIUS, is under commissioning in the country. SESAME has started operations only recently, and Gihan Kamel emphasised the impact that such a facility will have on the scientific development of the Middle East and neighbouring regions. Finally, Andreas Roodt made the entire audience dream of a brighter future by presenting the concept and long-term planning for the African Light Source.

At the 29th General Assembly of the IUPAP, *LAAMP* was presented during the Commission Chairs Meeting and the General Assembly. In addition, a special 25-min session entitled '*The LAAMP Project: Advanced Light Sources for Development*' was held as part of the workshop 'New Challenges in Pure and Applied Physics'. IUPAP President Bruce McKellar (now Immediate Past President), in his welcome speech, stated that *LAAMP* is one of the highlights of his term. Sandro Scandolo then introduced all actions and tasks of *LAAMP*, while José Roque da Silva (Director of LNLS, Brazil) spoke about the impact of the Brazilian light source and how it opened many new avenues of research for his country. He used the Latin American experience to explain the great impact that high-level scientific infrastructure can have not only on scientific development but also on the socio-economic conditions of a region at large.

CALL FOR APPLICATIONS

The last call for applications from FAculty-STudent (FAST) Teams (new and continuing) to spend two months at participating AdLSs will be out in 2018. The faculty should be employed at a university in Africa, the Caribbean, Mexico or the Middle East and accompanied by his/her PhD student. *LAAMP* will provide 1818 Euros per person to cover transportation. Any excess will be applied to accommodation/subsistence. The remainder of accommodation/subsistence should be negotiated with the host AdLS and other sources of support. After the visit, the team should provide a description of the research conducted, including any resultant publications, and an evaluation of the non-scientific aspects of the visit, including positive experiences as well as ways that the visit could be enhanced in the future. Please watch for news of this third call at laamp.iucr.org. A list of the successful FAST teams from the first call can be seen at laamp.iucr.org/calls/first/awardees.

Michele Zema, Sandro Scandolo and Sekazi Mtingwa (LAAMP EC)

IYCR LEGACY

São Paulo School on Scattering: Diffraction and Imaging using Light, Neutrons and X-rays

The IUCr Outreach and Education Fund enables the continuation of many of the initiatives successfully launched during IYCr2014 and the fulfilment of the objectives stated in the declaration 'Crystallography for the next generation', *i.e.* to continue to increase awareness of crystallography, to build capacity in crystallography and related fields of science in the developing regions of the world, and to forge collaborations with governmental, scientific and educational institutions.

The Fund is being used to support the IUCr-UNESCO OpenLab initiative and other events/activities, such as that below, aimed at pursuing the above main aims. To donate to the Fund or find out more, please visit http://www.iucr.org/iucr/sponsorship/iucr-outreach-fund.



IUCr booth. Iris Torriani (left; IUCr delegate) and Marcia Fantini (school organizer).

This winter school, which took place in the Institute of Physics, U. of São Paulo (IFUSP), Brazil, from 17 to 21 July, 2017 (http://fep.if.usp.br/~spslnx/), was organized by Cristiano L. P. Oliveira (IFUSP) together with Marcia Fantini (IFUSP), Eduardo Granado (U. of Campinas, Brazil) and Heloisa Bordalo (U. of Copenhagen, Denmark).

In Brazil, there are several groups with international relevance to the use of scattering techniques for the structural investigation of systems at the nanoscale. With the advent of the Brazilian Synchrotron Light Source (SIRIUS) and the future Brazilian Multipurpose Reactor (RMB), a broader range of scientific applications will be open to Brazilian and Latin American researchers. For an efficient use of these facilities, it is necessary to have a qualified user community. With this in mind, we aimed at an advanced school on scattering diffraction and imaging using X-rays, neutrons and light.



Worldwide key researchers on the school topics - Otto Glatter (Graz U. of Technology, Austria), Nikolay Kardjilov (Helmholtz Zentrum Berlin, Germany), Frank Scheffold (U. of Fribourg, Switzerland) and Leopoldo Suescun (U. de la Rep□blica, Montevideo, Uruguay) - gave lectures and stayed throughout the week, permitting intensive interactions with the participants. The school had 65 attendees, with 5 undergraduate students, 40 MSc/PhD students, 12 postdocs and 8 professors. Two thirds of the participants were from São Paulo state but we also had attendees from other states (22%) and from other countries in Latin America and Europe (12%). The official language was English.

A grant from the Provost for Research at USP covered the travel and per-day allowance for the speakers. As the school could not provide support to the participants, many of the applicants were granted free registration. The support we received from the commercial sponsors (Bruker, Excillum and Xenocs) along with the registration fees paid for the school materials and coffee breaks and lunches; the sliced 1 m-long sandwiches were very important for several participants with limited resources.







Poster-prize winners: (l-r) Alysson Morais (IFUSP, Brazil; 1st prize), Isabel Galain (U. de la República, Montevideo, Uruguay; 2nd prize) and Sylvia Mutisya (U. Federal do ABC, Santo André, SP, Brazil; 3rd prize), with Prof. Oliveira.

The participants presented their research results as posters in a special session. In addition to a booth, the commercial sponsors also had a lecture slot to present their products. Iris Torriani, representing the IUCr and the Brazilian Association of Crystallography (ABCr), presented a lecture describing IUCr/ABCr activities in Brazil and worldwide. On the last day, we heard lectures from José Roque, LNLS/CNPEM coordinator and director of the SIRIUS project, and José Perrota, IPEN and coordinator of RMB. These excellent talks were very important to show the present and future scientific opportunities in the Latin American region.

The organizing committee selected the three best posters and awarded prizes to the winners (certificates from Xenocs and IUCr, gifts from Bruker, and IUCr Journals vouchers for free open-access publication in *Acta Cryst. E*).





Latin American students supported by the IUCr grant. l-r: Fabiana Nakary (U. de los Andes, Mérida, Venezuela) and Marcos Imer and Isabel Galain (both from U. de la República, Montevideo, Uruguay).

We received sponsorship from the IUCr Outreach and Education Fund. This was used to support the attendance of three Latin American students (see photo on Page 6), who have provided the following testimonials:

Fabiana Nakary:

In this school we improved our knowledge about scattering and other techniques related to crystallography; in addition, it was useful to find out which projects are in progress around the world. As an attendee I think this school was an enriching experience and an opportunity to gain more knowledge and improve my laboratory work and analysis of the data. I am thankful to the IUCr for the opportunity to participate in this school and for all the attention I received from Cristiano Oliveira and all the crew of SPSLNX 2017. Without your help I couldn't participate in this great school.

Marcos Imer:

I would like to express my gratitude for the IUCr's support to come here for this great school. The topics and schedule were fantastic; I could learn about soft matter and I was introduced to new techniques like SAXS, SANS and imaging. The professors' level was really great. Actually, these lectures about the latest technologies and developments allow me to have a broader view of what I can do. Now, I have a good background in new techniques, really important to grow in knowledge. Finally, I would like to say thank you again.

Isabel Galain:

I want to thank you again for the opportunity to participate in the 1st SPSLNX, and for offering me the IUCr support, which I greatly value. Without it, it would have been impossible for me to attend the School. The School was a very important chance to improve my knowledge about materials characterization techniques, which are so useful for my PhD work. To share the School with worldwide experts and have learned from them the theoretical aspects of the School topics was an invaluable opportunity. I believe that opportunities like this provide the necessary tools to enhance our research work, and give us the possibility to establish new collaborations. In addition to this, I think that attending the School opened new doors to find the explanation for some of my research questions, and gave postgraduate students the opportunity to find new ways of developing their research area.

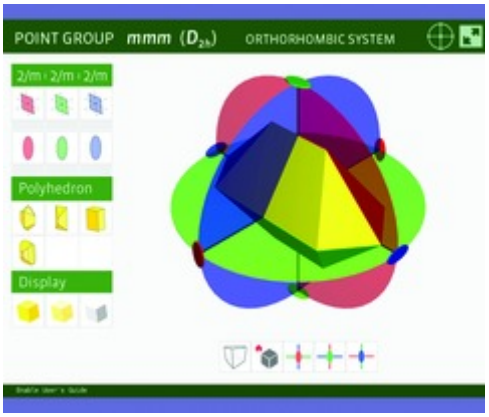
As described above, we were able to organize a school of high academic standard with very active participation by the students. An anonymous survey indicated a high level of satisfaction from the participants. We can conclude that the school reached its main objectives and certainly provided a solid basis for the development and use of the presented topics and techniques on the research activities of the participants.

We acknowledge the Provost for Research at USP for the financial support for our school, the USP for the availability of the infrastructure and technical support, the supporting companies and the grant from the IUCr for the support of three Latin American students.

Cristiano Luis Pinto de Oliveira

IUCR ACTIVITIES

New developments of the symmetry database



The symmetry database at http://it.iucr.org/resources/symmetrydatabase/ has been updated and expanded to include a wealth of new data. Information is now available for the Euclidean, chirality-preserving and affine normalizers of the space groups; these aid many crystallographic calculations, including the comparison of different but equivalent coordinate descriptions of a crystal structure (and the accompanying changes in structure factors) and the derivation of phase restrictions for use in direct methods, as described in Chapter 3.5 of the new edition of *International Tables* Volume A (http://it.iucr.org/A/). For those interested in molecular symmetry and the physical properties of materials, the generators, general and special positions, and Wyckoff positions of the three-dimensional crystallographic point groups are presented and can be transformed to different settings, enhancing and extending the data presented in Chapter 3.2 of Volume A. Users will also enjoy the simple, clear and instructive interactive visualization of the symmetry elements of the crystallographic point groups.

Throughout the database, symmetry operations are now presented in four different ways to suit a range of purposes: as *x*, *y*, *z*-based coordinate triplets, in matrix form, by geometric symbols (indicating the type and order of the operations, and the orientation of the corresponding symmetry elements) and in Seitz notation. Site-symmetry groups, whose oriented symbols show how the symmetry elements at a site are related to the symmetry directions of the crystal lattice, are now also listed for the space and point groups.

The symmetry database allows the generation of data for any space-group setting (not just those included in Volumes A and A1). The point-group visualization allows the user to turn different symmetry elements on and off and rotate the view so one can see the position of the planes and axes; it makes an excellent teaching tool.

The symmetry database is available to institutions that have access to **International Tables Online**. Please see http://it.iucr.org/services/purchase/.

IUCR ACTIVITIES

News from the IUCr Executive Committee



The new IUCr Executive Committee for the triennium 2017-2020. Front row (l-r): Alex Ashcroft (newly appointed Executive Secretary), Marvin L. Hackert (Immediate Past President), Sven Lidin (President), Hanna Dabkowska (Vice-President), Luc Van Meervelt (General Secretary and Treasurer), Jane Robinson (Administrative Assistant to the Executive Secretary). Back row (l-r): Graciela Díaz de Delgado, Masaki Takata, Santiago García-Granda, Radomír Kuzel, Jennifer L. Martin, Wulf Depmeier.

A successful 24th IUCr Congress and General Assembly took place on August 21-28, 2017, in Hyderabad, India. The total number of Congress participants exceeded 1700 with 73 countries represented (see http://www.iucr2017.org), making it a truly international scientific gathering. The Ewald Prize was awarded to Sir Tom Blundell, recognizing his very broad contributions to the field of crystallography, and the Gjønnes Medal was awarded to Richard Henderson and Nigel Unwin. Innovations at the Congress included a parallel programme and special activity microsymposia, which were held in the same time slots as the regular microsymposia.

A new IUCr Executive Committee for 2017-2020 was elected by the General Assembly: General Secretary and Treasurer:

President:	Sven Lidin
Vice-President:	Hanna Dabkowska
Immediate Past-President:	Marvin L. Hackert
General Secretary and Treasurer:	Luc Van Meervelt
Regular Members:	
Graciela Díaz de Delgado	Radomír Kuzel
Wulf Depmeier	Jennifer L. Martin
Santiago García-Granda	Masaki Takata

Other important decisions taken at the General Assembly included:

1. It was confirmed by the General Assembly that the 25th IUCr Congress will take place in Prague, Czech Republic, in 2020 (http://www.iucr25.org). Melbourne, Australia, will host the 26th IUCr Congress in 2023.

2. Albania and Kosovo, Bangladesh, Singapore and Tunisia were accepted by the General Assembly to become new category I members of the IUCr.

3. Gender representation: the policy of the IUCr should provide a balance with respect to gender at all levels of Union activities. A resolution confirming this approach was presented and accepted at the General Assembly.

4. A new Prize in the name of W. H. & W. L. Bragg was established. See the article here for more information.

5. Chairs, Members and Consultants of IUCr Commissions for 2017-2020 were approved (for further information, see http://www.iucr.org/iucr/commissions).

The IUCr Finance and Executive Committees met before and during the Congress. The IUCr has run a deficit in recent years and both committees identified savings and new income streams to address this deficit and to return the IUCr finances to safer grounds. New income streams include the Associates programme (http://www.iucr.org/people/associates), which was launched during the Congress; savings include reductions to honoraria and transferring the production of the *IUCr Newsletter* to Chester.

Here are some other updates from the Executive Committee and the Congress:

1. IUCr Journals are doing well despite the fact that the publishing environment is very challenging. The journals are the main source of financing for all IUCr activities.

2. In January 2016, the IUCr launched a new open-access data publication, *IUCrData* (http://www.iucr.org/news/newsletter/volume-23/number-4/iucrdata), which enables authors to rapidly publish brief, peer-reviewed *Data Reports* on individual crystal structures.

3. A detailed list of the schools and meetings supported by the IUCr is provided at http://www.iucr.org/iucr/sponsorship/meetings.html/meetings-supported-since-2006. Proposals for future meetings must be submitted nine months in advance. All the schools applying for IUCr financial support must obtain a Letter of Support from the IUCr Teaching Commission. The IUCr recommends that the presentations of the young scientists supported by the IUCr should be in English.

4. UNESCO supported 17 scientists from Africa (excluding South Africa) with partial bursaries to attend IUCr2017.

5. The Executive Committee created the IUCr Outreach and Education Fund (see http://www.iucr.org/iucr/sponsorship/iucr-outreach-fund). This Fund supports activities such as the Africa initiative, IUCr-UNESCO OpenLabs and similar.

6. The IUCr successfully applied to the International Centre for Theoretical Physics and the International Union of Pure and Applied Physics (IUPAP) for funding of a joint workshop in Senegal in 2017; see http://www.iycr2014.org/events/openlabs/iucr-iupap-ictp-openlab-senegal.

7. The Lightsources for Africa, the Americas and Middle East Project (LAAMP) promotes utilisation of light-source and crystallographic sciences to facilitate the enhancement of knowledge and improve the economic and social conditions in targeted regions of the world. For this project the IUCr is partnering with IUPAP and ICSU to enhance Advanced Light Sources (AdLSs) and crystallographic sciences in Africa, the Caribbean, Mexico and the Middle East. See the article here.

8. During the Congress a symposium in honour of Bill Duax was organized by Narasinga Rao. There was also a symposium in honour of Howard Flack, which was organized by the European Crystallographic Association.

Finally, as signalled previously, Mike Dacombe, IUCr Executive Secretary since 1993, retired at the end of the Hyderabad Congress. During both opening and closing ceremonies, IUCr President Marv Hackert sincerely thanked Mike for all the years of his excellent service to the crystallographic community. Alex Ashcroft was appointed the new Executive Secretary. He started in July 2017 and his email address is execsec@iucr.org.

Hanna Dabkowska, IUCr Vice-President

MEETING REPORT

XXIV Congress and General Assembly

Hyderabad, India, August 2017

Reports from some of the 119 IUCr2017 microsymposia are included here. Other microsymposia reports will appear in the next issue of the IUCr Newsletter.

Biological Macromolecules

MS-028: Long-wavelength applications in macromolecular crystallography

This methodology-based microsymposium addressed several aspects both on the theoretical background and challenges as well as on the practical application of energies lower than or equivalent to 6 keV for *de novo* structure solution of biological macromolecules. Intrinsic challenges of this technique, including absorption from the sample, its holder and the environment (use of a He atmosphere or vacuum), radiation damage (use of kappa geometry), air scattering and large scattering angles (special detector setups), were discussed. Two presentations on specialised synchrotron beamlines were given, introducing BL-1A at the Photon Factory, Japan, and I23 at Diamond Light Source (DLS), UK. The former reaches wavelengths of 2.7 and 3.3 Å and is equipped with an automated sample changer delivering samples in an He atmosphere and a laser setup enabling the removal of liquid surrounding the crystals. The latter beamline at DLS has a dynamical wavelength range from 4 to 1.5 Å, thus easily reaching the absorption edges of Ca, P, S and other light elements, and is equipped with a large semi-cylindrical detector allowing reflections at a 90° geometry to be recorded.

Chairs: Christoph Mueller Dieckmann and Dorothee Liebschner

MS-072: Solving the phase problem without experimental phasing

The microsymposium was organised first highlighting science cases in strong need of development for structure determination without experimental phasing, followed by the state of the art in new methods adopted at various places to tackle this common problem. M. R. Murthy (Indian Inst. Sci.) nicely introduced the encountered issues, taking as an example serendipitously crystallized proteins for which the structures were solved using a large-scale molecular replacement protocol. It was followed by two related presentations on biological crystal objects grown naturally in living organisms, where P. Montaville (Synchrotron SOLEIL) and L. Redecke (U. Luebeck) in turn highlighted the difficulties in adapting known experimental phasing techniques to their peculiar systems. S. Arold (KAUST) followed in describing the ContaMiner webserver, developed with the goal of quickly checking for known contaminants through fast MR-based screening of deposited crystallographic data. C. Millán Nebot (Inst. Biol. Mol. Barcelona) provided an introduction to the new implementations within the ARCIMBOLDO suite,

where small and accurate fragment search complemented by full structure expansion via autotracing appears a potential solution for structure determination of unknown folding. Finally, F. Simkovic (U. Liverpool) concluded with the applicability of the AMPLE pipeline towards phasing trans-membrane protein structures, again through tentative MR model building.

Chairs: Xiao-Dong Su and Leonard Chavas

MS-073: Minimizing radiation damage



MS-073: Minimizing radiation damage session chairs and speakers. (l-r) Richard Henderson, Yvonne Thielmann, Elspeth Garman, Mike Hough, Clement Blanchet, Go Ueno and Karol Nass.

Radiation damage is a phenomenon that presents challenges but also opportunities in many areas of structural biology. This microsymposium covered both the underlying principles and the practical implications of radiation damage in a range of different fields. The topic of radiation damage in macromolecular X-ray crystallography was introduced by the opening speaker, E. Garman (UK), who also described approaches to quantifying dose through the *RADDOSE* software and new methods to identify the location of specific damage caused by X-rays using the *RIDL* package. R. Henderson (UK) gave a perspective on radiation damage studies in structural biology and in particular, issues around radiation damage caused by electron bombardment in high-resolution cryoEM. This phenomenon is increasingly of concern with the current spectacular improvements in the resolution of cryoEM structures. K. Nass (Switzerland) described observations of radiation damage on very rapid timescales in certain XFEL experiments with longer X-ray pulse lengths, and work to characterise these by two-colour pump-probe approaches at the LCLS. C. Blanchet (Germany) presented studies of radiation damage in SAXS at the P12 BioSAXS beamline at PETRA3. This included discussion of strategies to minimize the effect of radiation-induced aggregation on SAXS data. G. Ueno (Japan) presented an interesting study of low-dose data collection with high-energy synchrotron X-rays to determine close-to-intact structures and compared these to XFEL results. Finally, an impressive new method of high-pressure cryoprotectant-free cooling of protein crystals with a very high success rate in freezing crystals grown in widely used commercial screens was presented by Y. Thielmann (Germany).

Chairs: Mike Hough and Ute Kaiser

MS-081: Macromolecular machinery

'Diversity' is probably the word which best describes the microsymposium on macromolecular machinery covering secretion systems, transcription control, protein trafficking and signal transduction. Well balanced in all important respects, and particularly geographically, the session counted on speakers from both North and South America as well as Asia, Europe and Oceania. However, diversity was most importantly represented by the range of techniques and approaches taken by the speakers in order to understand the full complexity of the molecular machines themselves and the underlying biological phenomena to which they relate. There was an overall feeling that structural biology and cell biology are rapidly merging into a single unified discipline with seamless borders.

The careful dissection (and reconstruction) of the type III secretion system (Strynadka) and the transcription anti-termination complex (Wahl) were spectacular examples of the success of combining X-ray crystallography with cryoEM. Other speakers (Duff, Ghai and Nivaskumar) often resorted to other approaches, including experimentally validated modelling techniques and SAXS, in order to gain biological insight. Imelio, giving his first presentation in English, clearly highlighted structure-function relationships in phosphotransfer reactions.

The session left no doubt that studies of macromolecular machinery will become an increasingly important component of future IUCr meetings.

Chairs: Richard Garratt and Soichi Wakatsuki

Crystal engineering

MS-003: Crystal engineering solutions to improve pharmaceutical tableting

The first presentation of this microsymposium focused on linking crystallographic features to tableting behavior of drugs. After introducing the bonding area-bonding strength (BABS) model for powder tableting, data of several polymorph pairs were presented to advance the idea that polymorphs with higher true density exhibit higher BS. This idea, if proven, can be adopted for qualitatively predicting tableting performance of polymorphs, which is useful for the pharmaceutical industry. The following lecture covered a recent attempt to explain different tableting behavior of several nitrofurantoin cocrystals by analyzing their structures, where the presence of active slip planes was shown to be an important criterion for exhibiting good tabletability. Consistent with this idea, an example was given in the third presentation where cocrystallization of griseofulvin with acesulfame deteriorated tabletability. In the fourth talk, a computational approach to qualitatively classifying or even predicting mechanical properties of crystals was presented, which considered slip planes and direction of Burgers * vector relative to the slip planes, both of which can be calculated from crystal structures. In the final talk, the BABS theory was applied to explain the tableting behavior of eutectic mixtures between aspirin and paracetamol.

Chairs: Changquan Calvin Sun and Thomas Hartmann

MS-030: Crystallization mechanisms of small-molecule organic materials



MS-030 speakers and chairs. (l-r) Isaac Rodríguez Ruiz, Jaime Gómez Morales (Chairman), Abdul Ajees Abdul Salam, Ian Rosbottom, Ilia Guzei and Tonglei Li.

Five interesting lectures covered the main aspects of crystallization phenomena. Tonglei Li (Purdue U., USA) spoke about solution speciation and implication on nucleation mechanism. Ian Rosbottom (U. of Leeds, UK) discussed the control of crystal morphology and its importance in downstream processes and filtration. Isaac Rodríguez Ruiz (Commissionnât de l'Energie Atomique de France) spoke about small-angle X-ray scattering (SAXS) coupled either to micro-batch precipitation or to a microfluidic platform, to elucidate the initial stages in the precipitation. Abdul Ajees Abdul Salam (U. of Manipal, India) showed the potential of laser-assisted crystallization to crystallize amino acids and proteins. Finally, Ilia Guzei (U.

of Wisconsin, USA) spoke about enantiotropic phase transitions in molecular solids involving Z' = 12. Besides these interesting talks, there was a high participation of communications as posters (22), many of them presented also as e-posters.

Chairs: Raj Suryanarayanan and Jaime Gómez Morales

MS-057: Charge-density studies in crystal and cocrystal engineering



MS-057 speakers and chairs. (l-r) E. Espinosa, T. S. Thakur, J. Contreras-Garcia, M. Ernst, A. Krawczuk, S. J. Coles and K. K. Jha.

This microsymposium highlighted the applications of charge-density studies and the newly developed topological descriptors towards the understanding of structure and properties of single and multi-component crystals. Invited talks from C. Matta (Canada) and J. Contreras-Garcia (France) focused on the applications of topological descriptors for studying intermolecular interactions and physicochemical properties calculations. C. Matta presented work on the use of the localization-delocalization matrix for the development of QSAR/QSPR models and its applications in predicting the pK_a and aromaticity of molecules. J. Contreras-Garcia on the other hand highlighted the applications of newly developed NCI descriptors of electron density for the analysis of attractive and repulsive interaction regions that can be very helpful towards the understanding of single and multi-component crystal formation. E. Espinosa (France) presented an invited lecture on the understanding of the effect of crystal environment on the nature of intermolecular interactions in molecular complexes involving a halogen atom in the two extremes (a salt and cocrystal) studied through charge-density analysis. Besides these, there were three interesting talks by S. J. Coles, K. K. Jha and M. Ernst that emphasized charge-density applications to pharmaceuticals and materials.

Chairs: Tejender S. Thakur and Anna Krawczuk

MS-075: Tailored properties of molecular co-crystals



MS-075 speakers and chairs. (l-r) Delia Haynes, Srinivasulu Aitipamula, Richard Cooper, Jenna Skieneh, Anilkumar Gunnam, Susan Bourne, Anil Kumar, Sreenivas Reddy Lingireddy and Anuradha Pallipurath.

Co-crystals have gained immense popularity in academia and in industry for their ability to fine-tune material properties. The session was aimed at providing an opportunity to senior and young researchers to present their recent results in this area of research. A total of seven speakers presented talks on

topics ranging from regulatory aspects and applications of co-crystals to optimization of co-crystal screening methodologies.

Co-crystals are currently in a stage of transition from lab to market and hence it is important to know how the regulatory bodies classify them. Sreenivas Reddy Lingireddy (Eli Lilly Company, USA) highlighted key aspects of the FDA's guidance on co-crystals and provided valuable information on regulatory pathways for the development of co-crystals as drug products. Streamlining co-crystal screening methodologies is valuable in understanding co-crystal formation. Richard Cooper (Oxford, UK) highlighted a data-driven approach to predicting co-crystal formation that reduces the number of experiments required to successfully produce new co-crystals. Delia Haynes (Stellenbosch, South Africa) highlighted guest exchanges in hydrogen-bonded frameworks; remarkably, stepwise and multiple guest exchanges occur within a given single crystal. Anil Kumar described the challenges in developing nutraceuticals for commercial use. The final three presentations were shorter talks by early career researchers. Jenna Skieneh described a co-amorphous phase with curcumin while Anuradha Pallipurath described a series of co-crystals that show irreversible thermochromism on converting to salts. Anilkumar Gunnam spoke about using co-crystallization to stabilize the neutral form in a series of zwitterionic molecules.

Chairs: Srinivasulu Aitipamula and Susan Bourne

MS-092: Bio-compatible porous materials for drug delivery



MS-092 speakers and chairs. (l-r) M. Gemmi, P. Falcaro, A. Bacchi, K. Sarkar, M. Fantini and P. Horcajada.
This microsymposium presented the hottest news on design, engineering, characterization and biomedical applications of diverse and technologically relevant porous materials. Metal-organic frameworks (MOFs), ordered mesoporous silica and self-assembled metal-organic polyhedra (MOPs) were discussed and their functional drug-delivery properties illustrated. Speakers presented results on bio-stability, bio-compatibility and bio-accumulation as a function of the administration route of MOFs (P. Horcajada), the external surface functionalization of MOF nano-particles and their biological compatibility (S. Wuttke), efficiency of the encapsulation of diphtheria anatoxin (D-ANA) into ordered mesoporous silica (M. Fantini), and encapsulation of other therapeutics into MOP nanocages (K. Sarkar). An overview of cutting-edge electron microscopy techniques was also presented to show how progress of this characterization can benefit the investigation of porous material systems (M. Gemmi). The focus of the session conjugated the synthetic strategies and structural characterization of different families of ordered porous materials with the assessment of their efficiency in biomedical applications. Based on the outcomes proposed in this microsymposium, it is indisputable that this research is quickly moving towards the development of novel smart materials for medicine.

Chairs: Alessia Bacchi and Paolo Falcaro

MS-102: Halogen bonding at the interface between small molecules and macromolecules



MS-102 speakers and chairs: (l-r) K. M. Sureshan (co-chair), Anssy Peuronen, J. A. Gavira (Chair), Kari Rissanen and Pierangelo Metrangolo.

Sunday was indeed the day of halogen bonding! The keynote address by G. Resnati set the platform for two microsymposia on halogen bonding. The afternoon microsymposium started with a talk by P. Metrangolo, who showed various examples of the use of halogen bonding as a decisive design element in various supramolecular systems. He demonstrated that a diblock copolymer substituted with terminal iodoalkyl chains showed organized assembly through halogen bonding. This is indeed an exemplification of the power of halogen bonding in organising an otherwise random polymer. Also he showed that halogenation of tyrosine residues in proteins leads to misfolding due to the halogen bonding. With systematic chemical mutation of a small amyloidogenic peptide DFNKN, he demonstrated the efficacy of halogen bonding in aggregation of the peptide, which led to the gelation of the peptide. By incorporation of the modified peptide in full-length fiber-forming protein, Metrangolo showed that fibrillation can occur much faster than the native protein. Current momentum and relevance of halogen bonding in designing small hosts were nicely highlighted by Kari Rissanen and Anssy Peuronen. They illustrated the design and synthesis of molecular cages or capsules thanks to the intrinsic properties of halogen bonds, i.e. directionality, strength etc.

Chairs: José A. Gavira and Kana M. Sureshan

MS-110: Phase transitions in alloys and molecular solids



MS-110 speakers and chairs: (l-r) Palwinder Singh, Kinga Suwinska, M. Sabeena, Philippe Guionneau, Zeljko Skoko, Mois Aroyo and Tony Linden.

Five oral presentations took place in the microsymposium: (1) Materials studies by the Bilbao Crystallographic Server by M. I. Aroyo (Spain); (2) Competing b.c.c. β to h.c.p. α phase transformations in Ti-1Mo alloy by M. Sabeena (India); (3) Multiscale structural view of phase transitions in spin-crossover molecular solids by P. Guionneau (France); (4) Phase-transition study of Ag-doped $Ge_2Sb_2Te_5$ thin films by P. Singh (India) and (5) Mystique world of acrobatic molecular crystals by Z. Skoko (Croatia).

From the first presentation one could get extended knowledge about the possibilities offered by the Server, which is equipped with a set of structure-utility programs including basic tools for transformations between different structure descriptions or transformations compatible with a specific

symmetry reduction. Phase-transition studies in composite materials of potential technological applications were presented by two young Indian researchers (Sabeena and Singh). The spin cross-over associated with structural modifications in iron(II) molecular complexes discussed by Guionneau was shown to start at the atomic level and then propagate from the coordination sphere to the crystal packing and to the sample scale. Finally, the negative thermal expansion in crystals known also as thermosalient crystals or, more colloquially, jumping crystals, was discussed in detail in an excellent presentation by Skoko.

Chairs: Kinga Suwinska and Anthony Linden

MS-119: Interactions in solids under stress



MS-119 speakers and chairs: (l-r) Kamil Dziubek, António dos Santos, Shanti Deemyad, Anton Targonskiy, Arianna Lanza, Andrew Cairns, Ines Collings, Alla Arakcheeva and Boris Zakharov.

This microsymposium highlighted issues related to unusual phenomena arising in solids at non-ambient conditions, from high pressures to acoustic excitation and studied by various techniques including spectroscopy, X-ray and neutron diffraction. The symposium included three long talks and four short talks. A. Arakcheeva (EPFL, Switzerland) showed new experimental results indicating that noble gases Ne and Ar, which are commonly used as pressure-transmitting media, influence high-pressure behavior of $CH_3NH_3PbI_3$ perovskite. K. F. Dziubek (LENS, Italy) presented new results on the phase diagram of urea at high pressures and high temperatures to show that solid-state reactions under high pressure are directed by the structure of the molecular crystal precursor. A. M. dos Santos (ORNL, USA) reviewed the state of high-pressure neutron scattering experiments. He showed that novel neutron sources coupled with innovative neutron guide geometries enable the delivery of much greater fluxes to the small samples which are common for high-pressure studies. In parallel, new developments in high-pressure devices allowed experiments that were only dreamt of a decade ago.

Chairs: Boris Zakharov and Shanti Deemyad



After the meeting in Hyderabad, we, a group of 22 IUCr 2017 participants, travelled to Delhi, being thrilled to start our golden triangle tour. The starting city, Delhi, houses amongst others the impressive Qutub minar, Bangla Sahib Gurudwara Sikh temple and India gates. Afterwards we continued to Agra where we were fortunate to visit the Agra fort and the marvellous Taj Mahal. On our way to the pink city Jaipur, we visited the interesting Fatehpur Sikri. In Jaipur itself, we visited the beautiful Amer fort and the Astronomical Observatory. After this exciting journey, we travelled back to Delhi where we said goodbye to our new friends, bus driver and excellent tour guide. Front row (l-r): Florencia Di Salvo, Hanna Dabkowska, Anna Schenk, Marv Hackert, Irina Makarova. Back row (l-r): tour guide Mina, Eddie Arnold, Ellie Francis, Aicardo Roa-Espinosa, Sue Byram, Eduardo Villalobos, Elke De Zitter (contributor), Stuart Mills, Kerry Goodman, Sebastian Klinke, Laurens Vandebroek, Elena Selezneva, Leo Sazanov, Kiyoaki Tanaka, Alex Vasiliev, Anne Tuukkanen, Umut Ozugurel, tour guide Sunil.

MEETING REPORT

AsCA 2016

Hanoi, Vietnam, December 2016

Single-Crystal School



School of Single-Crystal Structure Determination chairs and speakers. Front row (l-r): Y. Ohashi, S. Ward, D. Hashizume and T. Ozeki. Back row (l-r): H. Puschmann, T. Sato and C. Campana.

The opening ceremony of the AsCA meeting was preceded by a School of Single-Crystal Structure Determination on December 3 and 4, 2016. The basic theory of single-crystal structure determination was presented by Y. Ohashi (Tokyo Inst. Tech, Japan), and D. Hashizume (RIKEN CEMS, Japan) covered sample preparation and data collection. C. Campana (Bruker, USA) gave a summary of available programs and software for single-crystal data analysis and structure determination before focusing upon programs that specifically address the problem of twinned crystals. The program *ROTAX* identifies markers of twinning including the presence of forbidden reflection and inequality of 'equivalent' reflections and finds the relationship between the twins. Campana recommends using *Shake-and-Bake* after *ROTAX*. The talk illustrated the complexity of crystallization incorporating a lot of twinning and disorder that masquerade as single crystals. H. Puschmann (OlexSys, UK) talked about the details of single-crystal data collection, processing, structure determination and analysis and the use of the program *Olex2*. He described an automatically generated report with all the diagrams, pictures, tables and references required for publication. T. Ozeki (Nihon U., Japan) addressed the evaluation of results including crystal quality, proper space-group selection and other points addressed by Puschmann. He offered simple rules and went step by step over CIF file preparation. S. Ward (CCDC, UK) talked about the Cambridge Structural Database, which now contains over 850,000 structures and a set of 700 structures carefully selected to create a representative teaching database. She described deposition procedures in detail and many features of the standard output (chemical diagrams, molecular images *etc.*) that are useful for publication.

Opening ceremony

Dignitaries addressing the attendees at the opening ceremony on December 4 included Dang Vu Minh, President of the Vietnam Union of Science and Technology Associations, and Pinak Chakrabarti, AsCA President, who reported that of the 457 registrants, 86% were from Asia.



AsCA Council of National Representatives.

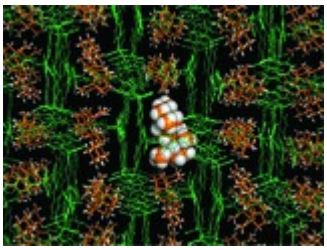
Plenary lectures

The first plenary lecture was given on crystallography and electron microscopy by S. Iijima (Meijo U., Japan). In 1970, using transmission electron microscopy (TEM), Iijima found evidence of carbon nanotubes. In the 1980s, he was publishing images that he eventually identified as carbon nanotubes. His Nature paper on carbon nanotubes [*Nature*, **354** (1991), 56-58] has had five times as many citations as the DNA paper of Watson and Crick. The 77-year-old Iijima's most recent publication is on one-dimensional nanowires of pseudoboehmite.

In his plenary lecture 'CryoEM of Molecular Machines', W. Chiu (Baylor, USA) demonstrated the power of cryoEM in the determination of the structure of a virus and a 2700 amino acid protein. The virus model begins as a 700 Å diameter cotton ball that becomes a textured cluster of 60 subunits of seven proteins, the backbones of which can be traced without human assistance. This is expanded to a model with side chains in which aromatics are easier to find and negatively charged residues are poorly defined. Two independent data sets were modeled independently and compared for consistency. The fold of the 7 x 60 proteins is excellent except at the termini where they diverge in seven ways.



Makoto Fujita with Gautam Desiraju (chair).



Crystalline sponge method. X-ray analysis without crystallization [M. Fujita *et al.*, *Nature,* **495** (2013), 461-466.]

M. Fujita (U. Tokyo, Japan) soaks target molecules in crystalline cage structures of the appropriate size to facilitate their structure determination. Encapsulated molecules in the cages take up fixed orientations and allow determination of structure. Over 70% cage occupancy is needed to get structure determination comparable to typical X-ray analysis. Heavy atoms in the cage structure remove the need to have an anomalous signal in the target for absolute configuration determination. He extracted three flavanoids from a piece of orange peel, separated them on HPLC and trapped each in a cage and

determined the three structures. A cycloelatanene study reversed an erroneous NMR conclusion. He is trying to capture reactions *in situ* and to design cages large enough for proteins.

Keynote lectures



Se Won Su (chair) and Jennifer Martin.

J. L. Martin (Griffith U., Australia) addressed antibiotic resistance *via* the disruption of disulfide bridge formation in virulence factors. Her research team is studying the crystal structures of a protein that forms disulfide bonds (DsbA). They found peptides that bound to DsbA and inhibited its function and discovered a disulfide shuffling protein that shuffles virulence factors back to their active form.

M. Li (Chinese Academy of Sciences) described structural studies of plant photosystem II (PSII) and contrasted the structure with those of the less complex plant PSI and cyanobacterial PSII. Her 3.2 Å structure of spinach PSII in a supercomplex with light-harvesting complex II (LHCII) has 25 protein subunits, 105 chlorophylls, 28 carotenoids and other cofactors. Based on the structure, the complete pigment network and the potential energy transfer pathways within the supercomplex were constructed, allowing analysis of the details of the evolution of photosynthesis from bacteria to plants.

Rising stars

Presentations by rising stars focused on techniques for chiral resolution (L. W.-Y. Wong, Hong Kong U. Science and Tech.), control of human zinc transporters (C. A. Cotrim, U. Queensland, Australia), photo-cycloaddition reactions inside MOFs (I. H. Park, Gyeongsang National U., Korea), symmetry and color symmetry properties of flat and round tilings (M. L. Loyola, Ateneo de Manila U., Philippines), synthesis and testing of redox active ligands for electron conductive networks (J. Y. Koo, Pohang U. Science and Tech., Korea), intercellular trafficking and recycling of E-cadherin, which is vital to cancer progression (J. Xu, Guangzhou Inst. Biomed and Health, China), *in situ* studies of MORF formation (Y. Wu, U. Cambridge, UK) and the attack mechanism of antimicrobial defensins (M. Jarva, La Trobe U., Australia).



Rising Stars chairs and speakers. Front row (l-r): Jin Young Koo, Mark Loyola, Camila Cotrim, Jinxin Xu and In-Hyeok Park. Back row (l-r): Ian Williams (co-chair), Michael Jarva, Yue Wu, Lawrence Wong and Alice Vrielink (co-chair).

Special session on materials science

T. Kamiyama (Inst. of Materials Structure Science, Japan) described using neutron diffraction to obtain accurate data on light atoms in functional materials. O. Sakata (National Inst. of Materials Science, Japan) surveyed synchrotron facilities for the study of materials in Japan and described the information one can obtain (valence band structure, occupied states *etc.*). A. Edwards (Australian Nuclear Science and Tech.) described the determination of the structures of multi kilodalton silver nanoparticles. She has found twinning in a structure where it had been overlooked. L. Q. Minh (Vietnam Materials Research Soc.) discussed the technology of rare earth nanomaterials. Vietnam has 22 million tons of rare earth minerals, many of which are important in electronics, optics, lasers, superconductors and optical emitters. Rare earth doping of LEDs can alter agriculture growth rate, and rare earth luminescent labels can produce imaging tools in biomedicine. Having expertise in phosphazane synthesis in solution, F. García (Nanyang Tech. U., Singapore) described how he explored mechanochemical (solvent-free) synthesis. He studied his starting material and goal, considered conditions that might work and experimented with dry cofactors. García reported that some syntheses that worked by mechanical techniques could not be synthesized in solution.



Special Session on Materials Science. Front row (l-r): Le Quoc Minh, Takashi Kamiyama. Back row (l-r): Nguyen Duc Chien (chair), Osami Sakata, Felipe García and Alison Edwards.

Chemical crystallography: general interest

L. Lindoy (U. Sydney, Australia) has created a molecular pressure switch involving a reversible Cu-N bond. S. Ward (CCDC, UK) illustrated the educational potential of 850,000 crystal stuctures. A. Rujiwatra (Chiang Mai U., Thailand), discussed a profusion of coordination polymers based on lanthanide ions and pyridine ligands. Y. S. Tan (Sunway U., Malaysia) described transformations of a binary cadmium dithiocarbamate. A. B. Zambrano (Philippines) discussed weaving colored tilings in hyperbolic space. B.-H. Chen (Taiwan) combined powder diffraction and absorption spectroscopy to study Co coordination polymers. C. I. Yeo (U. Malaysia) discussed Au...O and Au...π interactions. M. M. Jotani (Bhavan's Sheth R. A. College of Science, India) described intermolecular interactions and Hirshfeld surface analysis of a pyrimidine derivative. R. Yip (Hong Kong U. Science and Tech.) discussed oleanolic acid as a chiral resolving agent. E. R. T. Tiekink (Sunway U., Malaysia) analyzed the role of intermolecular interactions in crystal engineering.





Chemical crystallography: General interest chairs and speakers. Front row (l-r): Suzanna Ward, Chien Ing Yeo, Edward Tiekink (co-chair), Aliw-iw B. Zambrano, Rebecca Yip, Kittipong Chainok (co-chair). Back row (l-r) Len Lindoy, Yee Seng Tan, Mukesh M. Jotani and Bo-Hao Chen.

Structural biology: disease-related proteins

The microsymposium began with a talk on glutaminases as anticancer targets in which J. Sivaraman (National U., Singapore) showed a movie of an inhibitor causing a shift of six residues that inactivates the enzyme. A. Roujeinikova (Monash U., Australia) is investigating how a family of bacterial chemoreceptors (including carcinogenic *H. pylori*) sense and discriminate between attractants and repellents that can affect the potency of chemotherapeutic agents. H. Tanji (U. Tokyo, Japan) discussed how the binding of single-stranded RNA to toll-like receptor 8 induces innate immune response in relation to the treatment of auto immune diseases. M. I. Bin Anasjr (Australia) is studying pro-apoptotic and anti-apoptotic BCl-2 proteins in search of a way to increase production of the pro-apoptotic form to combat viral infection.



Disease-related proteins chairs and speakers. Front row (l-r): Saori Roppongi, Anna Roujeinikova, H. Tanji. Back row (l-r): Mohd Ishtiaq Bin Anasjr, Toshiyuki Shimizu (co-chair) and J. Sivaraman.

Macromolecular complexes: proteins/DNA/RNA

C.-J. Chen (Natl Synchrotron Radiation Research Center, Taiwan) described the capsid assembly and mechanism of infection of a virus that attacks the nervous system of large fish. They are exploring the basis of specificity of residues on the viral surface in order to find ways to disrupt viral assembly and protect the food source. M. Bostina (U. Otago, New Zealand) reported on a cryoEM study of a picornovirus with therapeutic potential to treat metastatic disease. He reported a similar fold of six different virus families including foot and mouth, entero and polio viruses. T.-H. Nguyen (Genetic Eng. Hanoi, Vietnam) compared the receptor-binding domains of non-human adenovirus capsids of turkey,

raptor, goose, lizard and snake with each other and with the human adenovirus. H. Song described the unwinding mechanism of a DNA helicase of *Bacteroides* based on crystal structures of several complexes. X.-D. Su (Peking U., China) discussed the ethylene-insensitive transcription factor family of the ethylene signaling pathway.



Macromolecular complexes: proteins/DNA/RNA speakers and chairs. Front row (l-r): Haiwei Song, Xiao-Dong Su, Thanh-Hong Nguyen (co-chair). Back row (l-r): Chun-Jung Chen, Mihnea Bostina, Nei-Li Chan (co-chair).

Membrane complexes: proteins/DNA/RNA

New membrane protein structures reported in the microsymposium included the first light-driven chloride pump rhodopsin (H.-S. Cho, Yonsei U., Korea), a long-lasting endothelin vasoconstrictor (T. Nishizawa, U. Tokyo, Japan), a glucagon receptor antagonist linked to the treatment of diabetes (A. S. Dore, UK), an ATP-binding cassette (ABC) transporter responsible for multi-drug cancer resistance (M. S. Jin, Gwangju Inst. of Science and Tech., Korea) and X-ray and NMR analysis of an electron-transfer complex of photosystem I and ferredoxin (H. Tanaka, Osaka U., Japan).

Ultra-high resolution protein structures

Reports of high-resolution studies included a charge-density analysis of an iron sulfur electron carrier protein (K. Takeda, Kyoto U., Japan), substrate specificity determination of an arabinofuranosidase at 0.97 Å resolution (A. Goyal, Indian Inst. Tech., India) and locating hydrogen atoms related to redox catalysis in a cholesterol oxidase (A. Vrielink, U. Western Australia). K. Hasegawa (SPring-8, Japan) described the properties of the latest ultra-high resolution beamline at SPring-8 and illustrated applications. P. Thaw (TTP Labtech, UK) described a system for the optimization of the crystal screening process.



Ultra-high resolution structures of proteins, chairs and speakers. (Front row) G. Kurisu (co-chair), P. Thaw. (Back row) K. Takeda, A. Vrielink and K. Hasegawa (co-chair).

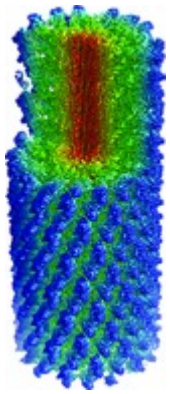
Hybrid methods



Hybrid/integrative methods in biological structure analysis, chairs and speakers. (Front row) Matthias Wolf, Lawrence Lee, Anna Nagai, Christopher Squire. (Back row) Mihnea Bostina (co-chair), Masaki Unno and Kurt Krause (co-chair).

M. Wolf (Okinawa Inst. Science and Tech., Japan) used cryoEM to achieve a complete structure of the bacterial flagellar hook structure. EM, atomic force microscopy and small-angle X-ray scattering (SAXS) were used to study artificially constructed supramolecular protein assemblies *in vitro* (L. Lee, U. New S. Wales, Australia); neutron diffraction was used to determine the first structure of a ferredoxin-dependent bilin reductase to reveal the protonation state of the biliverdin and surrounding residues (M. Unno, Ibaraki U., Japan); SAXS, NMR and X-ray diffraction were combined to elucidate the folding in bacterial surface adhesins (C. Squire, U. of Auckland, New Zealand); and X-ray crystallography and SAXS were used to determine the structural basis for substrate specificity in a family of peptidyl arginine deiminases (A. M. Nagai, Ibaraki U., Japan).

CryoEM reconstruction of the *Campylobacter* polyhook. 'Complete structure of the bacterial flagellar hook reveals extensive set of stabilizing interactions'. Matsunami *et al. Nature Commun.* **7**, 13425 (image credit: Matthias Wolf).

	
	Superposition of a SAXS model and X-ray structures from a study of bacterial surface adhesins, the work of Y. Yosaatmadja and C. Squire.

William L. Duax

OBITUARY

Philip Coppens (1930-2017)



Philip Coppens, born in 1930 in the Netherlands, died suddenly on 21 June 2017 while he was leaving his office at Buffalo U. This was a tremendous shock (both in scientific and personal terms) for the international scientific community, particularly materials science and crystallography. Since his first publications, which were focused on the potential impact of crystallography on the study of the quantum behavior of matter, he attracted young scientists from the whole world. He always emphasized the complementary capacities of his co-workers and helped them to develop their own successful careers. He was undoubtedly the 'father' of global developments in the study of the electronic behavior of matter (from simple systems to biological systems) using X-ray/neutron (X-N) scattering. Many young researchers who had recently enjoyed fascinating cooperations with Professor Coppens in the field of time-resolved crystallography, a prime area for future studies, were deeply dismayed to hear the sad news.

Philip Coppens started his research with Caroline MacGillavry in the area of crystal structures and photochemistry. His PhD (Amsterdam, 1960) was mainly carried out at the Weizmann Institute in Israel. He approached the study of the electronic behavior of condensed matter (at or out of equilibrium) through intense cooperation with Fred Hirshfeld and Gerhard Schmidt. One main result concerned the differentiation of the photo-induced behavior of two polymorphs of *p*-nitrophenol (at a time where lasers did not yet exist).

Just after his PhD, he was recruited by Walter Hamilton at Brookhaven National Laboratory (including stays at the Weizmann Institute and various places in Europe). His innovative work on X-N diffraction complementarity aided the study of the electronic behavior of solids. His paper in *Science* in 1967 [Coppens, P. (1967). *Science*, **158**, 1577-1579] showed the electron deformation density of *s*-triazine and created a worldwide research axis. He focused on the importance of mastering 'real' aspects of X-ray and neutron diffraction (such as absorption, extinction and thermal effects) for obtaining trustworthy electron density. The quality of his research led to his appointment as a professor at Buffalo U., where he stayed thereafter with his family. Philip and Robert Stewart were the source of every group that developed research on charge, spin and momentum density across whole continents. In cooperation with Richard Weiss and Vedene Smith, he also brought about important triennial conferences such as the Gordon Research and Sagamore conferences.

His paper in *Science* attracted me, as it gave a concrete sense to molecular wavefunctions, and I joined his group with my family for my PhD at the end of 1972. Amazingly, I was asked to work on extinction (both for X-rays and neutrons) and to propose a workable model; he also asked me to optimize step-scanned signal *versus* noise data. This was very hard, but all members of the lab used to exchange ideas, in particular through weekly meetings. It was said that Philip first experienced time-resolved research, since he came to us every 15 minutes asking how we had been improving! The experience was unforgettable and the final gift was the determination of the deformation density in tetracyanoethylene (with F. K. Ross), revealing simple, double and triple bonds plus lone pairs: at that time, quantum computations were not possible for such a molecule.

Philip had a fantastic chemical intuition and always put emphasis on finding the potential complementary talents of his co-workers. His priority was to further our international scientific

recognition - he never said 'I did', but always emphasized our work. This was extremely positive and opened up long-term international collaborations for us. Each of us could create personal groups and suggest young scientists who could interact with Philip. Another fundamental quality of Philip struck me concerning extinction: when the theoretical strategy was validated by referees, he proposed a simple scheme that would be easily transferable in refinement processes.

A fundamental scheme was proposed by Niels Hansen and Philip: the multipolar development of charge density, which has been used by all groups for nearly 40 years. With Guru Row, we proposed a complementary approach concerning the extension of radial functions, the application of which fits the Slater model for atomic orbitals. It also led to a first joint charge-spin density study with Tibor Koritzansky. The joint refinement of charge, spin and momentum densities is now a key issue in advanced crystallography (for the groups of Beatrice Gillon, Jean Michel Gillet and Claude Lecomte, and at SPring8, among others) and is leading to a promising project towards 'quantum crystallography'.

Another important approach was developed by Claude Lecomte's group, in parallel with Philip's group, and concerned the electronic behavior of proteins. A substantial database built on charge partitioning of molecular groups present in proteins was developed. Crystallography thus allowed this fundamental domain to be approached.

Philip also worked on structural evolution in phase transitions (*e.g.* the metal-insulator transition for TTF-TCNQ with Vaclav Petricek, involving incommensurate modeling) and charge-density evolution under an applied electric field. He also interacted strongly with Anatoly Volkov (from Siberia) and Tibor Koritzansky.

In 1997, Philip thought it was time to move to his 'childhood dream': photocrystallography. As usual, his intuition about which chemical compounds to study was correct. The first we tried was sodium nitroprusside (showing long-lived excited states), which was studied in the lab using laser flashes at low temperature. Then he used synchrotron sources, including at Brookhaven National Laboratory, with picosecond pulses, then the Argonne Advanced Photon Source. He welcomed many motivated young scientists from both Krzysztof Wozniak's and Claude Lecomte's groups, who became involved in fascinating new studies, such as those leading to the observation of the 0.28 Å contraction of Pt-Pt bonds in $Pt_2(P_2O_5H_2)_4^{4-}$ at 16 K for which the duration of the excited state was 50 µs. Then with Jason Benedict he developed studies of the time-dependent behavior of nanoparticles, again starting a new boundless area of solid-state science.

On October 22, 2016, Jason Benedict organized a retirement ceremony for Philip. It was an unforgettable day, where many collaborators came and enjoyed the strong long-term friendships that had started from their work with Philip.

Owing to his unique influence on developments in crystallography, Philip received many prizes, including the Aminoff Prize in 1996 and the Ewald Prize in 2005. He was President of the IUCr from 1993 to 1996, a member of the IUCr Executive Committee from 1987 to 1999, and a member of the IUCr Commission on Charge, Spin and Momentum Densities from 1972 to 1981, the Commission on Neutron Diffraction from 1975 to 1978 and the Commission on Journals from 2002 to 2015. His book *X-ray Charge Densities and Chemical Bonding* (IUCr/OUP, 1997) summarized in a highly pedagogical way the key aspects of his contribution to crystallography.

Philip remains an eternal guide for us, and his spirit will continue to guide international scientists.

*Pierre Becker, Acta Cryst. (2017). A**73**, 373-374*
https://doi.org/10.1107/S2053273317012475

OBITUARY

Davide Viterbo (1939-2017)



Davide Viterbo was a crystallographer, a chemist and a teacher, who will be remembered for his genuine love for science and research. Being endowed with great openness and humanity, he cultivated a variety of social and professional activities, aimed in particular at the national and international dissemination of science and culture.

On starting his career at the U. of Torino, Italy, in 1962, he pioneered X-ray diffraction techniques and mastered in crystal structure determination with the enthusiasm of the young chemist, being one of the first to start 'photographing' molecules and crystal structures. He realized how much there remained to do in methodologies, in particular concerning the solution of the phase problem, and moved into the theoretical area of direct methods. He managed to contact the most brilliant minds in the area, including Herbert Hauptman, the future Nobel laureate of 1985, and Michael Woolfson. In the late 1960s and early 1970s, he deepened his relation with Michael during long training periods in the UK (at the Universities of Oxford and York). People attending the historical 1974 Erice School on direct methods recall that Davide was already a recognized expert and a member of the teaching staff alongside other legendary names, including, besides Hauptman and Woolfson, 'stars' like David Sayre, Peter Main and others. On that occasion, Davide fully showed his natural skill for transforming complicated concepts into simple ones, as was apparent from his own lectures or just sitting next to him while attending seminars. His comments were never ordinary but enriched one's perception of the topic. The 1974 Erice School was also the start of a long-standing interaction with Carmelo Giacovazzo. As an apparent newcomer, the latter showed his already uncommon competence in all of the scientific discussions, thus anticipating his undisputed leadership in the field of direct methods. The partnership become highly synergic, in particular in Davide's role in the exploitation of Carmelo's innovative theories for the development and 'real-world' use of a computer package for structure solution (the SIR series), which has received worldwide attention and is still used now. The development of SIR was a complex task, which could be successfully fulfilled thanks to the full dedication of other excellent Italian minds such as various of Carmelo's pupils in Bari and collaborators from Perugia, Rome and Torino itself. Davide was also one of the authors of what can now be seen as the international crystallographer's bible, namely the textbook *Fundamentals of Crystallography*, edited by Carmelo Giacovazzo.

Davide Viterbo was highly respected among Italian crystallographers for his long and zealous activities on behalf of the Italian Crystallographic Association (AIC), of which he was one of the founders and then President from 1997 to 1999. He also worked at the international level, both in the IUCr and its Regional Associate, the European Crystallographic Association (ECA). For the latter, he served as a member of the Executive Committee in the years 2000-2002. Then in 2002 he was elected as a member of the IUCr Executive Committee, spending six years in that role. He chaired important committees, such as the Sub-committee on the Union Calendar (2008-2014), the IUCr/OUP Book Series Selection Committee and the Committee to select the winner of the eleventh Ewald Prize.

Davide was a highly respected Professor of Physical Chemistry at various Italian universities, where he contributed to the birth of new crystallography groups. Apart from his time in Torino, he founded from scratch the crystallography laboratories in Arcavacata di Rende (U. of Calabria, in the early 1990s) and in Alessandria (U. of Piemonte Orientale, since 1998). He raised funds for acquiring modern instrumentation and trained various young pupils, who went on to form flourishing research groups. As a spokesperson for these now not-so-young pupils, one of us (Milanesio) would like to emphasize the importance of Davide's role, formally as a supervisor and teacher, but also as a friend, advisor and supporter during every occasion in his pupils' scientific and personal lives.

As a scientist, Davide Viterbo produced a list of excellent publications, centered on direct methods in his early career and then on the extraction from single-crystal experiments of useful relations between the stereochemistry of molecules and materials with their properties. In the last two decades, with his keen foresight, he extended his interests to molecular modelling and powder diffraction, and these in combination with other techniques. It was an indication of his genuine passion that, at the AIC International School in Camerino, Italy, in 2011, he titled one of his memorable lectures *Love Diffraction, But Do Not Let It Alone!* In 2010 in Oviedo, Spain, he was awarded the first MISCA gold medal by the joint Italian and Spanish Crystallographic Associations for his work in disseminating crystallographic culture (he is proudly showing the MISCA medal in the photograph). On the occasion of his retirement in 2011, he was awarded a medal for his priceless contribution to the thriving of the association.

On all occasions Davide showed the greatest enthusiasm for tackling scientific and social tasks. An excellent storyteller, he recently presented numerous anecdotes about the history of crystallography and science, such as his personal memories of Herbert Hauptman and unprecedented viewpoints on personalities such as Primo Levi, Eligio Perucca and other historical characters. In January 2017, he reviewed the history of crystallography in Italy during the celebrations for the 50th anniversary of the AIC. Davide had a natural intellectual honesty and never indulged in any academic trickery. He also always offered unconditional support to people who asked for his help. In this respect, one of us (Carlo Mealli), as the Chair of the Florence IUCr Congress in 2005, wishes to express his eternal gratitude to Davide for the continuous encouragement and precious suggestions that transformed the event into a success.

The final words must be devoted to his beloved and now bereft wife, Mariella, who was always at Davide's side during his worldwide activities and represented for him an unconditional point of reference.

Carlo Mealli and Marco Milanesio, Acta Cryst. (2017). A73, 375-376
https://doi.org/10.1107/S2053273317011500

AWARDS AND PRIZES

The W. H. & W. L. Bragg Prize

A new Prize in the name of W. H. & W. L. Bragg has been established by the IUCr, in honour of the father-and-son team William Henry Bragg and William Lawrence Bragg. Both father and son were responsible from 1912 onwards for establishing the then new scientific discipline of X-ray crystallography. As a result, they both shared the Nobel Prize in Physics in 1915, W. L. Bragg still, at the early age of 25, being the youngest Nobel Prize winner in a scientific discipline.

Unlike most scientific awards that go to well-established scientists, often towards the ends of their careers, this Prize is to be awarded to one or possibly two promising crystallographers. This is very much in line with the characters of the two Braggs, who were instrumental in encouraging young scientists, both men and women without discrimination, to take up the field of crystallography. Their encouragement resulted in many young crystallographers achieving considerable distinction, for example the Nobel Prize winners Dorothy Hodgkin, Max Perutz and John Kendrew as well as Francis Crick and James Watson.

This Prize will be awarded at future IUCr Congresses, starting with the next one in 2020 in Prague, Czech Republic (http://www.iucr25.org). In order to deal with this, a special committee is being set up under the Chairmanship of David Billing (Dave.Billing@wits.ac.za) of South Africa, with the aim of establishing the working procedures to be used in selecting suitable persons for the Prize. Particular emphasis will be given to finding candidates who are at the early stages of their career, for whom this Prize would be of most benefit. The committee is tasked to take into consideration the different educational systems throughout the world and, for instance, what constitutes 'early stage' in different countries. It is intended that the Prize will be global in nature, including consideration of candidates from the developing world as well as from the developed world.

The financial value of the Prize is yet to be determined, but it should be substantial, depending on IUCr funds at the time. The decision on the actual value of the Prize to be awarded will be decided by the IUCr Finance Committee closer to the Congress year. It is intended that this award will be highly prestigious and given a special, high-profile place during the Congress. This will be determined in consultation with the Congress organiser.

Given the IUCr's financial situation, it is hoped that the Prize fund will eventually be self-sustaining. In order to build up a fund, donations from private individuals as well as from commercial companies and academic institutions will be welcome, in return for recognition if required. Those interested in donating to this Prize should contact Mike Glazer (glazer@physics.ox.ac.uk) or Jonathan Agbenyega (ja@iucr.org).

Mike Glazer

AWARDS AND PRIZES

Yue Deng wins fifth PANalytical Award





Yue Deng (center) with his supervisors, Christian Masquelier (U. of Picardie) and M. Saiful Islam (U. of Bath).

The PANalytical Award 2016 has been won by Yue Deng, a former PhD student at the U. of Bath (UK) and the U. of Picardie (Amiens, France). His article about fast lithium-ion conduction in solid electrolytes was highly rated by the selection committee who especially mentioned the excellent quality of the comprehensive work described in the paper. The winning article was selected from a record number of more than 100 contributions from young scientists all over the world.

Dr Deng and his co-authors were delighted by the good news. He said: 'This award is a great acknowledgement for the value of our work, and a great encouragement for me to apply my knowledge of diffraction and crystallography in my career.' He will receive the PANalytical Award in Shanghai, China, where he is currently working. More information about the award can be found here.

AWARDS AND PRIZES

Aminoff Prize awarded to Piet Gros



Piet Gros

The Royal Swedish Academy of Sciences has awarded the Gregori Aminoff Prize in Crystallography for 2018 to Piet Gros (Utrecht U., the Netherlands) 'for his fundamental contributions to understanding the complement system-mediated innate immune response'. The prize amount is SEK 100,000.

Prof. Gros received his PhD in 1990 from the U. of Groningen, the Netherlands. After postdoc studies at ETH Zürich in Switzerland and at Yale U., USA, in 1994 he returned to the Netherlands and founded a research group at Utrecht U. He is a member of the European Molecular Biology Organization and the Royal Netherlands Academy of Arts and Sciences. He has been the recipient of numerous scientific prizes, including an ERC Advanced Grant and the Spinoza Prize.

The complement system plays an important role in the body's defences against bacteria and viruses. When the complement system is activated, more than 30 different proteins interact in a highly intricate cascade-like manner. Prof. Gros has determined the three-dimensional structures of many complement proteins, studied the complicated protein complexes formed by these proteins, and succeeded in clarifying their three-dimensional structures. He has been able to describe the molecular mechanisms that lead to the activation of the complement system and explain their effects on the immune system. Congenital and acquired defects in the complement system have proven to be the cause of many medical conditions. The structural information produced by Gros' research is a foundation for the development of new treatments for autoimmune, inflammatory and degenerative diseases.

The Prize Ceremony will be held at the Royal Swedish Academy of Sciences' Annual Meeting on April 13, 2018. The Prize Lecture will be given on April 12, at Lund U., Malmö, Skåne U. Hospital, Sweden.

The Gregory Aminoff Prize rewards a documented individual contribution to the field of crystallography, including areas relating to the dynamics of crystal structure formation and dissolution. More information is available at http://www.kva.se/en/priser/gregori-aminoffs-pris.

ADVERTISING FEATURE

EIGER2 X detectors for the brightest X-ray sources

DECTRIS
detecting the future



The DECTRIS team in front of our booth at the IUCr Congress.

At the 24th IUCr Congress in Hyderabad, India, DECTRIS announced the EIGER2 X detector series, the latest Hybrid Photon Counting (HPC) detector for synchrotron applications. Over the last decade, HPC detectors have revolutionized X-ray sciences. For example, half of all new structures released by the Protein Data Bank are based on data acquired with DECTRIS HPC detectors. The new EIGER2 X detectors will allow researchers to answer more challenging scientific questions at the brightest new synchrotrons.

HPC technology is based on the direct detection of X-ray photons in a semiconductor with dedicated readout electronics for each pixel. By comparing the signal to a reference value in every pixel, electronic noise and possible fluorescence can be suppressed, and single-photon counting is enabled. Accurate data can be collected with superior signal-to-noise ratios. As a result, our users get better crystal structures, obtain more detailed structural information and extract more useful information from radiation-sensitive samples.

The parallelization of the readout system dramatically cuts down readout times. Acquiring a full data set is reduced to a few minutes at most, which opens up possibilities for high-throughput ligand screens, time-resolved studies of dynamic systems and high-speed characterization of heterogeneous samples. High frame rates combined with millisecond readout times enable shutter-less data-acquisition protocols and scanning of large sample areas with small step sizes. With a dead time of only 3 µs, EIGER detectors enable fine ϕ slicing at the highest angular speeds, again increasing the quality of the data that can be collected from a given crystal (https://www.dectris.com/ultrafine_slicing - see our success story).

Diffraction-limited storage rings with optical systems of corresponding quality enable much higher photon fluxes on the sample. The brilliant new X-ray sources that have already started operation or are under construction will provide unmatched opportunities to the crystallographic community. Small-angle X-ray scattering can be combined with stopped-flow devices to study reactions as they happen. The potential deterioration of battery materials with rising temperature can be visualized *in situ*. Protein microcrystals can be delivered to the beam in microchips holding hundreds of samples or even in liquid or viscous jets. Increasingly challenging biological systems can be understood in greater detail (https://www.dectris.com/Cpf1 - see our success story).

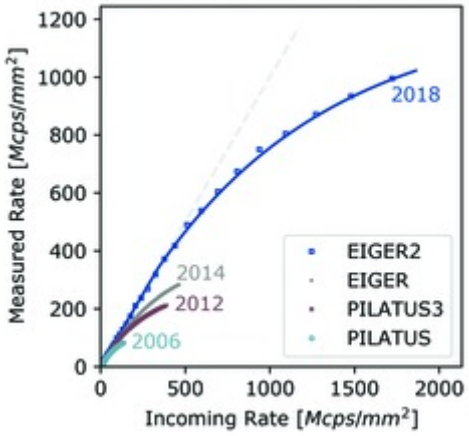


Fig. 1. Progress in count-rate capability of different detector generations.



Fig. 2. EIGER2 X detector series.

The prospect of peeking into the unknown with ever-brighter X-ray sources is the main driving force behind our detector developments. For this, a high count-rate capability is particularly important. DECTRIS has always set the pace in this field. PILATUS3 introduced instant retrigger technology, which substantially extends the count-rate capability. EIGER broke the record for count rate per unit area. EIGER2 X takes photon counting a big step forward. Featuring DECTRIS instant retrigger technology, it supports count rates up to 2 × 109 counts/s/mm^2 (Fig. 1). 'With the new EIGER2 X detectors series we match the power of 4th generation synchrotrons. I can't wait to see these system performing in the field', says Stefan Brandstetter, Head of Product Management at DECTRIS.

EIGER2 X detectors (Fig. 2) will be available early in 2019. Get a quote now at https://www.dectris.com to prepare your beamline for the future with an EIGER2 detector.

ADVERTISING FEATURE

Choosing a diffractometer - navigating a minefield of technology and jargon



On average, laboratories look to replace their diffractometers every ten years due to new technology becoming available, research taking a new direction or the need to replace aging parts. Starting your own research group - or setting up a central facilities laboratory - often requires a diffractometer that will ensure that your highest quality publications are supported with the gold standard of analytical techniques: a single-crystal X-ray structure.

Term	Translation	Meaning
HPAD	Hybrid Pixel Array Detector	Photon counting detectors including PILATUS, EIGER and HyPix detectors
CPAD	Charge-integrating Pixel Array Detector	Integrating detectors with glass taper or stub; including CCDs and CMOS/CPAD detectors

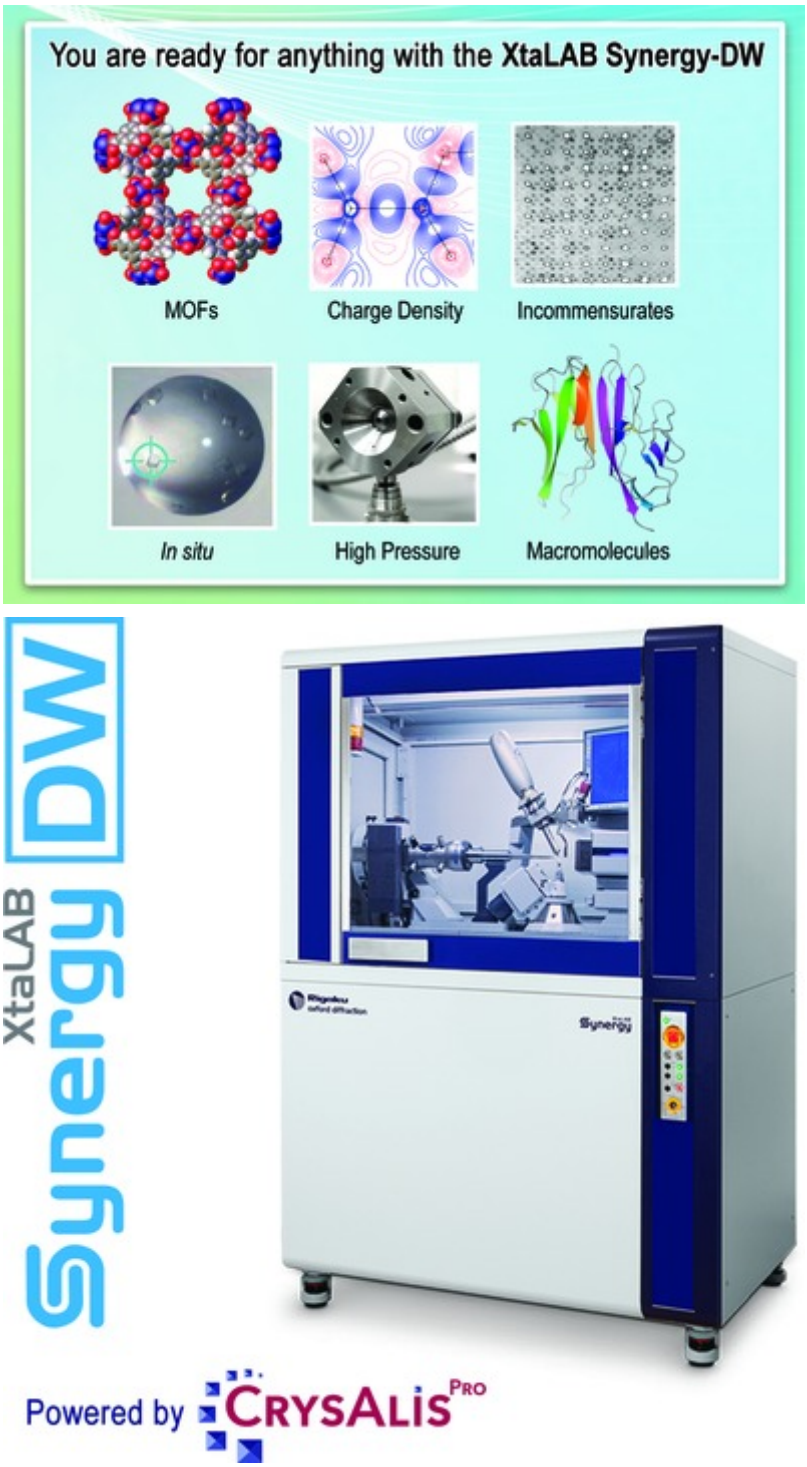
Commonly used X-ray detector jargon.

Purchasing a new X-ray diffraction system can be a time-consuming and difficult process, where the user needs to rapidly become an expert in the latest technology. Since this is a decision only made infrequently, the task can be daunting, especially with all the jargon associated with the technology.

Common but significant concerns during the purchase of a system are to ensure that (1) your investment will meet your changing research requirements over the course of the next ten or more years, and (2) you have a reliable system that will not require significant maintenance downtime or costs.

Rigaku understands these issues and has a solution that addresses these concerns. As there is no precise way to know which direction your research will take, why not have:

- one source capable of producing two wavelengths
- a high-flux source for even the most challenging small molecule or protein samples
- the latest technology HPAD detector
- a fully integrated system in a compact cabinet controlled by one user-friendly, powerful software program



In straightforward terms, the **XtaLAB Synergy-DW** diffractometer combines the increased flux of a rotating anode source with the flexibility of two different wavelengths, making it ideal for laboratories exploring a wide range of crystallographic research interests. The system is based on Rigaku's proven, low-maintenance MicroMax-007 HF microfocus rotating anode. The target is constructed with two different source materials (Cu and Mo, for example) and is coupled with an auto-switching dual-wavelength optic, meaning that you can select between copper and molybdenum X-ray radiation at the click of a button. The XtaLAB Synergy-DW offers up to 30x higher flux compared to the standard sealed tube sources, and utilizing only one generator means overall maintenance is reduced. Rounding out the XtaLAB Synergy-DW configuration is Rigaku's fast and efficient four-circle kappa goniometer, which is compatible with HPAD detectors, including the HyPix-6000HE.

At Rigaku, we like to refer to the XtaLAB Synergy-DW as the 'Swiss Army Knife' of diffractometers, as it is possible to gain high-quality data on a range of samples, from MOFs to macromolecules. No matter where your research leads you, this system will be ready.

One of the best ways to evaluate a system is to actually collect data on it to see how it performs on typical samples from your research lab. It is all too easy to become lost in the technical specifications and numbers of component parts when the data should speak for itself. Since we believe so emphatically in the superior performance of our systems, we welcome you to visit one of our application laboratories around the world for a demonstration using your own samples.

ADVERTISING FEATURE

Benefits of hard X-ray radiation

X-ray powder diffractometers are generally equipped with X-ray sources using Cu anodes. For specific applications, however, switching to shorter wavelength 'harder' radiation, like that obtained from X-ray tubes with Mo or Ag anodes, gives significant improvements over Cu, or even allows experiments that are impossible to do with Cu radiation. Often, people make use of synchrotron radiation, but new developments on source, optics and detector technologies allow a variety of hard radiation experiments in the home lab.

Below we present some of the key advantages of hard radiation.

Larger penetration depth

	Cu (1.54 Å)	Mo (0.71Å)	Ag (0.56 Å)
Al	60	572	1131
Cu	17	18	35
Steel	4	28	54
W	2	4	8
Inconel	7	26	37
Fe_2O_3	7	58	112
Co_3O_4	5	43	84
Si	54	527	1040
$LiFePO_4$	18	155	298

Table 1. Example of penetration depth in mm for different materials and different X-ray wavelengths.

For inorganic materials, the penetration depth of Cu *K*α is often only a few micrometres (see Table 1). In order to extract information from a larger sample volume, hard radiation is an advantage. Thanks to the larger penetration depth, it is possible to observe crystallographic changes in working devices, such as Li-ion batteries, and perform high-pressure experiments with diamond anvil cells. Hard radiation allows the use of transmission geometry for inorganic samples.

Optimizing the instrument

Effective excitation of hard radiation requires a higher acceleration voltage than used with Cu tubes. The Empyrean system is designed for continuous operation at 60 kV. X-ray tubes with Mo or Ag radiation, optimized to work with mirror optics, are developed in our in-house tube factory. The optical path is carefully optimized to prevent stray radiation, essential for proper PDF data free of instrument artifacts. The proprietary GaliPIX^{3D} detector based on Pixirad technology features a high-quality CdTe sensor allowing 100% detection efficiency up to 50 keV photon energy.

Better crystallographic information

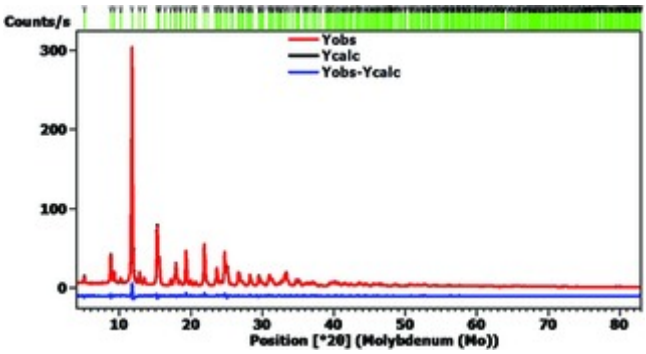


Fig. 1. Rietveld refinement of $Fe(IO_3)_3$ carried out with the *HighScore* suite [1].

Atom	Wyck.	x	y	z	B_{iso}(Å²)
O_1	6c	0.4772(2)	0.1879(2)	0.2686(3)	0.47(3)
O_2	6c	0.1319(2)	0.5499(2)	0.2191(3)	0.55(3)
O_3	6c	0.0566(2)	0.2238(2)	0.1212(4)	1.36(3)
I	6c	0.02189(1)	0.33716(3)	0.3636(1)	0.861(2)
Fe	2b	1/3	2/3	0.000000	0.483(7)

Table 2. Atomic coordinates obtained from the Rietveld refinement for $Fe(IO_3)_3$.

Preparing samples in glass capillaries is the best way to minimize preferred orientation effects of powdered samples. Working with Mo radiation in combination with optics focusing on the detector allows the usage of large-diameter capillaries which increases the irradiated volume of the sample without a loss in angular resolution or excessive absorption problems. Moreover, the use of Mo radiation suppresses the fluorescence from transition metal ions. In this example, we present a detailed investigation of the crystal structure of $Fe(IO_3)_3$ from powder data. Table 2 reports the atomic coordinates derived from the Rietveld refinement. As expected, we obtained an excellent precision of the position of the iodine atom but also of the lighter atoms such as the oxygen atoms. In particular, the error bars on these lighter atoms are 10 times better than previously reported [2,3].

In operando studies of batteries in the lab

Batteries are complex systems and in order to understand their functioning in detail it is important to be able to measure their phase composition and structure in real time and under non-equilibrium conditions [4]. This is possible with X-rays by using radiation that is sufficiently penetrating to go through pouch cells or thin prismatic batteries. Moreover, the possibility of performing such measurements in the home lab is crucial for aging studies, which are typically time consuming since the battery needs to be charged and discharged a large number of times.

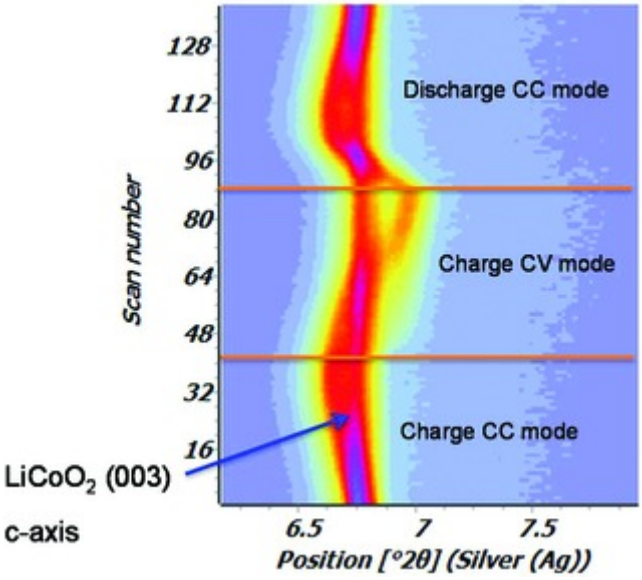


Fig. 2. Intensity of the (003) reflection of $LiCoO_2$ peak during one charge/discharge cycle.

In Fig. 2 is possible to see the modification in intensity and peak position for a $LiCoO_2$ cathode during a charge and discharge cycle. The so-called 'unit-cell breathing' is clearly visible, due to insertion of lithium ions in between the cobalt oxide layers which results in peak shift; but also the fact that part of the cathode material is not participating in the charge-discharge cycle and therefore reduces the charge capacity of this specific cathode. This information is of great value to battery manufacturers since understanding it can result in better batteries to fuel our future devices and cars.

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[1] T. Degen *et al.* (2014), *Powder Diffraction*, **29** (S2), S13-S18.

[2] M. Jansen (1976), *Journal of Solid State Chemistry*, **17**, 1-6.

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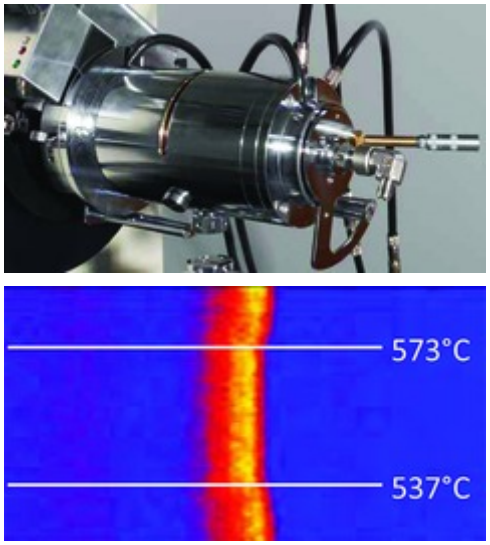
[4] V. K. Peterson *et al.* (2017), *IUCrJ*, **4**, Part 5, 540-554.

ADVERTISING FEATURE

Innovations in powder XRD - fast measurements in Debye-Scherrer geometry

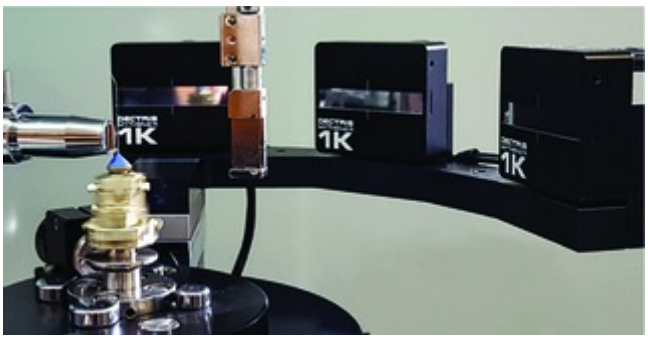
Founded in 1887, STOE is celebrating its 130th anniversary this year. STOE has been synonymous with superior quality and customer orientation. To celebrate this anniversary and to underscore its high-quality approach, STOE has launched its 10 Year Extended STOE Parts & Labor Guarantee for ALL new STOE Single-Crystal and Powder XRD systems.

Furthermore, STOE has presented new instrumentation to facilitate exciting powder XRD experiments:



Phase transition from α to β-quartz and back in a heating up and cooling down process.

STOE INSITU HT2 is the first commercially available *in situ* heating and reaction chamber in Debye-Scherrer mode for small sample amounts (5-20mm^3) in a temperature range from RT to 1600°C and gas flows between 0.01 to 0.1 l/min. It allows studies of solid state or solid state-gas reactions in capillaries on all vertically mounted STOE transmission diffractometers with Mo or Ag $K\alpha_1$ radiation.



STOE MULTI-MYTHEN DETECTOR has been developed to afford ultra-high resolution data collection in shortest measuring times. Depending on the sample material, excellent powder data can be collected with a MULTI-MYTHEN 3K from 2 to 110° 2θ in less than a minute, from 0 to 54° 2θ in only a few seconds. See the latest STOE newsletter for details on the results of an LaB_6 measurement, or contact STOE.

Both accessories are available for the STOE X-ray powder diffractometers STOE STADI P and STOE STADI MP.



STOE's STADI MP combines the two most common diffractometer configurations: transmission/Debye-Scherrer and Bragg-Brentano geometry. The change between geometries is done in only a few minutes, without the need for any realignment. All geometries of STOE STADI MP and STADI P are running with pure Co, Cu, Mo or Ag $K\alpha_1$ radiation.

ADVERTISING FEATURE

Emily ensures your screens are perfect every time



At Molecular Dimensions Ltd, we develop many of our products in collaboration with academics. After our product development team has created a new prototype, our production manager, Emily Harrison, has to scale that up to make a product for sale on our website.

How did you get the job of production manager?

I was first employed as a lab technician nearly 9 years ago and was then put in charge of custom production. The opportunity then arose to become Production Manager and I took it.

What qualifications do you have, did you do additional training?

BSc (Hons) Cell and Molecular Biology, Leadership skills training.

What's the first thing you do when given a prototype screen?

Check the availability and cost of the components. Also how safe the chemicals are for the lab staff to use.

What things do you commonly have to change when moving from a prototype to a full-scale product run?

Concentrations of components, particularly phosphates, pH of some buffers if they do not mix well.

What goes wrong?

Solubility problems, resulting in a potential change in the concentrations.

What common questions do people ask about screens?

Composition of individual conditions and how they are made. Specifically, which titrants are used to adjust our buffers.

Do you have any recommendations for how to get the best from Molecular Dimensions screens?

Use them as fresh as possible and store at 4°C.

Finally, what is the best thing about your job?

The variety that comes with the job and the day to day challenges.