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IUCR JOURNALS NEWS

Are you happy with your online persona?



What is the first item you see when you google your name? For many it will be a Facebook page, or maybe LinkedIn or Twitter. Whichever one it is, your online presence is now just as important as your physical day-to-day presence.

There are many tools and services available now to help build and maintain your online profile, tools such as ResearchGate, ORCID and your own departmental university page. All provide targeted content for those looking for experts in the field or to network and grow their community even wider.

Many will be satisfied with their online presence but for many professional scientists who also need this online exposure as a way to share and communicate their science with the global community, it is important to focus on the key messages you want to convey to the rest of the world so you become the authoritative figure in your field of research and the natural go-to person when scientists are searching your area of science online.

Alongside the aforementioned sites, researchers may want to consider blogging. A blog can provide you with a platform to communicate in a more liberated way. A successful scientific blog can give your community a true sense of who you really are; at the end of the day, this is what people want to know. How you present yourself, what are your interests, are you someone ultimately they can connect and work with?

For young research workers it can help improve their writing skills. It can also help them think about areas of communication and networking and how others may interpret them and their results.

A blog can help you promote yourself and what you are doing. It can publicise your name within a targeted community and it can help you build an effective and long-standing reputation within your chosen field, something that might be difficult or impossible to do until you have a quite a number of publications or have travelled extensively in the field to conferences and different research groups.

In a survey of 620 science bloggers, bloggers most often mentioned having started their blogs to practise their non-technical writing skills and to educate or explain science to a non-specialist audience. Motivations to continue blogging vary slightly to what might encourage you to begin, from developing an online writing portfolio, for instance, to blogging to explain, educate and popularise science. In general, what motivates scientists to continue blogging addresses the areas of outreach, self-improvement and enjoyment.

In a blog, the goal is not necessarily to publish breaking news or to explain. A new study reveals the primary goal of a blog is more to share the attitudinal aspects of science and society and to reach out to your colleagues and peers.

An excellent example for inspiration can be seen in the blog 'Reciprocal Space' by Stephen Curry of Imperial College, London, UK: http://occamstypewriter.org/scurry/. In a recent post, Professor Curry publishes an open letter requesting help in a project in which he is involved. Professor Curry cites the reason for using his blog: to widen the net of possible responses.

Having said blogs are an excellent vehicle to share comment and opinion on wider aspects in science and our society, they are also a popular way to share sometimes a more accessible version of your

recently published research article, with key messages summarised in about 1000 words, with the idea that it might reach a wider, more diverse audience who then have a vehicle to comment or contact you directly.

As you complete your next paper maybe take a second to have a look at your online profile and ask yourself, is this really me?

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

IUCR JOURNALS NEWS

The birth of IUCrData: a new era in data publication

The IUCr is delighted to announce the launch of a new open-access data publication, *IUCrData*. This innovative publication aims to provide short descriptions of crystallographic datasets and datasets from related scientific disciplines, as well as facilitating access to the data.

The first phase of this venture enables authors rapidly to publish brief, peer-reviewed *Data Reports* on individual crystal structures, making them readily available to the scientific community.

A global team of 25 editors forms the editorial board of *IUCrData*, bringing a wealth of experience and enthusiasm to the new data publication.

Data Reports in *IUCrData* include the following components:

- a short abstract
- an interactive 3D structure representation
- a structure description section
- a synthesis and crystallization section
- relevant figures
- tabular structural data
- literature references.

A key characteristic of *Data Reports* is the brevity of the discussion. The metric data and plots appear in the main body of the publication and provide the bulk of the information. Readers are able to access the complete diffraction data, the submitted crystallographic information file (CIF) and the full checking output.

By using the IUCr's *publCIF* software, which can be downloaded free of charge from http://iucrdata.iucr.org/services/cif/publcif/, submitting a *Data Report* to *IUCrData* is easy.

To find out more about the new open-access data publication *IUCrData* and keep up to date with announcements on future phases of this project, go to http://iucrdata.iucr.org.

IUCR JOURNALS NEWS

SESAME moves closer towards completion



Delegation in the experimental hall of SESAME.

There are some 60 synchrotron-light sources in the world, including a few in developing countries, but none in the Middle East. SESAME, which is a major facility under construction near Amman, Jordan, will not only be the first light source in the Middle East but also the region's first true international centre of excellence.

The aim of SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) is to foster scientific and technological capacities and excellence in the Middle East and neighbouring regions and help prevent or reverse the brain drain in the region by enabling world-class research in subjects ranging from biology and medical sciences through materials science, physics and chemistry to archaeology, much focused on issues of regional importance, *e.g.* environmental studies, health and agriculture. SESAME will also build scientific links and foster better understanding and a culture of peace through collaboration between different creeds and political systems.



(l-r) SESAME Director Khaled Toukan, CERN DG Rolf Heuer, CERN-SESAME Collaboration Coordinator Jean-Pierre Koutchouk and current SESAME President Sir Chris Llewellyn Smith admiring the magnets.

The council and advisory committees of SESAME met during the last week of November 2015 in Amman. It provided an opportunity to see the progress of the SESAME instrument and experimental beamlines. The construction project, defined as the storage ring and two beamlines (one for IR applications and the other for XAFS/XRF applications), is expected to be completed in early 2017. The macromolecular crystallography beamline, to be based on an in-vacuum undulator, received a boost with an initial grant of USD 2M given by Jordan Scientific Research Support Fund, a financially and administratively independent government institute responsible for encouraging and supporting scientific research in Jordan. The support came in response to a proposal jointly submitted by SESAME and Jordan U. for funding of construction of the macromolecular crystallography beamline and laboratory. This beamline, together with the materials science beamline based on a multipole wiggler, is expected to come online in early 2018, completing the suite of four beamlines due in Phase 1 of the project.



Installation of the 2.5 GeV storage ring has started. One of the 16 cells of the SESAME storage ring assembled on the girder. The components were constructed in collaboration between SESAME members and observers with the magnet assembly coordinated by CERN. The dipole magnets were manufactured in the UK, sextupole coils in France, quadrupoles and girders in Spain, vacuum chambers in Germany, sextupoles in Pakistan and quadrupole coils in Turkey.

The additional funding by a number of member countries supplemented by an EU grant has proved a pivotal point as the facility enters its final stages of construction. In addition to the extra funding by a

number of member countries, Italy, which is an observer country, has provided EUR 1.8M for the RF cavities. The European Commission (EC), which became an observer of SESAME in 2015, has provided EUR 5M to the construction of the magnetic system for SESAME's storage ring being led by CERN.



SESAME with its new white roof.

Staff numbers have gradually increased to 41, of which 28 are professional scientific and engineering staff directly involved in the construction project of the machine and Day-One beamlines. The staff strength is expected to increase to 67 by 2018.

Representatives of the member and observer countries' Governments as well as several other agencies including International Atomic Energy Agency (IAEA) and International Centre for Theoretical Physics (ICTP) attended the council meeting. On this occasion, EU Ambassador HE Mr Andrea Matteo Fontana said, 'We are delighted that we have become an observer of SESAME. In view of its importance of science cooperation and regional harmony we have invested close to USD 15M and have allocated a specific topic within the next framework to strengthen regional cooperation - step up our support so that we can help realise its full potential. Some earmarked funds are announced for training and capacity. Science diplomacy is very important in this complicated world.'

Samar Hasnain, SESAME Council Observer Delegate (UK) and Editor-in-Chief of IUCr Journals

As reported in Volume 22, Number 1 (2014) of the IUCr Newsletter, the IUCr has been pleased to support the SESAME project by providing free online access to IUCr Journals for 2014-2016 as part of the IYCr2014 celebrations.

IYCR LEGACY

Lighting the Way for a Brighter African Future

A movement is growing to construct an advanced light source somewhere on the African continent in the near future. It has been dubbed the African Light Source (AfLS) and has been long discussed within Africa and globally. To formally initiate that goal, many of those in the discussion called for nominations to an Interim Steering Committee for the AfLS (ISC-AfLS). On August 18, 2014, the ISC-AfLS was formally launched on the Forum Day of the 'African School on Fundamental Physics and its Applications', held at the U. of Cheikh Anta Diop in Dakar, Senegal. ISC members represented a broad spectrum of countries from both inside and outside of Africa, including Egypt, Ethiopia, France, Japan, Nigeria, Rwanda, Senegal, South Africa, Sweden, United States and Zimbabwe.



Fig. 1. Group picture, 1st AfLS Conference and Workshop, ESRF, November 2015. (Photo courtesy of ESRF)



Fig. 2. Several researcher and student participants, 1st AfLS Conference and Workshop, ESRF, November 2015. (Photo courtesy of ESRF)

The role of the ISC-AfLS was to initiate a transparent, inclusive and democratic process, culminating in a Conference and Workshop, where it could dissolve itself so that a more inclusive, fully mandated Steering Committee for the African Light Source (SC-AfLS) could be elected. With that foundation, the vision of an AfLS would gradually be able to take form and mature, attracting support. Thus, a subgroup of the ISC and the leadership of the European Synchrotron Radiation Facility (ESRF) convened the First African Light Source Conference and Workshop during November 16-20, 2015, at the ESRF (Grenoble, France). Fig. 1 is a group photo of the participants, and Fig. 2 shows several of the researcher and student participants along with two traditional African ceremonial sticks. The larger stick metaphorically summoned the participants and 'allowed' the opening of the meeting, and each speaker held up the smaller stick, which gave the authority to speak. This was the first in a series of AfLS meetings, with most of the subsequent meetings to be held in Africa. The organizers decided that the first meeting's venue should be at a flagship international facility so that policymakers, students and others not familiar with advanced light sources would be able to tour a fully operational facility.

The first international AfLS meeting was a huge success. Divided into two parts, the first two days took the form of a conference that consisted of presentations on research at light sources by African scientists, as well as research by both Africans and non-Africans on topics highly relevant to Africa. The second part of the meeting was a workshop where the participants, numbering approximately one hundred, discussed strategy and policy. One of the main outputs of the workshop was the adoption of a set of overarching statements that provide the WHY for an AfLS. They decided to call those statements the *Grenoble Resolutions*, and they are as follows:

- Advanced light sources are the most transformative scientific instruments similar to the invention of conventional lasers and computers.
- Advanced light sources are revolutionizing a myriad of fundamental and applied sciences, including agriculture, biology, biomedicine, chemistry, climate and environmental eco-systems science, cultural heritage studies, energy, engineering, geology, materials science, nanotechnology, palaeontology, pharmaceutical discoveries, and physics, with an accompanying impact on sustainable industry.
- The community of researchers around the world is striving collaboratively to construct ever more intense sources of electromagnetic radiation, specifically derived from synchrotron light sources and X-ray free-electron lasers (XFELs), to address the most challenging questions in living and condensed matter sciences.
- The African Light Source is expected to contribute significantly to the African Science Renaissance, the return of the African Science Diaspora, the enhancement of University Education, the training of a new generation of young researchers, the growth of competitive African industries, and the advancement of research that addresses issues, challenges and concerns relevant to Africa.
- For African countries to take control of their destinies and become major players in the international community, it is inevitable that a light source must begin construction somewhere on the African continent in the near future, which will promote peace and collaborations among African nations and the wider global community.

To move the project forward, the participants also adopted a Roadmap to guide future activities. It consists of short- (within 3 years), medium- (within 5 years) and long-term (5 years and beyond) goals. Major activities in the short term include training large numbers of African scientists, engineers, students and technicians in the design and utilization of advanced light sources; enhancing the existing community of light source users; establishing formal partnerships with existing international light sources; promoting the involvement of industry; establishing and enhancing Africa's current and needed critical feeder infrastructure that empowers light-source science; promoting outreach and communication around light-source-based science; studying the feasibility of constructing African multinational beamlines at existing light sources, perhaps with partners from other regions of the world; developing a *Strategic Plan* for submission to African Ministries; and developing an AfLS non-site specific Pre-Conceptual Design Report, which specifies the scientific case for an AfLS along with its various components, including the accelerator complex, experimental beamlines and ancillary facilities. In the medium term, the main elements include studying the feasibility of constructing an AfLS, including costs, and appointing a Task Team approved by African governments to develop a detailed Business Plan and Governance Model for an AfLS. In the long-term, the Roadmap calls for the completion of an AfLS Technical Design Report that includes site selection and, when approved by a sufficient number of African governments, the construction of a fourth-generation light source with requisite infrastructure. Finally, to drive the Roadmap forward, the AfLS meeting participants and others *via* online balloting elected a fully mandated Steering Committee for an AfLS, with one of us (SHC) as Interim Chair.

By far the largest community of advanced-light-source users in Africa is in South Africa. Over the years, one of us (SHC) has documented that history. The first users were Trevor Derry and Jacques Pierre Friederich 'Friedel' Sellschop, both from the U. of the Witwatersrand (Wits). In 1994, Derry performed studies of diamond surfaces at both the ESRF and the Synchrotron Radiation Source-Daresbury

Laboratory (UK). During the same year, Sellschop participated in other diamond studies at the ESRF. In 1996, Giovanni Hearne, then at Wits and currently at the U. of Johannesburg, used the ESRF to study materials under extreme temperatures and pressures. From those experiences, he urged his government to study the feasibility of constructing a South African synchrotron light source in partnership with neighboring countries. Then in the 1999 timeframe, Bryan Doyle, also now at the U. of Johannesburg, served as a postdoctoral researcher at the ESRF. From those early efforts, the synchrotron-light-source user community started to grow.



Fig. 3. Group picture, Synchrotron Science Workshop, Pretoria, Dec 2011. (Photo courtesy of South African Institute of Physics)

To advocate for themselves, South African light-source users began to establish organizations, with one of the most successful being the Synchrotron Research Roadmap Implementation Committee (SRRIC), chaired by Tshepo Ntsoane of the South African Nuclear Energy Corporation, with Wolf-Dieter Schubert of the U. of the Western Cape as Deputy Chair. In collaboration with the South African Institute of Physics (SAIP), led by SHC as Council President and Brian Masara as Executive Officer, SRRIC convened a synchrotron science workshop during December 1-2, 2011, in Pretoria, which was attended by South African researchers and government policymakers, as well as a number of international partners, including Francesco Sette, Director General of the ESRF; Angus Kirkland of Oxford U., who served as Workshop Facilitator; Herman Winick of Stanford U. and SLAC National Accelerator Laboratory; and one of the authors (SKM). Fig. 3 provides a group photo of the meeting. The goal was to provide input into the development of a document entitled 'Strategic Plan for Synchrotron Science in South Africa', which was chaired by SKM. SRRIC and the SAIP submitted that document to South Africa's Department of Science and Technology and its National Research Foundation, the country's main funding agencies. One of its most important recommendations was for South Africa to enter into a formal financially supporting relationship with the ESRF. Indeed, that recommendation was adopted by the government and on May 21, 2013, South Africa signed a medium-term arrangement with the ESRF at a level of 0.3% of the ESRF budget and, in doing so, became the 20th member country of the ESRF.



Fig. 4. Countries with ALC member institutions. (Map courtesy of ALC)



Fig. 5. ALC organizers, Pretoria, November 2003. (Photo courtesy of ALC)



Fig. 6. Several participants, ALC Student Training Workshop, U. of Zambia, Lusaka, 2007. (Photo courtesy of ALC)

An excellent model already exists for African countries collaborating around a scientific theme. It is the African Laser Centre (ALC), which is a nonprofit organization based in Pretoria and consists of more than 30 member laboratories at universities and various research institutions across the African continent. Fig. 4 shows the countries with ALC member institutions. Launched in 2003, the ALC was the first to call for a pan-African synchrotron light source. From its inception, this has been one of its long-term goals as defined in its *2002 Strategy and Business Plan*. Fig. 5 is a group photo of the organizers, with the second from the right on the first row being Philemon Mjwara, the first ALC Board Chair and currently Director General of South Africa's Department of Science and Technology. Through its educational and research programs, the ALC awarded 87 grants during the period 2006-2013, allowing its participants to achieve a number of milestones. During that period, participants contributed 151 articles in refereed journals, 210 publications in conference proceedings, 12 book chapters and 59 student theses. Moreover, between 2003 and 2013, 1249 students were trained in workshops, symposia and various short courses. Fig. 6 shows several participants at a student-training workshop at the U. of Zambia in Lusaka during 2007.

As argued by Herman Winick and SKM in an article published on the lightsources.org website entitled 'A Synchrotron Radiation Research Facility for Africa' (www.lightsources.org/news/2014/09/05/synchrotron-radiation-research-facility-africa), the time is ripe for African governments to make the bold move and invest in a pan-African synchrotron light source in the near future. Highly successful models of such an international facility already exist. For example, the ESRF is a collaboration of 18 European governments, plus South Africa and Israel, and has been in operation since 1992. Even earlier, there was the high-energy physics laboratory, CERN (European Organization for Nuclear Research), in Geneva, Switzerland. Indeed, the CERN model has served well the SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) light source in the Middle East, which is scheduled to start its research program during 2016 (see 'SESAME moves closer towards completion' in this issue of the IUCr Newsletter). Concluding construction in Allan, Jordan, approximately 30 km from Amman, it is a collaboration of nine Middle Eastern governments, namely Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestinian Authority and Turkey. UNESCO serves as the umbrella organization for both SESAME and CERN. Thus, a proven path is already laid for an African Light Source.

Sekazi K. Mtingwa and Simon H. Connell

Sekazi K. Mtingwa, an accelerator and high-energy physicist, is a member of the AfLS Steering Committee, a founding Board Member of the ALC, retired from the faculties of MIT and North Carolina

A&T State U., and currently is Principal Partner at Triangle Science, Education & Economic Development, LLC, in the Research Triangle of North Carolina, USA.

Simon H. Connell, an accelerator, nuclear, high-energy and condensed matter physicist, is Interim Chair of the AfLS Steering Committee, Chair of the Organizing Committee for the First AfLS Conference and Workshop, former Council President of the South African Institute of Physics, and former Professor of Physics at the U. of Johannesburg.

The IUCr was represented at the First AfLS Conference and Workshop by Michele Zema (IUCr Outreach Officer). Michele Zema and Claude Lecomte (Chair of the IUCr Crystallography in Africa initiative) are both members of the AfLS Steering Committee. Please send any ideas about projects to help implement the AfLS to Michele (mz@iucr.org).

IYCR LEGACY

First India-Bangladesh Structural Chemistry Conference

Kolkata, India, September 2015

The two neighbouring Asian countries India and Bangladesh share a long history and culture, but have hardly any scientific ties. With the intention to break this artificial barrier, the first India-Bangladesh structural chemistry conference was held at the Indian Institute of Science Education and Research (IISER), Kolkata, India during 18-19 September, 2015. The focus of the conference was to discuss and acknowledge recent advances in the field of crystal engineering happening in East Asia. This bilateral conference, co-organized by C. Malla Reddy (IISER Kolkata, India) and Altaf Hussain (Dhaka U., Bangladesh) as part of the extended celebrations of the International Year of Crystallography 2014, dealt with the topics related to crystal engineering of small molecules and macromolecular structural chemistry, covering synthesis, structure and dynamics, which indeed are the issues at the heart of this contemporary multidisciplinary science.



Presentation of the IUCr prizes for the best student posters. Winners M. H. Mesbah Ahmed (Jagannath U., Dhaka, Bangladesh), Pritam Gosh (inset; CSIR-Central Mechanical Engineering Research Institute, Durgapur, India) and Rima Paul (Pandu College, Guwahati, India) are flanked by poster-prize judges A. Ramanan and Michele Zema on the left and convenor C. Malla Reddy and poster-prize judge M. Qumrul Hassan on the right.



The conference started with the inauguration by R. N. Mukherjee (Director of IISER Kolkata, India), followed by welcome addresses from Gautam R. Desiraju (IISc, India), C. Malla Reddy, Altaf Hussain,

Michele Zema (IUCr) and Rajesh Parishwad [Royal Society of Chemistry (RSC)] and then the Inaugural Lecture by Pinak Chakrabarti (President, AsCA; Bose Institute, India). Next came the first scientific lecture by Kumar Biradha (IIT Kharagpur, India) on 'Crystal Engineering of Coordination Polymers', which was followed by Md Manzurul Karim (Jahangirnagar U., Bangladesh) talking about metal-sulfur-nitrogen-bonded complexes of manganese and rhenium; Sakhawat Hussain (Dhaka U., Bangladesh) about the optimisation of multiquantum well structure for high-efficiency yellow-green emission; and Debajyoti Ghoshal (Jadavpur U., India) about metal-organic frameworks. Other speakers on the first day were Alok Mukherjee (Jadavpur U., India), Md Nizam Uddin (Shahjalal U. of Science & Technology, Bangladesh), Ashok K. Varma (ACTREC, India), Syed Rashel Kabir (Rajshahi U., Bangladesh) and Arun K. Shukla (IIT Kanpur, India), who enlightened the participants about many interesting topics related to structural chemistry.

On the second day, Parthasarathi Dastidar (IACS, India) outlined an interesting project on 'Exploiting Supramolecular Synthons in Designing Supramolecular Gelators for Drug Delivery'. This was followed by scientific lectures from Md Anamul Haque (Dhaka U., Bangladesh), Binoy K. Saha (Puducherry U., India), Md Aftab Ali Shaikh (Dhaka U., Bangladesh), Soumyajit Roy (IISER Kolkata, India), A. K. M. Atique Ullah (Atomic Energy Centre, Bangladesh), Tejender S. Thakur (CDR, India), Md Abu Hasan Howlader (Bangladesh U. of Engineering & Technology, Bangladesh), Ranjit Thakuria (Gauhati U., India) and Linia Tashmim (Dhaka U., Bangladesh). Prizes for the best student posters were then presented by RSC and IUCr, and the day ended with a vote of thanks from C. Malla Reddy.

The gathering offered the opportunity for scientists and young researchers from India and Bangladesh to exchange their scientific ideas as well as to engage in cooperation and future collaborations.

C. Malla Reddy, Convenor

IYCR LEGACY

Bruker/CCDC OpenLab Senegal, 5-10 October, 2015



Hands-on lesson with the powder and single-crystal diffractometers.

The travelling laboratory concept was defined by UNESCO and IUCr in 2013 as one of the most important projects of the International Year of Crystallography: it is the conjugation of a conventional crystallography school with real hands-on experiments using single-crystal and powder diffractometers made available on site. In this way the students learn basic crystallography and diffraction to enable them to understand how to solve a structure (single crystal) or how to analyze a complex crystalline powder like clays, which are one of the most studied materials in Africa. To achieve this goal a strong collaboration has been built between IUCr, UNESCO and Bruker. Bruker shipped and lent for free two portable diffractometers to U. Ziguinchor. The teachers of the school were from African and European universities, large facilities and Bruker: L. Le Dréau (Bruker), A. H. Barry (U. Nouakchott, Mauritania), M. Camara (U. Zichinchor), P. Kenfack (U. Dschang, Cameroon), C. Lecomte (U. Lorraine, Vandoeuvre-les-Nancy, France), F. Porcher (LLB,CNRS/CEA, Gif sur Yvette, France) and J. Pradon [Cambridge Crystallographic Data Centre (CCDC), UK]. Drs Pradon and Le Dréau were supported by their own companies, whereas the others were supported by IUCr and AUPELF (Association des Universités Partiellement ou Entièrement de Langue Française). This diversity of the lecturers added value to the school. The diffractometers installed in Dr Camara's laboratory were used extensively during the school and until the end of October.



The participants of the Ziguinchor school, the first travelling laboratory in sub-Saharan Africa.

A total of 45 students attended the travelling laboratory; most were from Senegal with the remainder from Benin, Burkina Faso, Cote d'Ivoire and Madagascar. Two thirds of them were Master and PhD students and the others were chemistry, physics and pharmacy professors. The gender balance was excellent with approximately one third of the students and lecturers being female. The foreign students and the accommodation of most of the Senegalese participants were supported by UNESCO, IUCr and U. Ziguinchor. The programme of the school (www.iycr2014.org/openlabs) was divided into two parts: theoretical background (taught at the master level) and hands-on lessons. The difficulty of the school was that some students had had almost no previous crystallographic education (25%), some had some crystallographic knowledge and some were already able to solve structures (10%); all lecturers and tutors were aware of this disparity and dealt with it very well. The students were able to collect X-ray data from their own crystals and powder samples. They performed data reduction, crystal solution and refinement themselves under the tutors' supervision. Seven crystal structures were solved and 15 clays characterized; all resolved structures were unknown and will be submitted to *Acta Crystallographica* journals by all participating students. This will be published as a highlight of the school. Some of these new structures were analyzed using the Cambridge Structural Database as, thanks to CCDC, the software was freely available to students until the end of the year.



Visit of the Minister for Superior Education and Research to Dr Camara's laboratory.

The location, work conditions and accommodation of the school were perfect thanks to the rector of the University and to the local chair and his students, who made all participants feel at home. The ambiance of the school was extremely friendly with many fruitful discussions not only at the scientific level but also at a professional level, allowing future collaborations in crystallography between Senegalese universities to be built and person-to-person networking in western Africa and Madagascar to be established. Last but not least, Mary Teuw Niane, Minister of Superior Education and Research of Senegal, unexpectedly

visited the school and was impressed by its quality (his background is in mathematics). The subsequent discussions between the Minister and school lecturers and students about the role of crystallography in chemistry, physics, geology, life sciences and applied mathematics convinced him about the need for well equipped crystallography laboratories in Senegalese universities.

A questionnaire about the school was completed by all the students and fully confirms the quality of the school and the interest of the students in crystallographic methods: 33 students gave high grades for the quality (average grade 3.9/5); 15 students out of 33 attested that this school fitted very well with their expectations, and for 10 of them it perfectly fitted their expectations. Some students suggested the need to teach a preliminary course on Fourier transform and linear algebra. Also, 60% of the students asked for more documents to be deposited on the website in advance, and all doctorants and most professors asked for an internet book built from all the lectures. It was decided to write this ebook in French and make it freely available to all participants; UNESCO sponsorship would be welcome.

Claude Lecomte, scientific chair, and Magatte Camara, local chair

IYCR LEGACY

Bruker OpenLab Vietnam, 7-11 December, 2015



The second edition of the IUCr OpenLab Vietnam 2015 was held at the Faculty of Chemistry, VNU Hanoi U. of Science (VNU-HUS) in conjunction with Hanoi National U. of Education (HNUE) and the IUCr from 7 to 11 December, 2015.

The course was opened on Monday, December 7, with a welcome speech given by Phan Tuan Nghia, Vice-President of the VNU-HUS, followed by a short introduction to the IUCr and its worldwide activities by Luc Van Meervelt. After that, Prof. Van Meervelt initiated the audience in the field of symmetry and X-ray diffraction during an intensive three-day course. Throughout these lectures a number of exercise sessions were supervised by Nguyen Hung Huy (VNU-HUS) and Nguyen Bich Ngan (HNUE) further illustrating the theory of point, plane and space groups, as well as the concept of X-ray diffraction and structure factors.



Participants at the IUCr OpenLab in Hanoi, Vietnam.

During the last two days, a selection of the participants was divided into two smaller groups for a hands-on session, demonstrating crystal selection and mounting, and diffraction data collection. Additionally, a second group was able to perform data reduction, structure solving and refinement on their own with the assistance of Thanh-Ha Nguyen (Bruker AXS Singapore). Moreover, thanks to sponsorship from the

Cambridge Crystallographic Data Centre, the participants were introduced to the CSD Enterprise 2016 by tutorials during a hands-on session showing the use of the database during structural research.

Thanks to the financial support from the IUCr, VNU-HUS, HNUE and VLIR-UOS (Belgium), the OpenLab Vietnam 2015 could be organized successfully. The five-day course was intensive and very informative so that all participants were enthusiastic. In total, 82 participants attended the course, including 25 from outside Hanoi coming from universities in many regions in the middle and north of Vietnam. Notably, the variety in background of the participants proves that crystallography will play an important role in their future research. They all greatly appreciated the OpenLab's combination of theory and hands-on sessions, and hope to present their first results during the AsCA2016 meeting in Hanoi (www.asca2016.org/) and the IUCr Congress in Hyderabad, India in 2017 (www.iucr2017.org/).

Nguyen Bich Ngan, local organiser

IYCR LEGACY

Winners of the IUCr worldwide crystal growing competition 2015



Category 1, gold-medal-winning video.



Category 2, gold-medal-winning video.



Category 3, gold-medal-winning video.



Following the great success of the IYCr2014 competition, schoolchildren were invited to take part in the 2015 edition and convey their experiences of growing crystals through a video.

An international panel of judges has evaluated all the entries using the following criteria: creativity, aesthetic value, description of the working plan and experimental work, clarity of explanations and scientific background. Gold, silver and bronze medals were assigned to each of three categories based on the age of the participants.

Congratulations to all laureates! Enjoy watching the winning videos at www.iycr2014.org/participate/crystal-growing-competition-2015/winners.

Category 1: 15-18 (high-school upper forms)

Medal	Team name	School	Country
Gold	Lourdes R. Diaz - Mateo B. Martinez - Candelaria S. Molina	Escuela Industrial 'Domingo F. Sarmiento', San Juan	Argentina
Silver	Tessa Loh Yun Yi	Bedok South Secondary School	Singapore
Bronze *ex aequo*	Cecilia Caivano - Virginia Laguzzi - Catalina Seinhart	Colegio Nacional de Buenos Aires	Argentina
Bronze *ex aequo*	10A1-Xuan Hoa	Xuan Hoa High School	Vietnam

Category 2: 11-15 (high-school middle forms)

Medal	Team name	School	Country
Gold	Prerana Pai	Delhi Private School, Sharjah	United Arab Emirates
Silver	Krystalise	Presbyterian High School	Singapore
Bronze	Colon 2455	Escuela 'Luis Federico Leloir', Buenos Aires	Argentina

Category 3: under 11 (primary school)

Medal	Team name	School	Country
Gold	Alumnos de sexto grado	Escuela 'Luis Pasteur', Villa Urquiza, Buenos Aires	Argentina
Silver	3A El Cañaberal	Escuela No. 65 'Juana Elizalde de Urán', Treinta y Tres	Uruguay
Bronze	3B La Rama	Escuela No. 65 'Juana Elizalde de Urán', Treinta y Tres	Uruguay

FEATURE ARTICLE

War, Peace and Crystallographers



William Henry Bragg

X-ray crystallographers around the world have traditionally formed a closely knit community, even as the community size has increased significantly in the last 30 years. This community has recently seen a burst of celebratory activities around the world, and rightly so, as 2012 marked the centenary year of the discovery of X-ray diffraction. Moreover, to the delight of crystallographers around the world, 2014 was declared as the International Year of Crystallography by the UN. The discovery of diffraction by X-rays indeed marked a landmark development in modern science, and has had an enormous impact on our understanding of fundamental aspects of nature - possibly beyond even the imagination of its early proponents. From the very early days, it has been apparent that properties of matter depend upon relative juxtaposition of atoms within molecules, to the extent that properties of even highly complex biological assemblies can be understood elegantly by studying the relative positions of atoms in these assemblies. As early as in 1925, William Henry Bragg noted in his essay 'Concerning the Nature of Things', the title borrowed from Lucretius's two thousand year old treatise, that 'The properties of the metals must depend, in the first place, on the properties of the individual atoms, and, in the second place, on the atomic arrangement, which is in effect the state of crystallization'. Over the years following the early developments, as X-ray crystallography became an important tool to address properties of matter, the practitioners of this technique slowly spread over the world, many of them tracing their roots to the British school led by the father and son Braggs. Social closeness among crystallographers is therefore not surprising given the common roots amongst most of them.

One of the interesting aspects of being such a closely knit community appears to be that related to the involvement of X-ray crystallographers in issues of social importance from the very early days. It is not surprising that among the scientists that took upon themselves to address societal issues were leading figures such as J. D. Bernal, Kathleen Lonsdale, Linus Pauling and Dorothy Hodgkin, all of whom shared another passion - using X-ray crystallographic tools to understand nature. All of them strongly argued for participation of scientists in societal matters, apart from their own outstanding contributions to science. The fact that they were all in their prime in the period between the two world wars, and that they were all known to each other closely, might have prompted their passion for the constructive use of science in society.



William Lawrence Bragg at the Third Congress and General Assembly of the IUCr in Paris, France in 1954. Photo contributed to



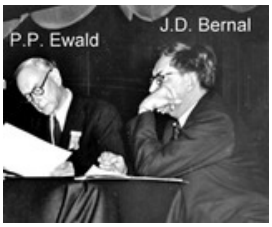
Linus Pauling at the American Crystallographic Assn Annual Meeting in Philadelphia, PA, USA in 1988. Photo



Kathleen Lonsdale at the Eighth Congress and General Assembly of the IUCr in Stony Brook, NY, USA in 1969. Photo contributed to the IUCr archive by Sidney C. Abrahams.



Dorothy Hodgkin at the Ninth Congress and General



J. D. Bernal sits alongside P. P. Ewald at the Third Congress and General Assembly of the IUCr in Paris, France in 1954. Photo contributed

the IUCr archive by William L. Duax.	contributed to the IUCr archive by William L. Duax.		Assembly of the IUCr in Kyoto, Japan in 1972.	to the IUCr archive by William L. Duax.

Even before crystallographers began involving themselves in the cause of promoting peace in the world, there were disturbing events due to the mindless violence of the two wars. Three of these related to iconic crystallographers deserve special mention. Foremost of these names are the Braggs and Moseley. Both of William Henry Bragg's sons had been drafted into military service during the First World War. Robert Bragg was posted to the Turkish front and died in an attack at Gallipoli. William Henry Bragg apparently never recovered from this personal loss, and consequently refused to travel to Stockholm to receive his Nobel Prize. His other son, with whom he shared the Nobel Prize, William Lawrence Bragg, eventually delivered the Nobel lecture and received the Prize, but nonetheless skipped the originally planned Prize ceremony.

Moseley had discovered the famous relationship between X-ray emission wavelength and atomic number of an element. This stunning discovery eventually led to the reorganization of the Periodic Table according to atomic number, instead of atomic weight as had been the practice earlier. He had learnt the technique of measuring X-ray spectra during a visit to William Henry Bragg's laboratory at Leeds. However, his brilliant academic career was cut short by the war in 1915. Moseley's death at the young age of 27 while fighting in the war at Gallipoli has been described by some authors as the single most costly death to mankind due to war. Indeed, what he might have achieved as a scientist in later years was cut short by the tragic event.

An unfortunate incident related to the ugliness of wars and historical monuments is related to that of Röntgen's famous house. The house where he had made one of the most profound discoveries of mankind - X-rays - was razed to the ground during the bombing of Wurzberg. Röntgen had passed away in the intervening period between the two wars, but ironically the house where he made the discovery was destroyed by bombing in his centennial year.

Kathleen Lonsdale is widely known as one of the first two ladies to be elected to the Royal Society. She was also the first woman President of the International Union of Crystallography. Her tutelage under William Henry Bragg and the first experimental evidence for the structure of benzene in 1929 have been as famous as her staunch anti-war personality. An important aspect of Lonsdale's remarkable personality is that despite the frenzy created in society about the imminent conflict, Kathleen Lonsdale refused to participate in the war when she was recruited by the armed forces. Although she could have reportedly sought pardon as her children were under the age of 14, she refused to do so for what she felt was denial of civil liberties. She demonstrated extreme courage by not paying the fine for refusing to do so, choosing instead to go to jail for this brave act of hers. Her forthrightness and anti-war sentiments have been recorded in her book on Removing the Causes of War.

Historians will debate whether these incidents had any influence on the likes of J. D. Bernal, Dorothy Hodgkin and Linus Pauling to take up the crusade for peace. Bernal, although he participated in the war by being the chief scientific advisor to the British Army, made compelling arguments on the value of science on societal development. In his highly influential book, The Social Function of Science, he notes that 'The millions who had suffered in the last War are aware that to a large extent their sufferings were directly due to scientific developments, and that science, far from having brought benefits to mankind, is in fact proving its worst enemy. The value of science itself has been put in question, and at last scientists have been forced to take notice of the outcry'.

Hodgkin and Pauling actively participated in movements against organized violence. Pauling was deeply concerned about the possible misuses of nuclear technologies, and actively organized protests against them. Hodgkin was a life-long supporter of non-violence and was an active supporter of the promotion of science in third-world countries. Out of these convictions, she chaired the Pugwash movement in the mid

1970s. One of the strongest supporters of Scientists for World Affairs was Mr Jawaharlal Nehru, the first prime minister of independent India. The first Pugwash conference was indeed understood to have taken place in Delhi at the invitation of Mr Nehru.



Shekhar Mande

Against this backdrop, one wonders if the crystallographic community will take up the cause of peace around the world once again. The International Union of Crystallography will do well to take cues from these people actively to persuade governments around the world to find peaceful solutions to problems. Areas that currently need special attention are those in the Middle East, central Africa, and the Koreas. With the IUCr Congress being hosted in 2017 in Hyderabad, India, crystallographers might think of their role in society once again.

Shekhar Mande

MEETING REPORT

ECM29

Rovinj, Croatia, August 2015

http://ecm29.ecanews.org



Venue of ECM29, the Adris exhibition and convention centre, a renovated old tobacco factory complex which is listed as a historical monument of *fin-de-siècle* industrial architecture.



Aleksandar Višnjevac, Chair of the Organizing Committee, officially opened the Meeting.

The 29th European Crystallographic Meeting took place in Rovinj, Croatia, August 23-28, 2015, and was extremely successful. A total of 1052 crystallographers from 52 countries met in Rovinj to attend the scientific sessions in the fascinating location of a renovated old tobacco factory complex representing an extraordinary example of the *fin-de-siècle* industrial architecture of the late 19th century. A high participation of young researchers was registered, with over 200 students, and 80 exhibitors who contributed to profitable discussions and a very lively atmosphere aside the lectures. The Congress was opened with the Ode to Joy performed by A. Rucner (Croatia), followed by welcome addresses given by the ECA President A. Roodt (South Africa), the chair of the organizing committee A. Višnjevac (Croatia) and the Assistant Minister of the Ministry of Science, Education and Sports of the Republic of Croatia, R. B. Lučić (Croatia).



John R. Helliwell, recipient of the 8th Max Perutz Prize.

During the opening ceremony the 8th Max Perutz Prize was awarded to J. R. Helliwell (UK) for his long, generous and fruitful dedication to developing all aspects of the use of synchrotron radiation for crystallography and for his boosting support to global development of synchrotron and neutron facilities.

The Opening Ceremony was animated by traditional Croatian songs *a capella* performed by klapa 'Motovun'.



Plenary speaker Henry Chapman.



Plenary speaker Andrea Ferrari.

The scientific program was opened by the plenary lecture 'Serial crystallography with X-ray free-electron laser pulses' by H. Chapman (Germany), and was closed with the plenary lecture 'Graphene future emerging technology' by A. Ferrari (UK). Over the four days of the conference, 50 microsymposia and 16 keynote lectures embraced the latest advances in all aspects of crystallography; a very well attended special session 'How to' was devoted to give young crystallographers hints and suggestions on their next future career outside academia. Besides the main conference, ten well-attended satellite meetings were run, among them the very successful young crystallographers' satellite meeting.



IUCr President, Marv Hackert (left), with IUCr Poster Prize winners Anton Brausemann (Germany) and Eleonora Conterosito (Italy).



Poster Prize winner Matteo Alvaro (Italy).



Marijana Đaković



Participants at the Welcome Reception.



Student mixer for Young Crystallographers



The Gala dinner.



The IUCr Executive Committee met during ECM29. (l to r) Front row: Santiago García-Granda, Malcolm Cooper, Mitchell Guss, Marvin Hackert, Jane Robinson, Hanna Dabkowska and Michael Dacombe; back row: Luc Van Meervelt, Radomir Kuzel, Wulf Depmeier, Mike Glazer, Masaki Takata, Brian McMahon and Peter Strickland.

There were 20 poster prizes awarded at the closing ceremony which was officiated by M. Đaković, Co-chair of the Organizing Committee. Additional photos can be found at http://ecm29.ecanews.org

Alessia Bacchi, ECA President

MS4: Advances in phasing, refinement and autobuilding

Speakers in this session on macromolecule techniques included:

I. Uso (Italy), developer of *ARCIMBOLDO*. This software (i) uses molecular replacement techniques to find positions of small structural fragments in the unit cell, and (ii) tests how well they kick-start autobuilding. The procedure works in cases where the resolution is 2 Å (or better) and there are sufficient computing resources to run the multiple tests.

V. Lamzin (Germany) described new developments in Arp/Warp. The detection of NCS at early stages of the rebuilding process means it has been successful at resolutions down to 3 Å. Another powerful feature is the detection of ligand density. Likely 'shapes' are evaluated against a library of common fragments.

A. D. Finke (Switzerland). As synchrotrons allow more seamless data-collection protocols, old methods can be reintroduced. It is possible with careful crystal alignment on a multi-axis goniometer to collect high-multiplicity data of equivalent Bijvoet pairs at much the same time, reducing the systematic errors in the anomalous signal introduced by radiation damage and enhancing the chance to solve the phase problem.

K. Diederichs (Germany) urged the community to beware of RULES for data-quality evaluation, which can be useful but need to be re-examined in the light of first principles. He gave two examples: (i) Data-processing statistics such as R_{merge} measure the precision of data (*i.e.* how well multiple observations agree) and not their inherent accuracy. For instance, measuring multiple reflections with different absorption pathways will increase R_{merge} but improve the accuracy of the observation. (ii) R values based on different selections of observations cannot be validly compared.

A. Thorn (UK) raised the issue of the relatively poor agreement between observed and calculated F_{obs}. She showed how plots of F_{obs} *versus* resolution did not fully fit the predicted Wilson plot features, and sparked a vigorous debate on why this might be so - suggestions included 'Ice rings?', 'Poor solvent modelling?' 'Secondary structure artefacts?'

Navraj Pannu and Eleonore Dodson

MS5: Structure and function of enzymes

It is now possible to visualize successive steps of an enzymatic reaction *via* the use of XFEL, where one can collect serial femtosecond X-ray data. P. Fromme (USA), 'SFX - The dawn of a new era in structural biology'. In parallel, the development of general photoactive reagents makes it easier to trigger enzymatic reactions in crystals. D. Monteiro (UK), 'Towards a general approach for the time-resolved crystallographic study of enzymes'. As more enzymes are found in integral membranes, it has become very exciting to compare their structure and functions to equivalent soluble enzymes. A. Goldman (UK), 'New structures of *T. Marittima* integral membrane pyrophosphatase suggest a conserved coupling mechanism for proton and sodium transport'. Finally, it has now become standard practice to combine crystallography with a multitude of additional techniques to fully characterize the targets of interest, if in healthy systems or disease. M. Cygler (Canada), 'Effector proteins from pathogenic bacteria: focus on kinases' and A. Wang (Taiwan), 'An integrative approach targeting phophatase substrate complexes for new cancer drug design strategy'.

Joel Sussman and Ute Krengel

MS13: New instrumentation, methods and approaches in inorganic crystallography

The symposium covered a broad range of topics from X-ray powder diffraction analysis (R. Cerny, Switzerland) to the ultimate electron diffraction analysis, based on statistical approaches (A. Eggeman, UK) or dynamical refinement of 3D data (L. Palatinus, Czech Rep.). Applications of the free electron laser snapshot crystallography at the SwissFEL (C. Dejoie, Switzerland), and the benefit of the 'cluster approach' for the X-ray analysis of intermetallic compounds (D. Proserpio, Italy) were also described. Six posters concerned both X-ray and electron diffraction developments.

Damien Jacob and Anton Meden

MS14: Mineralogical crystallography: Nature as a source of inspiration for new materials

The papers presented in this symposium ranged from the hydrothermal synthesis and structural characterization of new phases, to the study of imogolite nanotubes and naturally occurring metal-organic framework (MOF) compounds. Several papers were focused on the use of porous materials in

different applications, such as the treatment of nuclear waste or the polymerization of organic molecules. Many non-ambient studies, HT and HP, on various mineral and mineral-like phases were presented.

Nikolay Eremin and Rossella Arletti

MS15: Structure property relationships

Detailed understanding of structure-property relationships is a key motivation for many crystallographic studies and this session attracted attention from practically all branches of the community. It highlighted the overlap between different areas of crystallography and covered neutron and X-ray diffraction, physical and chemical properties, as well as hard, soft and hybrid materials. The session included contributions with variation of sample composition, pressure and temperature for materials as diverse as molecular materials, metal oxynitrates, borohydrides/boranes and metal-organic frameworks.

M. Lusi (U. of Limerick) talked about 'Design and synthesis of molecular materials: mixed crystals for finer engineering' and emphasized the possibilities of solvent-free synthesis of mixed crystals. J. P. Attfield (U. of Edinburgh) discussed the 'Structure property relationships arising from anion order in solid oxynitrides', an emerging class of materials with interesting optical, photocatalytic, dielectric and magnetoresistive properties that may be sensitive to oxide-nitrade order.

P. Schouwink's (U. of Geneva) talk 'Energy-related aspects of complex metal borohydrides and higher boranes: beyond hydrogen storage' demonstrated that there is a great potential for achieving high ionic conductivity and that the numerous compounds studied for their hydrogen sorption properties are promising candidates for other energy-related applications. A. Comotti (U. of Milano Bicocca) 'Molecular rotors in nonporous periodic architectures' provided insight into the dynamics of molecular rotating dipoles. I. Collings (U. of Bayreuth) 'Structure-property relations in multiferroic metal-organic frameworks at high pressure' discussed how the magnetic metals MOFs couple to the ferroelectric guest ions and how physical pressure studies can guide the design of the MOFs with improved multiferroic properties.

Kari Rissanen, Martin Bremholm

MS18: Thermoelectric materials - from fundamental science to applications

For the first time an ECM featured a symposium on thermoelectric materials. These materials are challenging for crystallographers, due to their complex crystallographic structures and the impact of micro/nanostructure on thermoelectric properties. Methods covered included neutron and X-ray diffraction, theoretical calculations and electron microscopy. Y. Grin (Switzerland) demonstrated the crucial role of the inhomogeneity and anisotropy of chemical bonding in thermoelectric materials. The problem of 'rattling atoms' was addressed by M. Koza (France) who used neutron spectroscopy to show that the classical view on the vibration of rattlers is much too simplified.

O. Oeckler and S. Herbert

MS20: High-pressure solid-state chemistry

Contributions to this symposium included studies of inorganic and organic solids, minerals, polymers, pharmaceuticals and other materials. 25 scientists from 10 countries took part in MS20 and related poster sessions: four oral presentations were given by representatives of Austria, Denmark, Germany, Japan, and UK; 21 posters were on display presenting research in Austria, Croatia, Denmark, Germany, Italy, Poland, Russian Federation, South Africa and UK. Young scientists made great contributions. M. Schmitt (Austria) presented high-pressure synthesis and characterization of the new nickel borate HP-NiB_4O_7, whose structure type was hitherto unknown in the field of borate chemistry, underlining the importance of the parameter 'pressure' in synthetic solid-state chemistry. J. Sotelo (UK) presented high-

pressure structural data on the microporous scandium framework, Sc_2BDC_3 (BDC = benzene-1,4-dicarboxylate) with included methane molecules from 2 to 25 kbar. This research is providing in-depth structural insight into the adsorption/desorption mechanism of metal-organic frameworks (MOFs) that might have important implications for the development of new methods of storing, trapping or separating light gases, such as CO_2 or CH_4. An invited talk delivered by U. Schwarz (Germany) on high-pressure high-temperature synthesis of new covalent metals offered insight into recent preparation, results and physical properties of binary compounds comprising covalent framework patterns.

Natalia Dubrovinskaia

MS23: Nanoscale structures

The symposium featured many high-quality contributions, with 27 abstracts in total. The subjects of the oral and poster presentations extended from electron microscopy *via* X-ray diffraction, absorption and scattering studies to theoretical modeling and software development, with a strong focus on nanoscale diffraction techniques. Metal nanoparticles, semiconductor nanowires and quantum dots, functional oxides, electronic materials and organic-inorganic hybrid nanostructures were highlighted. The important contribution of crystallography to this emerging field of science became obvious.

During recent years, substantial instrumental developments in electron diffraction, such as aberration-corrected TEM and STEM, X-ray analysis and X-ray nanoprobe beamlines at various synchrotrons worldwide, have revolutionized the possibility of crystallography on nanoscale structures. The invited talks at the microsymposium, given by internationally recognized experts (P. Boullay, France, and U. Pietsch, Germany), provided an exciting overview including excellent examples of the novel potential within both fields. Contributed talks covered total scattering (A. Guagliardi, Italy), coherent diffraction imaging and ptychography (V. Favre-Nicolin, France) and *in situ* studies of nanoparticles in liquid environments (M. Zobel, Germany). The symposium included experienced senior scientists and promising young researchers.

J. Hadermann, R. Timm

MS26: Modulated, modular and composite materials

Aperiodic structures were the focus of this symposium. A. Abakumov (Belgium) presented a superspace description of a complex superstructure of a perovskite, supporting the displacive-like origin of the distortion instead of a phase separation proposed in previous models. C. Müller (Sweden) reported a superspace model of the intermetallic compound Cu_3Sn, which shows an intriguing feature: only odd satellites are observed. She was able to explain this fact using triangle-like occupation domains.

C. Mariette (France) analyzed critical phenomena in a composite compound where alkane chains are confined in honeycomb-like urea sublattices. Together with the phonon branches in incommensurately modulated composite structures, the low-frequency phason excitations could explain the large length correlations along the direction of the misfit. B. Stöger (Austria) focused on the phenomenon of allo-twinning, the oriented association of two or more polytypes of the same compound. Some examples of structure determination of allo-twinnings were presented. Finally, A. Gagor (Poland) analyzed the commensurate-incommensurate phase transition of the semiconducting hybrid $(2\text{-}MI_m)BiI_4$. The possible relation between the variation on the Bi-Bi distance coming from the sinusoidal modulation and the physical properties of the material were also discussed.

Luis Elcoro and John Claridge

MS27: Electron crystallography methods

Invited lectures covered the extreme ends of the field, with J. P. Abrahams (Netherlands) discussing techniques for imaging and diffraction of biological and biomedical samples, while David Cooper (LETI, Grenoble) highlighted the current state-of-the-art for strain mapping in semiconductor samples.

R. Beanland (UK) showed the latest developments from digital LACBED measurements, combining automated beam controls, image processing and fast simulations for accurate refinement of diffraction data. M. Gemmi (Italy) contrasted the various protocols for 3D electron diffraction measurements to optimize the amount of information recorded for a given electron dose. Finally, T. Gorelick (Germany) reported the application of PDF analysis to electron diffraction data.

The poster sessions continued to highlight the range of research in electron crystallography, with presentations on the methods for 3D electron crystallography of a wide range of organic, inorganic and hybrid materials. A special mention should be made of the two electron crystallography poster prizewinners: D. Johnstone (UK) and C. Correa (Czech Republic).

Alex Eggeman and Lukáš Palatinus

MS29: Quasi-crystals and aperiodic materials

This microsymposium focused on the latest theoretical and methodological advances with structure determination and analysis of aperiodic crystals and how structural features influence their physical properties.

In his talk on 'Statistical description of icosahedral quasicrystals,' R. Strzalka (Poland) proposed three-dimensional structure modeling in physical space as an alternative to modeling in higher-dimensional space. In 'Long-range ordered magnetic and atomic structures of the quasicrystal approximant in the Tb-Au-Si system,' G. Gebresenbut (Sweden) described a new strategy for crystal synthesis with first results on atomic and magnetic structures. S. Ben-Abraham (Israel) addressed in 'Three-dimensional eight-color structure' a two-dimensional chair substitution tiling based on eight cubic prototiles, and showed how to generalize the structure to additional dimensions. In 'Quasiperiodic canonical-cell tiling with cubic symmetry,' N. Fujita (Japan) discussed a new inflation rule for the canonical cells, proposing an inflation step factor (being the golden mean); E. Zupanič (Slovenia) considered 'Unit-cell twinning in quasi-crystals', an alternative understanding of the unit cell to recover quasi-crystalline reciprocal space.

A. Schönleber and J. Wolny

MS33: Mechanical effects and properties of ordered matter

Elastic materials that are capable of mechanical reconfiguration induced by external stimuli are indispensable for the fabrication of mechanically tunable elements for actuation and energy harvesting, including flexible electronics, artificial muscles and microfluidic elements. The most challenging practical difficulties with structural analysis of deformations of macroscopic-size single crystals are those caused by the large molecular structural changes and the significant strain that develops over the long-range structural order in these closely packed structures. Accumulation of strain can cause deterioration, sublimation, twinning and other forms of undesirable crystal disintegration. In order to maximize the performance of the mechanical response while keeping the fatigue at a minimum, these issues can be resolved by a combined approach that includes both intrinsic and external factors. This microsymposium included lectures that reflect the historical developments as well as the current status in the emerging field of mechanically-responsive crystalline materials. By including talks both from some of the leading researchers as well by some rising stars in the field, the symposium highlighted the recent interest in mechanical characterization of molecular crystals.

E. Boldyreva (Russia) opened the symposium with a wonderful overview of over three decades of research on mechanical effects in crystals, focusing on bending of single crystals induced by linkage isomerization. L. Alimi (South Africa) presented a report on a new compound that shows the thermosalient effect, where crystals explode as they undergo thermal phase transition. D. Levendis (South Africa) described an interesting case where a new mechanical effect is observed with a 'classical' photochemical reaction - photodimerization of *o*-ethoxycinnamic acid whose crystals undergo multiple mechanical effects during the reaction. P. Zolotarev (Russia) gave an in-depth overview of the topological and energetic aspects of identification of cleavage planes in crystals. G. Ramon (South Africa) concluded the session with a beautiful example of a solvent-responsive coordination network that 'breathes' by uptake and release of solvent.

Panče Naumov and Helena Shepherd

MS39: Recent advances in diffraction instruments, detectors and data processing

S. Capelli (UK) described recent developments for 2D detectors, data collection and data-processing software in single-crystal neutron diffraction. M. Brunelli (France) addressed structural disorder in doped ceria compounds. Defects were investigated by following the structural evolution of doped ceria compounds at different length scales. M. Blakeley (France) discussed neutron macromolecular crystallography at the Inst. Laue-Langevin and exciting new details of protein-ligand interactions relevant to HIV, and protonation shifts related to enzyme pathways. A. Casanas (Switzerland) described the advantages of the EIGER detector for combining fast frame-rate, very short dead-time and higher rotation speeds in collecting data, and highlighted the numerous advantages associated with higher rotation speeds data collection on challenging crystals. Finally, S. Smeets (Switzerland) described the collection of data, in broad-bandpass mode, and a new algorithm for the indexing of data collected in single-snapshot mode with either monochromatic or broad-band pass radiation.

Rosanna Rizzi and Trevor Forsyth

MS44: New applications of old algorithms in crystallography

This symposium revisited classical algorithms that with new twists are being applied to current crystallographic problems. It covered structure solution, refinement and validation in macromolecular, chemical and materials crystallography. Both single-crystal and powder diffraction methods were presented.

D. Turk (Slovenia) addressed the problems that are caused by omitting the test set of reflections that is used to calculate the free *R* factor. This has been used for almost 30 years to validate macromolecular structure refinements. The test set is also used to parameterize maximum likelihood (ML) refinement. As an alternative that does not require data to be omitted, he presented the ML free-kick refinement algorithm that removes model bias by small random displacement of atomic positions.

C. Jelsch (France) presented subatomic charge-density refinement of small macromolecules against ultra-high resolution data, now extended to predict molecular properties through developments in the program *MoPro* that has its roots in the Hansen and Coppens program *MOLLY*. *MoPro* is endowed with automation, visualization and analysis tools, a charge-density database and a graphical user interface.

R. Oeffner (UK) convincingly illustrated progress in the most widely used macromolecular phasing method, molecular replacement, targeted to increase the success in difficult cases with borderline models. He described and evaluated improvement of the located models by occupancy refinement against the ML target. He showed how to rescue solutions that would have been eliminated by phantom packing clashes. The resulting solutions provide superior starting structures for model building and refinement by removing the model bias burden of the incorrect regions.

M. Schmidt (USA) imparted a clear and engaging exposition of the use of cross-correlation functions on non-indexed powder data for the structure solution of nano-crystalline organic compounds. Successful solution of this challenging problem by global optimization of all parameters, including the cell constants, from random starts is implemented in his program *FIDEL*.

C. Millán (USA) presented the use of clustering algorithms in reciprocal space, evaluating mean phase differences and correlation coefficients using methods stemming from the low-resolution phasing context. Her implementation attempts to combine partial molecular replacement solutions from small fragments and has already succeeded in phasing some macromolecular structures that had resisted all previous attempts to solve them.

George M. Sheldrick and Isabel Usón

MS45: Chemical information as prior knowledge in crystallography

The symposium addressed the use of prior knowledge in macromolecular and small-molecule crystallography. In the opening talk, 'Fitting ensemble models of disorder using *a priori* chemical structure information', R.Cooper (U. of Oxford, UK) discussed the Squeeze algorithm. Rather than using an explicit atomic model of disorder, Squeeze adds a reciprocal space correction, improving geometry and parameter estimates in modelled regions. He discussed fitting ensemble models of disorder involving random sampling of occupancies, conformations and positions, utilizing prior information from known structures, providing a detailed description of disordered regions.

Addressing 'Chemical restraints in *Phenix*', N. Moriarty (USA) discussed the use of *eLBOW* for the generation of ligand restraints, derived from various sources, for use in refinement and validation, and the Conformation Dependent Library, used to generate main chain restraints based on protein backbone conformation.

In the third talk, '*SEQUENCE SLIDER*: a multi-sequence evaluator and its application in venomics', R. Borges (Spain and Brazil) described how to ascertain a protein sequence from a list of possibilities. Starting from a partial model, side chains are modelled and results evaluated against diffraction data, utilizing complementary experimental information.

D. Kratzert (Germany) described 'DSR-enhanced modelling and refinement of disordered structures with *SHELXL*', which performs automatic fitting of models in disordered regions. This utilizes a database of fragments and restraints, allowing multiple conformations with varying occupancies.

In the final talk, 'Deriving a chemical context for protein-bound monosaccharides', J. Agirre (UK) discussed using structural fingerprinting to assess monosaccharides in the PDB, revealing the prevalence of errors in sugar conformations. *Privateer* utilizes such knowledge for validation.

R.Nicholls and A. Linden

MS47: History of crystallography and the ECA

The European Crystallographic Association (ECA) has a General Interest Group organized by Senior Crystallographers (GIG-SC). The GIG-SC addresses the needs and interests of enthusiastic but ageing crystallographers. GIG-SC has distributed a written statement addressed to the organizers of crystallographic meetings. A further document is in preparation concerning the means for senior crystallographers to publish scientific articles as open-access and to access crystallographic databases. The GIG-SC also organizes microsymposia at ECMs. At ECM29 a microsymposium entitled 'History of Crystallography and the ECA' was organized. B. Kojic-Prodic (Croatia) gave a lively talk on the development of crystallography in Croatia. S. Popovic (England) enlightened us on scientific activities of the Croatian-born physicist and engineer, N. Tesla (Croatia), who was very active at the time of the

discovery of X-rays. D. Viterbo (Italy) gave a personal account of well known crystallographers that he had known. A similar theme could be found in the poster presentation of Mike Glazer, which presented the crystallographic lives of Kathleen Lonsdale and H. Megaw. J.-Louis Hodeau (Germany) took us further back in time by talking about crystallography before the discovery of X-ray diffraction. A. Wlodawer (USA) gave us a fascinating talk on the history of macromolecular crystallography.

For ECM30 in Basel, Switzerland, 2016, the organization of a microsymposium on 'Contributions to the development of crystallography' is already underway. More complete information on the GIG-SC may be found on its website.

S. Larsen and H. Flack

MS48: Teaching and outreach of crystallography

In the wake of the IYCr, distinguished teachers and popularizers of crystallography from academic institutions and industry presented accounts of their work related to IYCr.

A. Linden (Switzerland) provided an overview of the well known Zurich School of Crystallography, 'Bring your own crystals' (www.chem.uzh.ch/linden/zsc/), which was launched in 2007 and is organized and directed by Linden and H.-Beat Bürgi.

V. Stilinović (Croatia), co-editor of a Croatian popular science journal *Priroda (Nature)* and an avid science historian, presented 'History as a tool for a crystallographic storyteller'.

D. Šišak-Jung (Switzerland), on behalf of M. Fark (Germany), described a joint project of the IUCr and several companies. They sponsored a series of worldwide admission-free schools and workshops designed to quicken the development of crystallography in less-privileged regions. After being introduced to the basics of crystallography, the students receive hands-on tutorials using modern instruments and software.

M. Zema (Italy) described an initiative of the IUCr and UNESCO. The OpenLab project was to develop crystallography in Africa, South America and Southeast Asia. A total of 15 OpenLabs, each with 20 to 30 selected participants, were organized, providing high-level educational opportunities to local students and young professors, taking advantage of the scientific and educational expertise of the IUCr, the diplomatic and educational channels of UNESCO and the partnership of crystallographic instrument manufacturers.

N. Eremin (Russia) described a Russian initiative to teach crystallography to school children. Many workshops throughout Russia were attended by hundreds of students. Since school curricula lack instruction in crystallography, the authors have created a textbook, 'Entertaining Crystallography', aimed at primary- and high-school students.

Krešimir Molčanov and Bart Kahr

MS50: Cultural and historical aspects of crystallography

G. Cavallo (Italy) explained the role of X-ray powder diffraction in mineralogical studies of various ochres useful in dating archaeological artifacts. G. Artioli (Italy) gave a lecture about the contributions of crystallography and archaeometric approaches to understanding cultural heritage. C. Groom (UK) presented an overview of the scientific life of Frank Allen and his critical role in the creation, maintenance and use of the Cambridge Structural Database system.

In the corresponding poster session, M. Wildner (Austria) presented his 'pattern zoo' - the 17 plane groups and related periodic tilings and patterns that played and still play an important role in art and cultural history over the centuries, and P. Bezdička (Czech Rep.) explained the role of X-ray powder

diffraction and Raman spectroscopy in studying the naturally irradiated fluorite, called antozonite, a rare violet pigment used in Europe in the Middle Ages.

Petr Bezdička and Aleksandar Višnjevac

NOTICE

Eleventh Ewald Prize Call for Nominations



The IUCr is pleased to invite nominations for the Ewald Prize for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography. Prof. Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of the IUCr publication Acta Crystallographica from 1948 to 1959, and the President of the IUCr from 1960 to 1963.

The prize, consisting of a medal, a certificate and a financial award, is presented once every three years during the triennial International Congresses of Crystallography. The next prize will be presented at the Hyberabad Congress in August 2017.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible for the Ewald Prize, irrespective of nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a Nobel Prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognised. Current members of the Selection Committee and the President of the IUCr are not eligible. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor, but not more than three, for the same scientific achievement.

Nominations for the Ewald Prize should be submitted electronically using the Ewald Prize Nomination Form to the Executive Secretary of the IUCr (execsec@iucr.org). The closing date for nominations is August 31 2016.

Further information and the Nomination form can be found at www.iucr.org/iucr/ewald-prize.

NOTICE

Gjønnes Medal in Electron Crystallography Call for Nominations



The Gjønnes Medal in Electron Crystallography recognizes an outstanding contribution to the field of electron crystallography. The award is accompanied by a certificate and funding to present an invited Keynote Lecture at the triennial International Congress of Crystallography. The award is named in honour of its first recipient, Jon Gjønnes of the U. of Oslo, who received the award at the XXI IUCr Congress in Osaka in August 2008.

This award is managed by the Awards Sub-committee of the Commission on Electron Crystallography (CEC) of the IUCr. This Sub-committee is responsible for soliciting, evaluating and recommending a nominee to members of the CEC for final approval, or recommending that no award be made.

Nominations are now open for the Gjønnes Medal in Electron Crystallography. Nomination is open to scientists and engineers in all areas of electron crystallography. The next Gjønnes Medal will be awarded at the Hyderabad Congress in August 2017. Further details of the award and the nomination procedure can be found at www.iucr.org/resources/commissions/electron-crystallography/gjonnes-medal.

The deadline for receipt of nominations is April 30, 2016.

E. Orlova, chair of Commission on Electron Crystallography

AWARDS AND PRIZES

American Crystallographic Association 2016 Awardees

The following awards will be presented at the 2016 American Crystallographic Association Annual Meeting, 22-26 July, in Denver, CO, USA.

2016 Trueblood Award to Axel Brunger



Axel Brunger (Howard Hughes Medical Inst., Stanford U., USA) will receive the 2016 Trueblood Award for 'exceptional achievements in computational or chemical crystallography'. Brunger carries out cutting-edge research on the structural mechanisms of synaptic neurotransmitter release, complementing X-ray crystallography with single-molecule microscopy, and is exploring the new possibilities that X-ray free electron laser techniques offer for the structural determination of large macromolecular assemblies.

2016 Fankuchen Award to Elspeth Garman



Elspeth Garman (Oxford U., UK) will receive the 2016 Fankuchen Award. Elspeth is being recognized for her absolute dedication to teaching crystallography in seminars and workshops all over the world, and her great contributions to improve cryo-methods in crystallography.

Garman introduced mitigating measures such as the use of small molecules as radical scavengers. She experimentally determined the maximum X-ray dose that can be delivered to a macromolecule before compromising its structure - the 'Garman limit' - and presented a method to predict the lifetime of proteins exposed to certain radiation doses. She also pioneered the use of an online UV-visible spectrometer to detect the early signs of radiation damage.

2016 Bau Award to Benno Shoenborn



Benno Shoenborn (Los Alamos National Lab, USA) is the 2016 recipient of the ACA Bau Neutron Diffraction Award for his pioneering work on neutron crystallography and its application to biology. Benno has published over 100 publications on the subject, and has mentored, trained and inspired numerous students, post-docs and early-career researchers, expanding the reach of neutron crystallography to a larger community of scientists and setting the grounds for its further development.

Being one of the pioneers of the technique with Paul Langan, Benno promoted the creation of the first neutron protein crystallography beamline in North America, the Protein Crystallography Station (PCS) at the pulsed neutron source at Los Alamos Neutron Science Center (LANSCE), a state-of-the-art facility that helps users in every step of a neutron diffraction experiment, from protein production and deuteration, to data collection and analysis.

2016 Etter Early Career Award to Jason Benedict



Jason Benedict, (U. of Buffalo, USA) is the recipient of the 2016 Margaret C. Etter Early Career Award. Jason has been recognized as an outstanding mentor to students. He received national attention for launching the US Crystal Growing Competition in 2014, which aims to teach the fundamentals of crystallography to students and educators in the K-12 level across the nation. With Benedict at the helm the event has grown to almost 100 participants from over 15 regional institutions.

For more information on these award winners, visit www.amercrystalassn.org/2016-award-winners.