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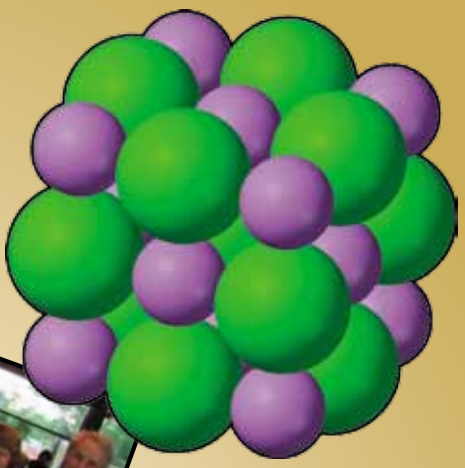
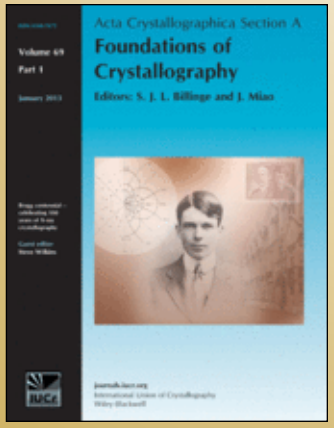
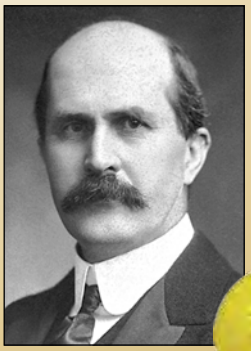
INTERNATIONAL UNION OF
Crystallography
NEWSLETTER
Volume 20, Number 4 ♦ 2012

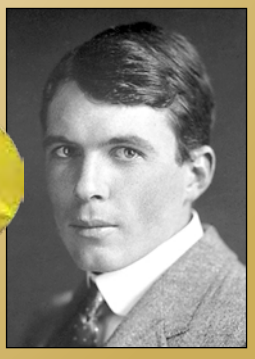
BRAGG CELEBRATION





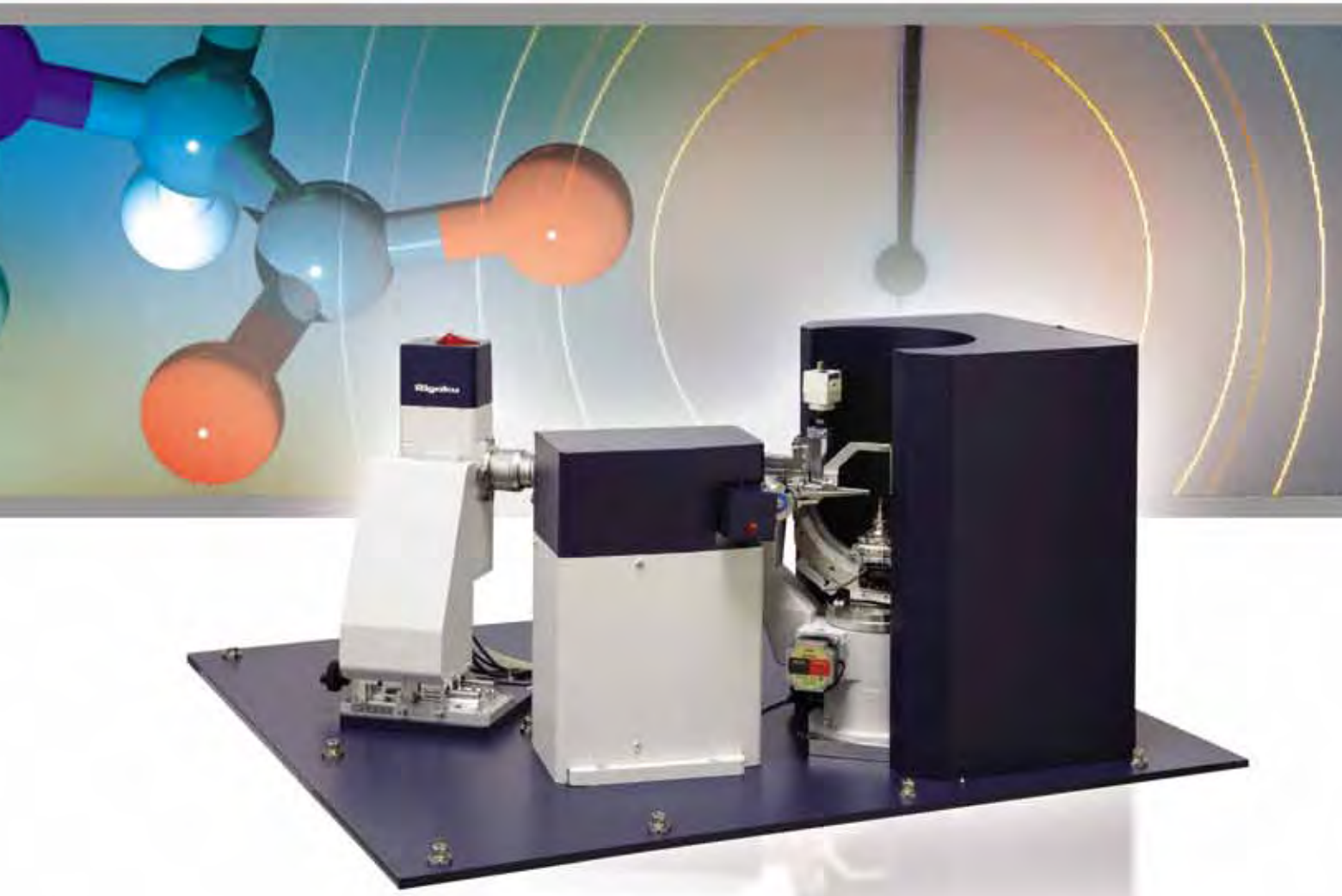


1915 Nobel Prize
"For their services in the analysis of crystal structure by means of X-rays"



The DualSource RAPID II

The most flexible diffractometer in the world



- **Small molecule crystal structures**
- **Powder diffraction**
- **Protein crystal structures**
- **Absolute determination of chiral compounds**
- **Diffuse scattering**
- **Supermolecular structures**
- **Twinned and disordered crystals**

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On the Cover: Celebrating Braggs: Top right: space filling image of sodium chloride; photos from the AsCA meeting and Bragg Symposium; cover of January *Acta Cryst.* A; W.H and W.L. Bragg received the Nobel Prize in 1915.

Contributors: S. Hasnain, J.-L. Hodeau, T. Janssen, A.J Katrusiak, F. Marone, M. Mukherjee, T.A. Munro, T. Pijning, D.J. Rigden, B. Stöger, J.J. Vittal, and S. Wilkins.

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Gautam R. Desiraju

The Executive Committee (EC) of the IUCr met recently in Adelaide and took some important decisions regarding the International Year of Crystallography (IYCr), and our journals. IYCr is going to be a very important occasion for all of us to celebrate and commemorate our subject, to build bridges with the student community and with the general public at large. I hope that the Year will see a number of new country-to-country exchanges and also region-to-region ones. Members of the EC have been entrusted with independent charge of various activities. These include regional activities in Africa, Latin America, Eastern and South Eastern Europe and upcoming regions in Asia. Planned also are interactions with large facilities and especially the SESAME project in the Middle East. IUCr wishes to be actively involved with our Commissions, Regional Associates and National Committees. These activities will be organized and monitored by individual EC members. Educational activities of all types will be planned by an individual member. All names and details will be posted on the IYCr web page the planning and execution of which is the responsibility of yet another member. An IYCr Project Manager will be appointed shortly and will coordinate the activities of the EC, our Chester office, and all of you. We are also aware that the IYCr coincides with a Congress Year and our (two North American) members will plan IYCr related activities for the Montreal Congress. I hope to see as many of you as possible in Montreal in August, 2014.

Our journals will also play an important role during IYCr in terms of increasing and improving our outreach to the research community. To celebrate the IYCr, the Union will be launching a new open access, high impact journal that will cover all areas of crystallography. When the Union began its activities in 1948, *Acta Crystallographica* was the journal where the most important results in the subject were published. We are aiming for this new journal to be the flagship journal of the Union where similarly important results will be published. At this time, I would like to welcome Samar Hasnain, University of Liverpool, the new Editor-in-Chief of our publications. Prof. Hasnain has had a very successful tenure as Section Editor of Journal of Synchrotron Radiation and is no stranger to the Union. I would like you to join me and extend all cooperation to him and his team of very dedicated section editors and co-editors and make us all feel proud of our journals and our Union.

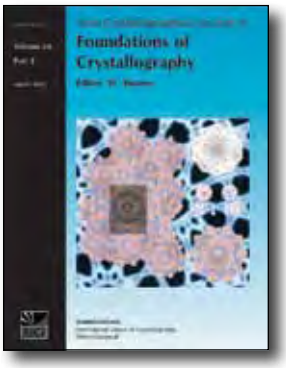
The EC meeting in Adelaide was held to synchronize with the joint meeting of AsCA and SCANZ and as usual, the talks and posters in this meeting were of a very high standard indeed. A unique celebration was also held at that time to celebrate the contributions of W.H. Bragg and W.L. Bragg to the subject of crystallography. Considering that W.H. Bragg was a professor in the University of Adelaide and that W.L. Bragg was born and raised in Adelaide, the timing and location of the symposium were particularly appropriate. A large number of distinguished crystallographers, and associates and family members of the Braggs were present. It was truly a memorable occasion.

I wish all of you the best wishes of the season and a happy, peaceful and scientifically rewarding 2013.

Gautam R. Desiraju (desiraju@sscu.iisc.ernet.in)

The International Union of Crystallography Newsletter is distributed by print to 587 libraries and various crystallographic meetings and electronically to 12,000 crystallographers and other interested individuals in 102 countries. The IUCr also runs Crystallography Online, available at www.iucr.org, as a complement to the IUCr print newsletter. Feature articles, meeting announcements and reports, information on research or other items of potential interest to crystallographers should be submitted to the editor at any time. Submission of text and images by electronic mail is requested. Items will be selected for publication on the basis of suitability, content, style, timeliness and appeal. The editor reserves the right to edit. Address changes or corrections and requests to be added to the mailing list can be made at www.iucr.org/news/newsletter.

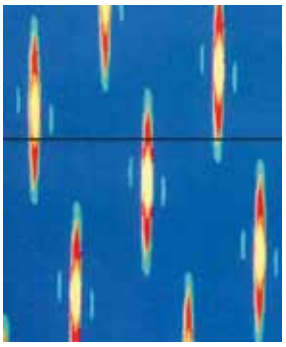
Acta Cryst. (2012). A**68**, 667–674 (http://doi.org/jww)



Fifty years of aperiodic crystals

T. Janssen

After von Laue had shown, in 1912, that crystals diffract X-rays and have ordered arrays of atoms, it was assumed that an essential property of crystals was their lattice periodicity. In 1982 quasicrystals were discovered showing crystals with fivefold symmetry axes, which exclude lattice periodicity. This was, however, not the first case of a crystal without lattice periodicity. In the beginning of the 1960s more and more examples were found, such that in 1982 quite a number of crystallographers were aware of their existence. A brief history of the slowly growing idea that crystals are not necessarily lattice periodic, culminating in the discovery of quasicrystals, is given.



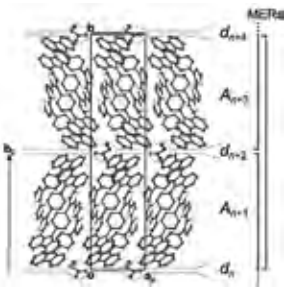
Patterson pattern for a Fibonacci chain: the chain appears along a horizontal line, the 'physical space'.

Acta Cryst. (2012). B**68**, 667–676 (http://doi.org/jwx)

Solvatomorphism of 9,9'-[1,3,4-thiadiazole-2,5-diylbis(2,3-thiophendiyl-4,1-phenylene)]bis[9H-carbazole]: isostructurality, modularity and order–disorder theory

B. Stöger, P. Kautny, D. Lumpi, E. Zobetz and J. Fröhlich

The title compound features an unusual tendency to cocrystallize with solvent molecules. The resulting solvates do not feature strong hydrogen bonds, nor are the molecules arranged in framework structures. To describe the structural diversity of six solvates of the title compound, we applied the concept of modularity which was originally developed for inorganics and minerals. Moreover, for one structure we used the formalism of order–disorder theory to explain the pseudo-symmetry and the twinning of the structure.



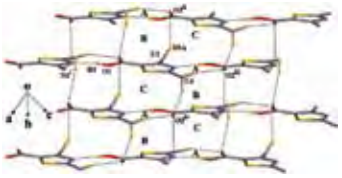
The order–disorder structure of the MEK solvate. The largest regions that are equivalent in all polytypes are indicated to the right by brackets.

Acta Cryst. (2012). C**68**, o452–o455 (http://doi.org/jwz)

2,4-Dimethyl-1,3-thiazole-5-carboxylic acid: an X-ray structural study at 100 K and Hirshfeld surface analysis

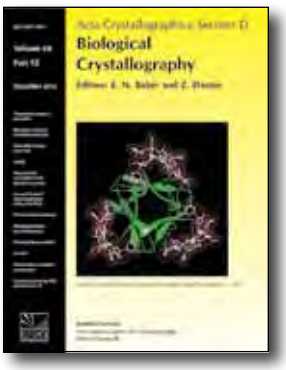
D.K. Hazra, M. Mukherjee, M. Helliwell and A.K. Mukherjee

Single-crystal X-ray structure analysis of a new thiazolecarboxylic acid derivative (I) determined using a high-quality data set collected at 100 K shows an interplay of strong and weak hydrogen bonds. Three types of eight-, ten-, and fifteen-member supramolecular synthons are edge-fused to form a two-dimensional framework in (I). Additional reinforcement within the framework is provided by S···S interactions. Intermolecular contacts in (I) are predominantly of H···H, N···H, O···H and S···H type, which can account for about 80% of the Hirshfeld surface area.



Formation of the two-dimensional framework in thiazolecarboxylic acid derivative (I).

Acta Cryst. (2012). D**68**, 1622–1631 (http://doi.org/jw2)



AMPLE: a cluster-and-truncate approach to solve the crystal structures of small proteins using rapidly computed *ab initio* models

J. Bibby, R.M. Keegan, O. Mayans, M.D. Winn and D.J. Rigden

Ab initio protein structure prediction, by programs such as *Rosetta*, can provide starting models for solving novel structures from crystallographic data. Rather than trying to construct the single best model, we generate ensembles which are known to work well in molecular replacement (MR). We have demonstrated the feasibility of an approach based on identification and extraction of incomplete but locally accurate search models from rapidly obtained *ab initio* predictions. 43% of a set of small (<120 residues) proteins were successfully solved.

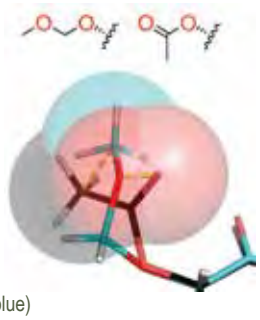
Snapshots along structure solution by *AMPLE*. A cluster of *ab initio* models is generated by structural alignment (top). Multiple truncated ensembles (e.g. lower left) are derived from it, varying in their treatment, and trialled by MR. A successful solution and rebuild are compared to the final structure lower right.

Acta Cryst. (2012). E**68**, o3225–o3226 (http://doi.org/jw3)

Salvinorin B methoxymethyl ether

T.A. Munro, D.M. Ho and B.M. Cohen

MOM-salB is a derivative of the naturally occurring κ-opioid salvinorin A, with higher potency and a longer duration of action. In the crystal structure, the MOM ether adopts a "classic anomeric" conformation. Counter-intuitively, this permits both the terminal oxygen atom and the methyl group to overlap with their counterparts in salvinorin A. This suggests a possible common bioactive conformation. The weaker preference for the classic anomeric conformation in substituted acetals may contribute to the reduced potency of substituted derivatives of MOM-salB.



The MOM ether of MOM-salB (blue) overlaid on the acetate group of salvinorin A (black) in their respective crystal structures. Overlapping van der Waals radii are shown as translucent spheres. Note how counter-intuitive this overlap appears from the structure diagrams.

Acta Cryst. (2012). F**68,** 1448–1454 (http://doi.org/jw4)

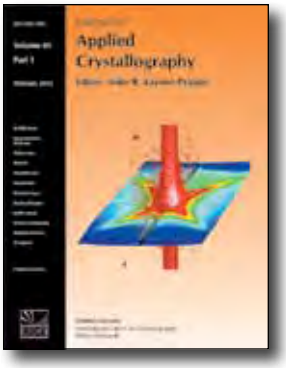
Structure of the α-1,6/α-1,4-specific glucansucrase GTFA from *Lactobacillus reuteri* 121

T. Pijning, A. Vujicic-Zagar, S. Kralj, L. Dijkhuizen and B.W. Dijkstra

Glucansucrases are bacterial enzymes that synthesize extracellular α-glucan polysaccharides from sucrose. We determined the first crystal structure of an α-1,6/α-1,4-specific glucansucrase, the fully active N-terminally truncated reuteransucrase GTFA-ΔN, using crystals with an unusually high solvent content of 85%. The GTFA-ΔN structure revealed differences when compared with other glucansucrases, notably in the region following the transition-state stabilizing residue. In accordance with the conclusions from earlier mutation studies on GTFA, residues in this region are likely to orient acceptor sugar molecules, thereby determining the product specificity of different glucansucrases.

Crystal structure of GTFA-ΔN determined at 3.6 Å resolution.

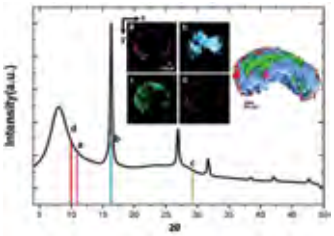
J. Appl. Cryst. (2012). **45**, 1109–1124 (http://doi.org/jw5)



Diffraction/scattering computed tomography for three-dimensional characterization of multi-phase crystalline and amorphous materials

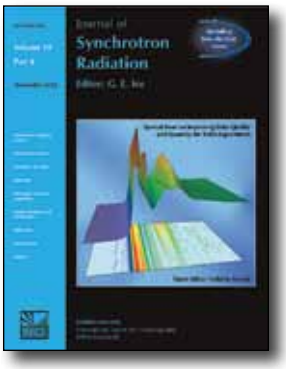
M. Álvarez-Murga, P. Bleuet and J.-L. Hodeau

X-ray diffraction computed/scattering tomography provides nondestructive three-dimensional structural images of crystalline or amorphous multi-phased heterogeneous materials. Diluted phases are discriminated with very high spatial and local resolution. The method is suited for numerous practical applications, in static, dynamic or multi-modal variants, as demonstrated by an increasing number of publications in this field. As reconstruction artefacts can degrade the quality of the rendered images and limit their interpretation, the sources of error and limits of this method are discussed and compared with other diffraction-based techniques.



Reconstructed volume and structural selective slices of polycrystalline cubic diamond (b), sp^3-like amorphous carbon (c), sp^2-graphitic carbon (d), short interlayed carbon (a), obtained from scattering patterns.

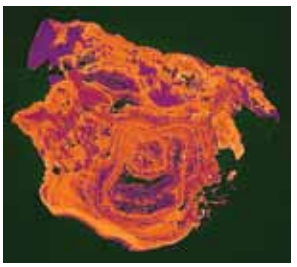
J. Synchrotron Rad. (2012). **19**, 1029–1037 (http://doi.org/jw6)



Regridding reconstruction algorithm for real-time tomographic imaging

F. Marone and M. Stampanoni

A fast algorithm for tomographic reconstruction (*gridrec*) based on the Fourier method and an optimized regridding approach is presented. On CPU, it provides an up to 20-fold performance increase compared with filtered back-projection routines with negligible accuracy degradation. These characteristics make *gridrec* an invaluable tool for efficient online quality assessment and data evaluation during the emerging high-data-rates tomographic microscopy experiments, which guarantee sub-second temporal resolution and enable new science where dynamic processes can for the first time be captured in 3D through time.



2D axial tomographic slice through a Ca-apatite human kidney stone.

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Innovation with Integrity

Crystallography

The most important crystal?

BY WILLIAM L. DUAX

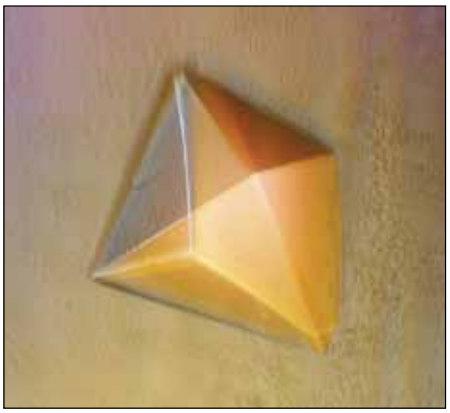
Since lysozyme may have been crystallized more often and by more people than any other protein, lysozyme crystals may qualify as the most important crystals of all. Many protein crystallographers have cut their crystallizing teeth on lysozyme. More experiments to study the relationship between crystal quality and pH, temperature, pressure, and solvent selection have probably been conducted with lysozyme than any other protein.

Nevertheless when you are able to grow your first really beautiful perfect crystal of any substance there is a feeling of satisfaction and accomplishment that is one of the rewards of a life in crystallography. No matter that it's been done before. The crystal is a joy to behold, you have learned a lot and suddenly you have a new skill. So it was for undergraduate summer intern Moiela Halimy when she grew the lysozyme crystal pictured here. When she was told a picture of her lysozyme crystal would appear in the *IUCr Newsletter*, Moiela wrote," First of all, thank you so much for the opportunity. It was a pleasure for me to work at your lab with you(Joe Luft) and Jen. I had a great time. I appreciate the fact that you trusted me with that project and let me do it. Today you gave me one of the greatest news that I've ever got, I would love it if my name would be associated with the picture. Please let me know when the newspaper is published."

I appreciate the help of Joe Luft (Hauptman Woodward's Crystal Guru) in giving us the photo of Moiela's crystal. The first reference Joe finds to crystallization of lysozyme is a paper by E.P. Abraham and R. Robinson, Crystallization of lysozyme, in *Nature* 140 (1937) page 24. A Google search for lysozyme got 2,150,000 hits. Perusal of a few dozen entries found "How to use lysozyme in a sentence", "Wine Maker Magazine" and 23 pages of lysozyme related images including crystals, structural ribbon diagrams, photos of Linus Pauling, Janet Thornton, Brian Kobalka, Marie Curie, and Ada Yonath.

Please take the time to email us your candidate for "Most important crystal ever!"

Since 1997 The Dept. of Chemistry at the National U. of Singapore (NUS) has held National Crystal Growing Challenge Competitions. This years 10th biennial competition attracted 118 teams from 47 secondary, junior college and polytechnic schools in Singapore and an audience of 300 guests attended the award ceremony (details on page 19). The next competition is scheduled to be held in 2014 as part of Singapore's celebration of the IYCr. Every National committee could follow Singapores lead as part of their plans for the IYCr and open up the world of crystallography to thousands of students. ❖



Chicken egg white lysozyme

IUCr Journals Development

BY SUMAR HASNAIN

The IUCr is embarking upon a project to extend and expand the scope of its Journals to meet the needs and serve the interests of the crystallographic and wider scientific community that utilize structural information for addressing their scientific questions. The Editor-in-chief, Samar Hasnain, in consultation with appropriate committees and commissions of the IUCr as well as the wider community has developed a plan to make the IUCr's journals the natural home for many of the high-quality scientific publications that are currently published in NSMB, Structure, PNAS, JACS, Angewandte Chem.,Chem. Commun. etc, where structural data underpin these publications.

Chemists, biologists, physicists and material scientists will be actively encouraged to report the best of their crystallographic studies in the IUCr's journals. Significant changes will be implemented in Journal organization and management to coincide with the celebration of the International Year of Crystallography.

Today's scientific advances require multidisciplinary research and new journals covering a wide range of technologies and applications. Because crystallographic studies are critical to understanding the structural basis for chemistry, physics, biology, and materials science the IUCr will inaugurate a new open access mega journal as part of the celebration of the IYCr. The new Journal will be simply called "IUCr Journal" (IUCrJ). IUCrJ will be fully open access striving to reach high impact and influence appropriate for the best of our science. Our aim is to capture a fair share of high profile papers on all aspects of sciences and technologies supported by IUCr via its commissions including emerging fields where diffraction plays a role. Much of the exciting crystallographic results that are published in other journals appeared first in presentations at IUCr congresses, AsCA, ECM, and ACA meetings. The goal for 2014 will be to publish 100 articles in IUCrJ covering as many aspects of crystallographic development and application as possible. As much as half of these will be solicited from the presentations of cutting edge research at ECM, AsCA and ACA meetings. A Management Board has been appointed that will be responsible for (a) increasing the influence of IUCr journals among the wider scientific communities (b) serving the interests of all of its Commissions, (c) broadening the scope of the journals so that high quality science papers that use crystallography are attracted to the journals, and (d) improving the visibility of IUCr journals at non-crystallographic conferences.

A Journal Development and Promotions Officer will be appointed in early 2013 with a mandate to (a) reach out to wider science community, (b) encourage closer integration of the journals with the Commissions, (c) develop social media marketing, (d) boost article citations by writing press releases highlighting the most significant papers, (e) prepare market research reports including citation and usage trend analysis, (f) identify subject trends and new journal opportunities,(g) identify target authors and encourage them to submit to the journals, and (h) exploit opportunities arising from IYCr2014. The Development and Promotions Officer will work closely with the Editorial staff.

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ACA 2012

Boston, MA, USA, July 2012
www. amercrystalassn.org
taken from ACA RefleXions, Fall 2012

The 2012 Annual Meeting was held in Boston, Mass., July 28 through August 1. 785 participants presented 258 posters and 294 lectures. Thirty-nine exhibitors participated in the Exhibit Show, beginning with the Opening Reception on Saturday and running through Tuesday. Attendees traveled from 30 counties with 23% coming from outside the USA. Young scientists (students and postdocs) represented 32% of the total meeting attendance. The meeting was financially supported by 33 organizations whose contributions were used to support young scientists, speakers and social events.

The meeting began on Saturday with workshops on *Modeling and Refinement of Nanoparticle Structures from Diffraction Data, Crystallography - World of Wonders, Refmac and Coot,* and *Structure Refinement and Disorder Modeling with OLEX2* on Saturday.

ACA Awards

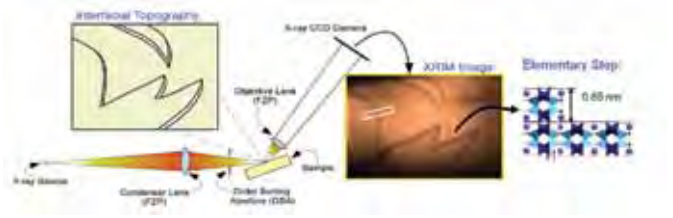
Five ACA awards were presented at this meeting. The Buerger Award to John Spence, the Warren Award to Paul Fenter, the Etter Early Career Award to Emmanuel Skordalakes, the Supper Instrumentation Award to Ron Hamlin, and the Elizabeth Wood Writing Award to Daniel Nocera.

In his Buerger Award lecture *TheFuture of Diffraction Physics in Crystallography*, John Spence noted that due to advances in instrumentation, crystallography continues to have a bright future. He focused upon two discoveries of the last decade - *lensless imaging*, pioneered in Janos Kirz's group, and the *diffract-before-destroy* approach to outrunning radiation damage, first suggested by Solem and demonstrated at Flash (the former Tesla Test Facility) in 2006. He reported the newest results from femtosecond diffraction experiments at XFEL. With lensless imaging, using oversampled diffraction data, electron density maps from single particles can now be reconstructed. The group at the LCLS in Stanford has published several milestone papers using the *diffract-and-destroy* method of serial femtosecond crystallography (SFX). Pulses of X-rays, brief enough to outrun the resolution limiting effects of damage, are generated in a micron sized beam from high energy electron bunches with frequency 120 Hz and about 1012 hard X-ray photons per pulse. A constantly refreshed supply of protein nanocrystals flows across the beam in random orientations. By using short pulses *instead* of freezing, data can be collected at room temperature for many proteins which fail to grow crystals large enough for conventional macromolecular crystallography. Instrumentation has been developed by the ASU group (Doak, Weierstall, Fromme, Spence), the Monte-Carlo method for merging data from size-varying nanocrystals was described in the dissertation of Rick Kirian, and software was developed by Tom White in the DESY group. SFX milestones include the achievement of atomic resolution, and new biology elucidated by images of a drug target. Spence concluded with a review of the rich opportunities for new experiments in time-resolved structural biology at XFELS, including pump-probe experiments, new solutions to the phase problem, and snap-shot biochemical dynamics, using correlated fluctuations in two-dimensional fast WAX patterns. These will be explored at a Royal Society Workshop on Biology with XFELS in October 2013. *Marius Schmidt*

John Spence during his Buerger Award lecture. *Photo by P. Mueller.*

Paul Fenter (ANL), winner of the 2012 ACA Warren Award, described his research on liquid-solid interfaces, and their importance to energy-related processes critical to society. The B.E. Warren award is given to recognize an important recent contribution to the physics of solids or liquids. Because liquid-solid interfaces are buried beneath a liquid layer that is opaque to surface sensitive structural tools, Paul and his colleagues developed phase-sensitive X-ray based scattering techniques to image structures at liquid-solid interfaces. He cited three examples: imaging of mineral-water interfaces and element-specific ion distributions at charged interfaces, and direct imaging of sub-nm lateral topography and structural variations. *Connie Rajnak*

George Phillips on the right, presenting the Warren Award to Paul Fenter. *Photo by P. Mueller.*



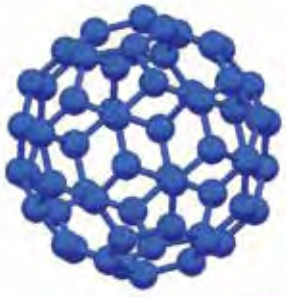
The X-ray reflection interface microscope (XRIM) images elementary topography on a solid surface through the use of phase-contrast. The dark lines on the XRIM image correspond to 0.65 nm highsteps, whose structure is shown(right).

The 2012 Margaret C. Etter Early Career Award was presented to Emmanuel Skordalakes (Wistar Inst., U. of Pennsylvania) for his elucidation of structure of telomerase, an RNA dependent DNA polymerase that stabilizes chromosomes and is commonly over expressed in age associated disorders. Emmanuel presented structures of telomerase, alone and in complex with cognate RNA and DNA substrates. He and his colleagues tested hypotheses about telomerase function with a series of experiments inspired by the structures. His findings set the stage for the design of better therapeutics for treating diseases associated with aberrant telomerase activity *Eric Montemayor*

Emmanuel Skordalakes, at left, accepting the Etter Early Career Award from Eric Montemayor. *Photo by P. Mueller.*

EMPYREAN

Laboratory X-ray diffraction equipment for pair distribution function (PDF) studies



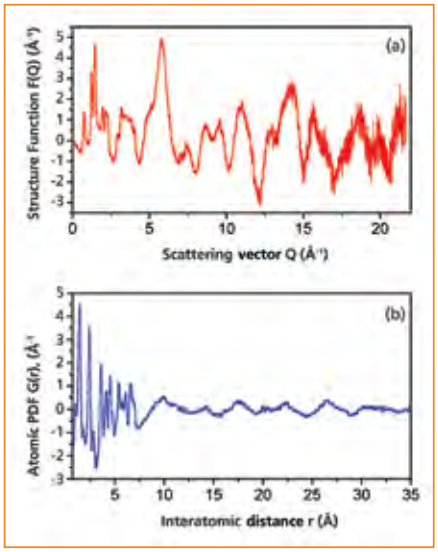
A buckyball molecule

C_{60} molecules in fcc type lattice

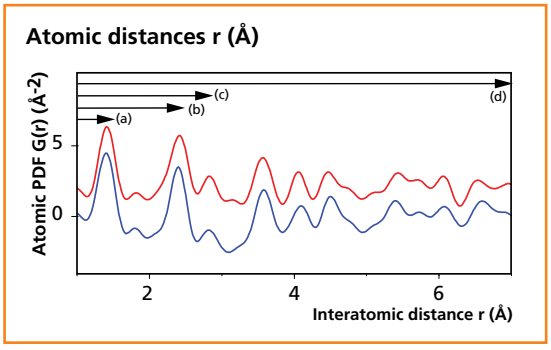
Any Empyrean system can be easily turned into an in-house PDF system by adding simple components such as an Ag or Mo tube and special anti-scatter slits.

A standard X'Celerator detector or scintillation counter give excellent results, allowing screening of PDF samples prior to synchrotron beamtime.

Example: probing the short- and long-range atomic ordering of C_{60} fullerene (buckyballs)



a) Structure function and b) atomic PDF of C_{60} fullerene (buckyballs). The experiment was performed with Ag Kα radiation, allowing a maximum scattering vector of 22 Å^{-1}. The PDF data shows sharp peaks up to 7 Å and broad features beyond this point. The sharp peaks correspond to the well-defined distance between atoms inside each C_{60} molecule. The broad features originate from the correlation of electron density between different buckyballs.



Comparison between the short-range interatomic distances of the experimental PDF (blue curve) and the calculated PDF from a single buckyball (red curve). The program RAD was used for the calculation (V. Petkov, J. Appl. Cryst. 1989, 22, 387)

The experimental results on the buckyballs are in excellent agreement with the calculated PDF and neutron studies reported in literature, proving the quality of our in-house PDF solution.

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Ron Hamlin, Area Detector Systems Corporation, was honored with the Charles Supper Instrumentation Award for his work in advancing the development of X-ray area detectors. His talk *2-D X-ray detectors -- What do we really want and how can we build it?* covered the development of X-ray detectors from film to the modern array detectors used today. His PhD project, with N-H Xuong, led to the construction of the first multiwire area detector - which became a national resource. Ron discussed the pros and cons of optical film scanners, single point scintillation counters, image intensified television cameras, 2-dimensional gas-filled, image plate, CCD and pixel array detectors. He discussed the characteristics of the "ideal" X-ray detector that Ron and others have long strived to achieve. Ron also told about the ups and downs he faced as a small business owner striving to keep pace with rapidly developing technology. His is an inspiring story about how the interest of a scientist/entrepreneur 30 years ago ultimately had an enormous impact on science. *John Rose*

Ron Hamlin on the left accepting the Charles Supper Award from ACA President George Phillips. *Photo by P. Mueller.*

Elizabeth Wood Writing Award winner Daniel Nocera (right) with John Spence at the Awards banquet. *Photo by P. Mueller.*

Poster Prizes

Seven Pauling Poster Prizes ($200, banquet ticket, and a copy of a Linus Pauling book) were awarded. The Herman R. Branson Pauling Prize, named for one of the first African American crystallographers, went to Amber Smith. The Muttaiya Sundaralingam Pauling Prize recognizing Sunderalingam's ground-breaking research on nucleic acids went to Tamaria Dewdney. The Louis Delbaere Pauling Prize, with Canadian sponsorship, for the best poster from a Canadian laboratory went to Kevin Kevin Leung. Three other Pauling prizes went to: N. Alicea-Velazquez ,Y-T Lai, and C.Boone. The IUCr Pauling Prize, online access to all IUCr journals for one year or a volume of the International Tables went to Serah Kimani. The RCSB Protein Data Bank Prize was awarded to Sergei Kalynych with an Honorable Mention to Rebecca Goldstein. The 2012 Crystal Engineering Prize sponsored by *CrystEngComm* published by the Royal Society of Chemistry went to Bo Wang. The 2012 *Journal of Chemical Crystallography* Prize went to Steffen Bernard and his co-authors D. Akey, S. Li, D. Sherman and J. Smith. The reported study revealed the presence of crystals of the same protein-substrate complex with different space groups and identical unit cell constants. This crystallographic anomaly occurred because a translation of layers within the crystal altered symmetry operators while maintaining the unit cell composition. Jennifer Wierman received an honorable mention.The 2012 Oxford Cryosystems Low Temperature Prize was awarded to Yimin Mao of Brookhaven National Laboratory and his co-workers who developed a specialized slam-freezing apparatus with rapid thrusting of the sample against a liquid-nitrogen cooled copper mirror allowing examination by grazing incidence X-ray scattering. *Bill Ojala*

Yimin was so excited to hear his name announced (this was his very first ACA meeting) - that he took the podium to tell everybody how happy he was. The audience gave him a big round of applause. *Photo by P. Mueller.*

Undergraduate Education

Undergraduate education was addressed at a lecture preceeding the opening night reception and a symposium on crystallographic research with undergraduates. E. Mazur (Harvard U.) described his interests, involvment and creative ideas in the realms of education, science policy, outreach, and the public perception of science. He reminded the audience that we learn not from lectures, but after class through self-study and discussions with fellow students. Mazur advocates peer instruction that capitalizes on the idea that the student knows the difficulty in understanding a concept better than the instructor. In the peer instruction environment the students can discuss the concepts presented by the instructor. Further information on Eric's teaching innovations is available at http://mazur.harvard.edu. In a half-day session J. Tanski (Vassar College) described strategies for X-ray diffractometer acquisition at a predominantly undergraduate institution and a teaching module that exposes undergraduate students to small molecule crystallography including publication. C. Slebodnick (Virginia Tech) described a summer undergraduate crystallography workshop covering theory and practical sessions. R. Rowlett (Colgate U.) created a protein crystallography laboratory with remote or onsite data collection, structure determination and refinement and the development fruitful collaborations. D. Juers (Whitman College) also emphasized protein crystallography at undergraduate institutions with crystallography-focused biochemistry course units and research projects. A. Norquist (Haverford College) described his undergraduate research program involving the synthesis and structural properties of chiral vanadium tellurites. He described best practices for including

Speakers in the session *Protein and Small Molecule Crystallography at Undergraduate Institutions*. (l to r) Douglas Juers, Alexander Norquist, Carla Slebodnick, Roger Rowlett and Kraig Wheeler. Inset: Joe Tanski.

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Speakers in *Past Reflections & Future Directions: 100 Years of Diffraction* (l to r) Christine Beavers, Louise Dawe, David Rae, Brian Toby, Curt Haltiwanger, Paul Swepston, Hilary Jenkins, Sue Byram, and Jenny Glusker.

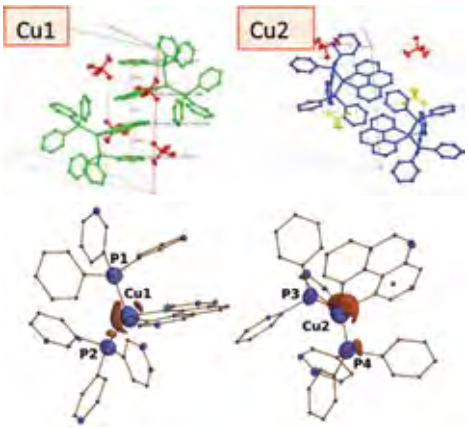
ray facilities. K. Wheeler (Eastern Illinois U.) related his strategy, pitfalls, and ultimate success in securing NSF-MRI funding. *Bruce Foxman, Bruce Noll and David Rose, Roger Rowlett & Kraig Wheeler*

Past Reflections & Future Directions: 100 Years of Diffraction

In her opening presentation J. Glusker (Fox Chase Cancer Centre) reflected on 100 years of structure determination and gracefully put our science in context for the next generation of crystallographers. S. Byram, (Bruker AXS) described the Evolution of Small Molecule Crystallographic Instrumentation with examples of hardware (and software) innovations by many major industrial contributors. B. Toby (ANL) forecast the future of service crystallography and offered practical suggestions for its survival. H. Jenkins (McMaster U.) described exciting new software for viewing data (MAX3D). P. Swepston (Rigaku Americas Corp.) talked about collaborations which could lead to great science. Especially challenging 'small molecules' and methods of refinement were discussed by C. Beavers (LBNL) and A.D. Rae (Australian National U.), respectively. *Louise Dawe and Curt Haltiwanger*

Transactions Symposium honoring Bruce Foxman

Transformations and Structural Oddities in Molecular Crystals covered crystal transformations, supramolecular assemblies and synthesis, polymorphism, and function and reactivity of engineered materials. Talks were presented by Bruce's friends, colleagues, and former students who also held a birthday party for him and shared anecdotes that highlighted Bruce's impact on their careers. At the symposium D. Watkin (Cambridge U.) discussed systematic studies of Z' > 1 structures, C. Brock (U. Kentucky) showed how optimizing hydrogen bonds within structures and using enantiomerically and diasteriomerically pure compounds can assist the formation of crystal structures with multiple molecules in the asymmetric unit. P. Coppens(SUNY Buffalo) discussed the use of dynamic photocrystallography to explore linkage isomerism and its application to stereoselective transformations of structures with Z' = 2. K. Wheeler(Eastern Illinois U.) designs J-shaped molecules that form robust supramolecular dimers which undergo photodimerizations via single crystal-single crystal processes, often with quantitative conversions. J. Bernstein (NYU Abu Dhabi) described some interesting aspects of crystallographic history including the fact that Reginald James, a physicist on Shackleton's 1914 Antarctic expedition later acquired a reputation as an authority in the newly developing field of crystallography. M. Kaftory (Technion-IIT) showed that UV illumination of a class of pyridines results in photodimerization in which reactants undergo molecular flips. M. Garcia-Garibay(UCLA) explained strategies for engineering reactions in crystals with examples of photodenitrogenation of diazo compounds, nitrenes, and azoalkanes. V. Young (U. Minnesota) described an ionic salt that exhibits enantiotropic phase transitions. The system starts from a non-twinned crystal structure and progresses to lower symmetry accompanied by twinning and an order-disorder transition. The transition was followed with the Dynamic Compression Sector (DSC) and X-ray data. B. Kahr (NYU) related his recent adventures with molecular crystals that grow helically with twisted lattice planes. J. Swift (Georgetown U.) described the impact of growth conditions and dye additives on the formation of uric acid crystals. Ö. Almarsson (Alkermes) addressed the importance of crystal structure analysis and data mining for pharma R&D. M. Hickey (Alkermes) discussed optimizing pharmaceutical material performance, the impact of chemical changes on crystal structure and properties, and the use of crystallographic data to understand solid-state reactivity in drugs. M. Hollingsworth(Kansas State U.)



Top: Cu1 and Cu2 show the difference in packing of two independent molecules in crystals of a Cu(I) phen anthroline complex. Bottom: Time-resolved photodifference map showing that the structural changes on photoinduced electron transfer to the microseconds lifetime excited state are different. Red: positive. Blue: negative. Isosurfaces ± 0.25 e/Å3. (*J. Phys. Chem.* A, **116**, 3359-3365 (2012), and *Acta Cryst.* A**67**, 319-326 (2011). *(Philip Coppens)*

Transaction symposium speakers (l to r) Bruce Foxman, David Watkin, Graciela Diaz de Delgado, Kraig Wheeler, Roger Bishop, Magali Hickey, Richard Adams, Menahem Kaftory, Larry Falvello, Carolyn Brock, Michael Ward.

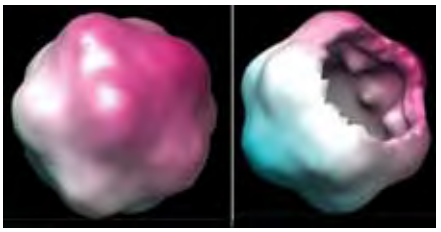
showed that co-crystallization of urea with alkanes, alkanones, and alkanediones, generates ferroelectric domain switching materials having twinning, phase transitions, and commensurate and incommensurate phases. M. Peterson (Amgen) described co-crystallization of urea with an α,ω-disubstituted hexane that produced stacked loops of ureas that form undulating channels. L. Falvello (U. Zaragoza) described his preparation of metal-citrate building blocks with a variety of cubane topologies and solid-state reactivity. The talk on iridium- and osmium-gold carbonyl clusters by R. Adams (U. South Carolina) drew attention to the complexities of CO labile systems. A. Rheingold (UCSD) showed that in mixed-valence iron acetates the rates of intramolecular electron exchange vary greatly, that local symmetry plays an important role in this phenomenon, and that it is solvent dependent. G. Diaz de Delgado (U. de Los Andes) described the sources of complex structural features of metal carboxylates. R. Bishop (U. New South Wales) addressed supramolecular synthesis, the structural preferences of molecular tweezers and the inverse relationship between clathrate formation and packing prediction. M. Ward (NYU) discussed assemblies of his guanidinium organosulfonate building blocks, with remarkable properties including soft matter microstructures that mimic Archimedean polyhedra. K. Harris (Cardiff U.) described the use of solid-state NMR to monitor the evolution of supramolecular assemblies as a function of time. *Graciela Diaz de Delgado, Magali Hickey, and Kraig Wheeler*

Emerging Sources: Theory and Practice

In the first of three sessions on Emerging Sources: Theory and Practice, J.Tainer (Scripps Inst.) discussed small and wide angle X-ray scattering (SAXS/WAXS) techniques, introduced the BioISIS data base as a resource for macromolecular SAXS, and predicted that time-resolved SAXS with millisecond time-resolution will soon become routine. F Schotte (NIH) illustrated pico-second time-resolved synchrotron experiments with a movie of structural changes immediately after carbon-monoxide was flashed away from the heme-iron position in carbonmonoxy-myoglobin. P. Schwander (U. Wisconsin) a major developer of embedding diffraction data into low dimensional manifolds, demonstrated how manifold embedding allows one to study structural heterogeneity, and removes the need for identical molecules. He showed that manifold embedding faithfully separates unlike particles at the experimental signal-to-noise ratio of cryo-EM. D. Saldin (U. Wisconsin), demonstrated how to determine the structure of viruses from diffraction patterns of random orientation without crystals by averaging the angular correlations of a large number of diffraction patterns from an ensemble of identical objects. Such diffraction patterns could be obtained using the ultra-short X-ray pulses available at the XFEL. P. Musumeci (UCLA) described the Pegasus, a source of relativistic electrons

Speakers in *Emerging Sources: Theory and Practice* (l to r) back, Henrik Lemke, Marius Schmidt, Yun-Xing Wang. In front: John Tainer, Dilano Saldin, Friedrich Schotte, Marc Messerschmidt, Peter Schwander.

for ultrafast, time-resolved electron diffraction experiments with high spatial and temporal resolution. The time-resolved melting of gold particles was given as an example U. Weierstall (Arizona State U.) concentrated on injector technology used to perform recent experiments at LCLS. He outlined some advantages of serial nanocrystallography : nanocrystals are readily obtainable, allow dynamic processes to be followed, and scatter intensity between the Bragg positions, which can be used to solve the phase problem. The small crystals are injected into the beam by a liquid jet whose diameter and velocity can be controlled by a surrounding gas stream. He described an international collaboration on nano sized crystals of lysozyme and photosystem *I. Marius Schmidt and Yun-Xing Wang*



3D images of the icosahedral satellite tobacco mosaic virus (STNV) reconstructed from simulated diffraction patterns from random orientations of the virus as expected from proposed "diffraction-before-destruction" experiments with an X-ray Free Electron Laser (XFEL). The image shows a computational slice through the image, revealing the hollow character of the protein capsid whose atomic coordinates from the PDB were assumed in the simulations of the diffraction patterns. D.K. Saldin *et al.*, *Optics Express* **19**, 17318-17335 (2011).

The second session, focused on SAS, was dedicated to the memory of Hiro Tsuruta, a pioneer in the field. P. Pernot (ESRF) described BM29 an instrument optimized to measure hundreds of protein solution samples quickly without user intervention. T. Weiss (SSRL,) described BM 4-2, an instrument capable of accommodating static and time-resolved experiments on proteins in solution and lipid membrane structures. L. Yang (NSLS) described the nearly completed LiX beamline which will permit time-resolved solution scattering using continuous flow cells, scattering-based scanning-probe tissue imaging, and scattering from membrane proteins embedded in single-layered lipid membranes. S. V. Pingali (ORNL) described Bio-SANS the only facility in the world specifically dedicated to biological applications of small-angle neutron scattering (SANS). The instrument operated by the Center for Structural Molecular Biology (CSMB) at the High Flux Isotope Reactor of ORNL. W. Heller (ORNL) described the Extended Q-Range Time-of-Flight SANS instrument that possesses a large dynamic measurement range at a single configuration and a high available flux suitable for weakly scattering samples and kinetics studies. J Barker (NIST) reported on the very small-angle neutron scattering (vSANS) diffractometer, currently under construction at NIST. *Volker Urban & Lin Yang*

In the third SAS session, T. Graber and Z. Ren (BioCARS) contrasted the properties of third generation sources such as the APS with those of spectacular new X-ray free electron (XFEL) sources such as the Linac Coherent Light Source at Stanford. Third generation sources offer ready accessibility to users, pink or monochromatic X-rays, high stability, a very high rep rate, and mature beamline instrumentation and experimental design, but cannot come close to XFELs in photons per pulse or brevity of their pulses. However, Ren described pump-probe experiments which offer a time resolution less than the X-ray pulse length. By systematically tracking the laser pulse across the X-ray pulse, the length of the trailing period is smoothly varied. Ren showed, in initial time-resolved crystallographic experiments, that this conceptually simple, general approach, 'poor man's pulse slicing', can yield a time resolution <100 ps. These experiments require systematic study of the

photophysics to achieve maximum yield of the desired species. J. van Thor (Imperial College London) described such a laser-lab-based study of the photocycle of photoactive yellow protein using fs laser pulses. The yield depends on pulse wavelength, intensity and duration, and on whether or not the pulse is chirped.Macromolecular crystallography increasingly focuses on tiny crystals, which requires the design and implementation of purpose-built beamlines that offer a tightly-focused X-ray beam, low X-ray background, the ability to visualize and center tiny crystals, and precision in crystal goniometry to ensure that the crystal remains centered in the beam. M. Yamamoto (Spring-8, Japan) described a new beamline at Spring-8 that has these characteristics. W. Kong (Oregon State U.) described a radically new, laboratory-based approach to structure determination of single proteins based on the incorporation of proteins into superfluid helium droplets at 0.38°K without significant unfolding. An elliptically-polarized laser beam is used to orient the droplets, and the electrons are scattered by the now-oriented protein molecules. The goal is to generate a complete, three-dimensional electron scattering pattern from which the structure could be reconstructed. This overall approach is technically challenging, and Kong presented results on successful initial steps in this high risk, high reward project. *Keith Moffat*

Extended Wavelength X-ray Crystallography

The session focused on the use of extended-wavelength X-rays (0.7Å to 3.5Å and above) in structural biology addressing new beamlines & equipment; sulfur phasing; phosphorous phasing and halide phasing. B.-C. Wang (U. Georgia/SERCAT/APS) described successful S-SAD phasing from a single insulin crystal with reduced radiation dose using a multiple-data-set (MDS) collection approach. He showed that the oxidation states of metals/ions could be monitored using data collected across the Fe absorption edge for crystals of bovine catalase. C. Mueller-Dieckmann (ESRF) described recent upgrades and plans to maximize the success of macromolecular crystallography experiments with the addition of the MASSIF sample evaluation and sorting facility and upgrades to ID29 to collect data with low energy (E = 5 keV, λ = 2.5 Å) X-rays. He also described methods of soft X-ray data collection including cluster analysis. N. Matsugaki (Photon Factory) described a beamline dedicated to SAD/MAD experiments that uses wavelengths greater than 2.7 Å to enhance weak anomalous signals. The beamline has loopless 'capillarytop-mounting' to reduce the background noise. Naohiro described recent sulfur-SAD phasing of the 2.5Å structure of a 43 kDa glucose isomerase for which automated model building was able to fit nearly all of the residues. J. Pflugrath (Rigaku, USA) illustrated the simplicity of using of halide (KI) soaks for SAD phasing with a video entitled 'Mastering the Halide Swish' produced by his colleagues S. Lee and J. Rieger. He stressed that highly redundant data is not essential for successful SAD phasing. M. Benning (Bruker AXS) presented statistics (year, resolution, and solvent content) on in-house SAD phased structures in the PDB, emphasized the importance of data optimization and presented successful results from crystals of moderate diffraction quality using S-SAD phasing. He noted that although his data sets were low-resolution they had high redundancy and one case required two crystals. He reported the successful phasing of a 42 kD protein soaked with $PtCl_4$. M. Weiss (Helmholtz-Zentrum Berlin) discussed challenges and problems in using long wavelength X-rays. He noted that over 50 methodological papers have been published and presented a statistics of S-SAD structures (wavelength, amino acids per asymmetric unit, and symmetry group). He gave details of three determinations, suggested ways to improve the success of S-SAD phasing, considering crystal mounting, data collection and data processing, and noted that based on the ratio of amino acid content to sulfur atoms more than 96% of all proteins could be possible targets for S-SAD phasing. A. Wagner (Diamond Light Source) emphasized that Beamline I23 will be the first MX beamline optimized for the long-wavelength region (1.5 - 4Å). He showed that the optimal wavelength for S-SAD is 4.5 Å for 0.05 mm sized crystals and 3.4 Å for 0.1 mm sized crystals. To minimize absorption effects, the complete beamline including sample, goniometer and detector will be operated in a vacuum. An X-ray tomography setup will be used for analytical absorption corrections. Sample cooling will be achieved using a conductive path running from a pulse tube cryo-cooler through the κ goniometer. A large curved detector will allow access to diffraction data up to $2\theta = \pm 90^{o}$. M. Wang (Swiss Light Source) described improving the signal to noise ratio in S-SAD and P-SAD phasing experiments using the X06DA super-bending magnet beamline which has a double channel-cut monochromator, PRIGo multi-axis goniometer and new PILATUS 2M detector. The PRIGo goniometer is able to place the best part of the crystal in the beam, align long-crystal axes to avoid overlaps, record Bijvoet pairs on the same image and carry out multi-pass data collection with different crystal orientations. Meitian presented stuctures determined with data from the new system of an RNA 14mer, the sarcin / ricin loop and three S-SAD proteins with amino acid lengths ranged from 84 to 387. Z.-J. Liu (Inst. of Biophysics, Beijing) described new tools for S-SAD phasing including X2DF, an updated version of the SCA2 system, and illustrated the use of X2DF in the structure determination of a 40kD protein. W. A. Hendrickson (Columbia U., NSL) reported using cluster analysis to merge S-SAD data sets collected from multiple crystals. Five examples discussed ranged from 22 to 1200 residues per asymmetric unit with resolutions ranging from 2.8 Å to 2.3 Å. The elemental identities for Ca, Cl, S, P and Mg associated with the structures were confirmed by f" scattering factor refinement using PHENIX. The procedures used in the analysis are robust and when aided by synchrotron beamlines optimized for low-energy X-ray diffraction measurements will offer truly routine structure determination of native macromolecules. *Bi-Cheng Wang and Robert Fischetti*

Speakers in *Extended Wavelength X-ray Crystallography* (l to r): Meitian Wang, Robert Fischetti, Jim Pflugrath, Armin Wagner, Christoph Mueller-Dieckmann, Matthew Benning, B.C. Wang, Manfred Weiss, Naohiro Matsugaki, Wayne Hendrickson, and Zhi-Jie Liu.

Advanced Hardware and Applications

The session focused on recent advances in X-ray area detector technology, robotics and automated data being incorporated at beamlines in the US and elsewhere. H. Robinson described the Qmx data collection system developed at NSLS. S. Waltersperger (Swiss Light Source) described the PRIGo multi-axis goniometer recently installed on beamline X06DA, D. Schuller (CHESS) gave an update on the installation of the second generation Berkeley Automounter (BAM-2) at MacCHESS. A. Cohen

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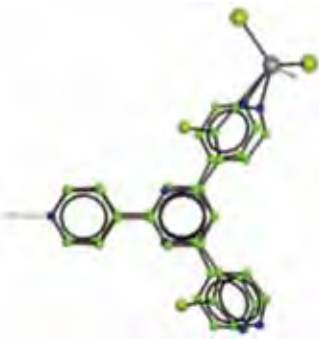
Speakers in *Advanced Hardware and Applications* (l to r): Malcolm Capel, John Rose, Howard Robinson, Michael Blum, Aina Cohen, Christian Brönnimann, Sandro Waltersperger, David Schuller. (Ron Hamlin not pictured)

(SSRL) conducted a live demo of a remote access *in situ* UV-visible absorption spectroscopy system to monitor metal oxidation states within protein crystals. C. Brönnimann (Dectris Ltd) described developments related to their PILATUS photon-counting detector, M. Capel (NE-CAT/Cornell U.) reported on the PILATUS 6MF pixel array detector installed on NE-CAT's undulator beamline 24-IDC, M. Blum (Rayonix LLC) described a new generation of detectors based on Split Frame Transfer CCDs, J. Rose (SER-CAT / U. of Georgia) presented plans for integrating the fast Rayonix MX300HS detector into the SER-CAT beamline 22ID, R. Hamlin (Area Detector Systems Corporation) described a new type of pixel array detector called the Dual Mode Pixel Array Detector (DMPAD) that ADSC is developing which addresses the problem of co-incidence loss common to PAD detectors at high-count rates. In related posters D. Szebenyi(CHESS) described high pressure cryocooling, J. Jenkins (TTP Labtech Ltd) reported on an automated gradient maker designed to rapidly generate screening or optimization crystallization plates, T. Allison (Labcyte Inc) described the Echo liquid handler that can transfer nanoliter quantities of reagents including viscous and osmotic fluids, and A. Gonzalez discussed the *'AutoDrug'* pipeline developed at SSRL. *John P. Rose & John Chrzas*

Public Domain Software

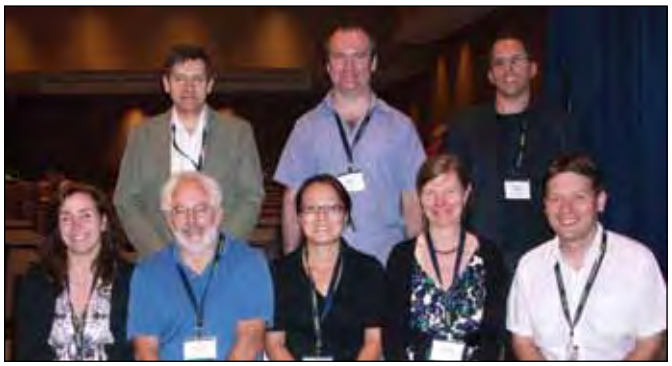
A. Spek (Utrecht U.) presented the latest developments in PLATON. Many changes for CIF Validation, SQUEEZE, TwinRotMat and Bijvoet analysis tools were implemented in the new SHELXL-2012. PLATON is available online at www.cryst.chem.uu.nl/spek/platon/. R. Von Dreele (ANL) presented The General Structure Analysis System -II (GSAS-II) has been rewritten in python. It is available in Windows, Linux and Mac OSX platforms and is now loaded with graphics and mathematical packages. GSAS-II has visualization tools for single crystal, powder, texture, and PDF analysis. Currently, GSAS-II handles only monochromatic CW X-ray/neutron data for powder, single crystal and PDF applications. The program has yet to be developed for neutron time-of-flight data, which was a distinctive capability of the original GSAS program. GSAS-II is available online at https://subversion.xor.aps.anl.gov/trac/pyGSAS. O. Dolomanov (OlexSys Ltd, UK) presented the newest version of Olex2, an open source project originated at Durham U. that combines crystallographic packages for small-molecule structure solution and refinement with a single easy-to-use interface that is available online at www.olex2.org. G.M. Sheldrick (U. Goettingen) presented his new SHELXL-2012 open source program that has been tested by 100 beta-testers. Precompiled binaries for Windows, Linux and Mac platforms are available to download. SHELXL-2012 includes many new features for modeling disorder, generating non-classical C-H..O hydrogen bonds, and extending rigid bond restraint. Improvements in data collection hardware and software now make it possible to determine absolute structure even when the anomalous scattering is extremely weak. For non-centrosymmetric structures SHELXL-2012 calculates the Flack parameter at the end of the refinement by two different methods. The hkl data and the .res file from final structure refinement are now embedded into the .cif output file with checksums included. This makes it possible to repeat any refinement exactly, and discourages cosmetic editing of the CIF file. More information at shelx.uni-ac.gwdg.de/SHELX/. CRYSTALS has been maintained in the Chemical Crystallography Laboratory in Oxford for 40 years. It is an X-ray & neutron crystal structure refinement package widely used in research, teaching and service. R. I. Cooper (Oxford U.) presented new features of parallel computation, asymmetric restraints and tools for modelling disorder in CRYSTALS (www.xtl.ox.ac.uk/crystals.html).



Disorder modeling in CRYSTALS.

R. Keegan (CCP4) introduced AMPLE, an automated software tool jointly developed by the U. of Liverpool and CCP4 for protein structure solution with the employment of *ab initio* protein structure modeling techniques in molecular replacement. Structures of smaller proteins or protein domains can now be reliably predicted for use as search models in cases where no homologous structure is available. AMPLE is designed to make this technique available to users in an automated way that requires only limited computational hardware resources. Initial tests on a set of 296 cases drawn from the PDB showed that the techniques employed in AMPLE can result in solutions for approximately 40% of the targets. A beta release version is included in the latest release of the CCP4 software suite: www.ccp4.ac.uk. New efficient software tools are needed for high -throughput work in data processing as light sources and detectors continue to improve. N. Sauter (LBNL) demonstrated a python-based software tool that provides a flexible platform for addressing these issues. The current BPCX package contains a python-based image viewer and a still-image data reduction toolbox, cctbx.xfel, capable of handling concurrent event requests with the use of a multiprocessing server, cctbx.so. *Xiaoping Wang*

Speakers in *Public Domain Software* (l to r): Xiaoping Wang, Richard Cooper, George Sheldrick, Anthony Spek, Ronan Keegan, Robert Von Dreele, Oleg Dolomanov, Nicholas Sauter.



Speakers in *Radiation Damage*: (l to r) back: Robert Thorne, James Holton, and Graeme Winter; front: Ana Gonzalez, Stephan Ginell, Zou Finfrock, Elspeth Garman, and Sandor Brockhauser.

Speakers in General Interest II: (l to r) back: Allen Oliver, Alexander Merriman, Renping Qiao, and Christopher Dettmar; front: Pranoti Navare, Constance Jeffery, and Karim Sutton.

Radiation Damage

The speakers in a session on Radiation Damage addressed different aspects of the phenomenon including how to measure and minimize it (J. Holton, BMB/PBD, U.C. San Francisco, and E. Garman, U. of Oxford), temperature and time dependence of it (R. Thorne, Cornell U.), spatial dependence and penetration depth of photoelectrons(Z. Finfrock, U. Washington), and modeling how to live with it (S. Brockhauser, EMBL-Grenoble and G. Winter, Diamond Light Source). To minimize damage Garman recommended back-soaking non-specifically bound heavier atoms out of crystals to reduce the absorbed dose per incident photon, matching beam size to crystal size, using a 'top-hat' shaped beam if possible, and making sure the beamline yielded enough information to estimate the dose for your experiment to determine what your crystals would tolerate. Thorne reported that by collecting data in ~1 μs, using dose rates which approach 1 megagray per second and a fast detector, approximately half of the radiation damage near room temperature could be outrun. *Stephan Ginell and Ana Gonzales*

General Interest

The first of two sessions organized by the General Interest SIG drew a packed house as speakers addressed the scandals surrounding fabrication of crystallographic data. E. Pozharski (U. Maryland) and B. Rupp (Hofkristallamt) provided examples of structural analyses that were either unintentionally in error or deliberately fabricated. They presented troubling and inconsistent characteristics in published data. The take-home message: it is easier to produce a *genuine* crystal structure than a fabrication. Reviewers, authors and readers need to be vigilant. E. Merritt (U. Washington) presented a methodology for translation, libration and screw analysis of molecular motion that reveals the quality of a structure determination. C. Campana (Bruker), Lee Daniels (Rigak U.), and M. Meyer (Agilent Technologies) discussed the merits of current hardware and software available for chemical crystallography. C. Dettmar (Purdue U.) discussed particle size analysis and ways to prepare amorphous samples using fluorescence. P. Navare (Worcester Polytech) demonstrated how enantioselectivity can be induced on solid surfaces by appending chiral SAMs (self-assembled molecules) to the surface of the substrate. C Hu (NYU) described the complexity of *in situ* crystal-to-crystal transformations of glycine. Etter Student Lecturer K.Sutton (Oxford, UK) demonstrated how a tunable source can be used to calculate populations of differing oxidation states of an element. This technique could be useful for structures in which doping or partial oxidation of an element as a charge carrier (semi-conductors, super conductors) is present. C. Jeffery (U. Illinois at Chicago) discussed "Moonlighting" proteins that have two distinctly different functions that are present in many species. M. Matho (La Jolla Inst. for Allergy & Immunology) discussed the virus envelope protein D8 and how its study may contribute to developing vaccines R. Qiao (Max Perutz Labs, Austria) described a membrane protein that simultaneously opens channels and provides rigidity.The final speaker, high school student A. Merriman (HWI), described using conserved three-dimensional folds and amino acid sequences of ribosomal proteins to determine a rooted phylogenic tree of all species. *Allen Oliver*

Speakers in General Interest I: (l to r) back: Allen Oliver, Ethan Merritt, Edwin Pozharski, and Bernhard Rupp; front: Lee Daniels, Mathias Meyer, and Charles Campana.

***In Situ* Parametric Studies**

At the Diamond Light Source in the UK, D. O'Hare (Oxford U.) used a custom built cell for the *in-situ* study of the flux growth of $Bi_5Ti_3Fe_{(1-x)}Mn_xO_{15}$. M. Wriedt (Texas A&M) presented his study of a copper based metal-organic framework material in which a single reaction led to the formation of three different crystals having different hydration states and magnetic properties. The hydration state was reversibly controlled *in situ* by temperature and humidity. At the Sequoia time-of-flight spectrometer at the Spallation Neutron Source, G. Granroth (ORNL) described a study that clarified details of two of the high field magnetic structures. of $MnWO_4$ which has at least 6 phases. S. Misture (Alfred U.) measured electrochemical properties of transition metal oxides using high temperature data collected under controlled atmosphere. The *in situ* electrochemical activity was related to the phases present under experimental conditions, mimicking the operational environment of fuel cells P. Khalifah (SUNY Stony Brook) described de-lithiation paths and degradation of $LiFeBO_3$, a high capacity battery material.

K. Wiaderek (ANL) studied the structure and size of nanoparticles in iron-based battery materials under operational conditions

Speakers in *In Situ Parametric Studies*: (l to r) Antonio dos Santos, Scott Misture, Kamila Wiaderek, Garrett Granroth, Dermot O'Hare, Mario Wriedt, and Peter Khalifah; inset: Xiang-Quiang Chu.

Speakers in *Magnetic Materials*: (l to r) Ovidiu Garlea, Ashfia Huq, Susan Herringer, Simon Parsons, Timothy Munsie, John Greedan, and Dimitry Khalyavin.

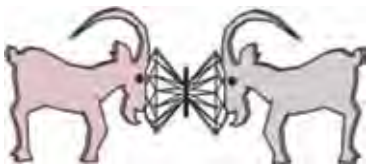
in a custom made electrochemical cell on both nano and meso scales. X.-Q. Chu (ORNL) discussed the use of quasi elastic neutron scattering to study the relaxational dynamics of lysozyme and an inorganic pyrophosphatase. The slow dynamics of these globular proteins could be adequately modeled by the mode-coupling theory. *Antonio dos Santos*

Magnetic Materials

This session featured materials synthesis, molecular magnets studied under pressure and three different families of compounds which have exciting magnetic properties. J. Greedan (McMaster U.) discussed short and long range magnetic order observed in vacancy ordered / disordered perovskite structures. D. Khalyavin (ISIS, Rutherford Appleton Laboratory) introduced the hexagonal lattice system RBaCo_4O_7 where a new exchange topology exhibiting geometrical frustration gives rise to varied degrees of spin correlation. O. Garlea (ORNL) described the effect of oxygen doping on the structural and magnetic properties of delafossite compounds. The second half of the session included studies of molecular based magnets under pressure, effects of random exchange in ferromagnetic copper chloride chains and studies of single crystal holmium titanate. *Ashfia Huq*

To be continued in the next issue.

Participants of the 5th Frolic Goats High-Pressure Workshop (l to r): Marta Lama Lopez, Armand Budzianowski, Weizhao Cai, Maciej Bujak, Kamil Dziubek, Michał Kaźmierczak, Reza Kia, Piotr Guńka, Michał Andrzejewski, Hamid Reza Shahsavari, Witold Zieliński, Magdalena Sikora, Anita Owczarzak, Ewa Patyk, Kinga Ostrowska, Michalina Anioła, Paulina Wawrzyniak, Anna Olejniczak, Kacper Rajewski, Hanna Tomkowiak, Damian Paliwoda, Jędrzej Marciniak, Marcin Stachowicz, Marcin Podsiadło, Waldemar Nowicki, Michał Dobrowolski, Maura Malińska, Dorota Stępień, Marek Jarek, Andrzej Katrusiak, Paweł Piszora; Absent from the photo: Paulina Pojawis, Jolanta Darul, Małgorzata Ratajczak-Sitarz, Marek Szafrański, Katarzyna Kowalska, and Hanna Piotrowicz.



Frolic Goats High-Pressure Diffraction

Poznań, Poland, April, 2012
hpc.amu.edu.pl/hpd2012/

BY ANDRZEJ KATRUSIAK

The 5th Frolic Goats High-Pressure Diffraction Workshop, held at the Adam Mickiewicz U. in Poznań, April 15-17, 2012, was attended by 36 crystallographers representing 5 countries. After an introduction to high-pressure techniques by A. Katrusiak, the lecturers spoke about methods of correcting high-pressure data measured for samples in a diamond-anvil cell (DAC) by X-ray diffraction (M. Kaźmierczak); high-pressure powder-diffraction crystallography (A. Budzianowski); high-pressure experiments at synchrotrons Michał Dobrowolski (ESRF); computation of interactions energy in molecular crystals (K. Dziubek and J. Marciniak); and graphical presentations of high-pressure structures (A. Katrusiak). Another session was dedicated to high-pressure results: transformed interactions in high-pressure (+)-sucrose polymorph (E. Patyk); the hidden polar phase of imidazole (D. Paliwoda); Carney's rule in chloroethanes (M. Podsiadło); remote switching of amine hydrophilicity (M. Andrzejewski); pressure-induced hydration in thiourea (A. Olejniczak); and a new high-pressure polymorph of KH_2PO_4, KDP (Weizhao Cai). The Workshop included hands-on laboratory exercises on DAC operation, alignment, loading, and diffraction experiments. A Frolic-Goats Spring Project has been announced, for encouraging the participants to start high-pressure experiments in their laboratories. The round-table discussion in the closing session was aimed at promoting the use of pressure in scientific investigations and collaboration involving high-pressure facilities.

The workshop was sponsored by the Faculty of Chemistry, Agilent Technologies and Bruker Poland, and was organized under auspices of Polish Foundation of Science. The participants experienced extreme conditions during the kayak excursion down the Warta River from the Wielkopolski National Park to the historical centre of Poznań, 17 km down the Warta River where strong winds and waves pushed kayaks upstream; otherwise it was warm and sunny in Poznań during the Workshop.

The kayak excursion down the Warta River.

10th Singapore National Crystal Growing Challenge

Singapore, October 2012
BY J.J. VITTAL

Crystals are one of the most beautiful objects found in nature. The wonderful colours, well-developed faces, sharp edges and artistic forms of crystals of naturally occurring minerals have given rise to their use in precious jewelry and as art objects. Growing large and aesthetically pleasing single crystals is an art that requires skills and patience. Crystal growing can also be a lot of fun and provide an opportunity to bring out one's creativity. Finally, crystal growing activities can get young people interested in the science of crystallography.

Winner of Best Display And Creativity Award from Senior Category - Temasek Polytechnic.

The Dept. of Chemistry at the National U. of Singapore (NUS) held the 10th Singapore National Crystal Growing Challenge Competition in October 2012 at the main building of Faculty of Science, NUS. This popular competition which began as an annual event in 1997 has been held biennially since 2000. This year 118 teams from 47 Secondary, Junior College and Polytechnics in Singapore participated in the competition.

There were three categories for this year's competition, Junior (Secondary school stu-

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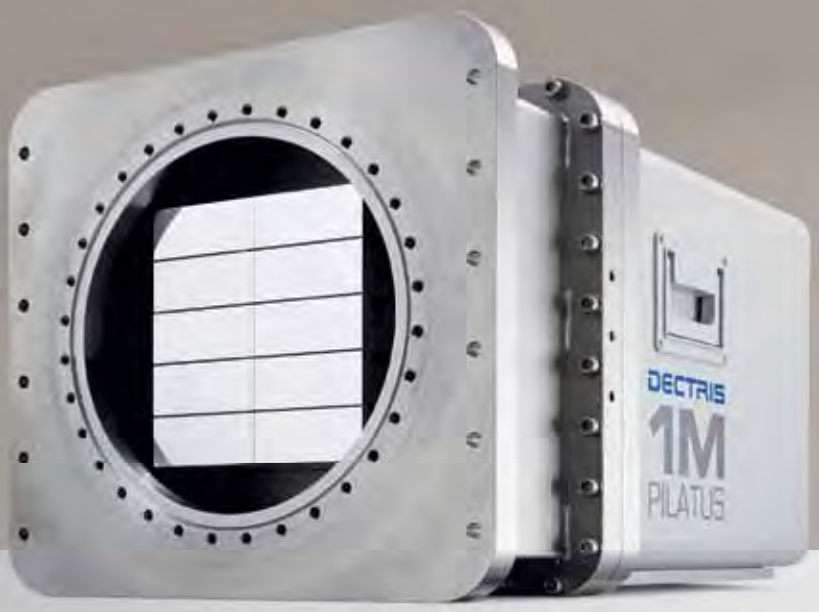

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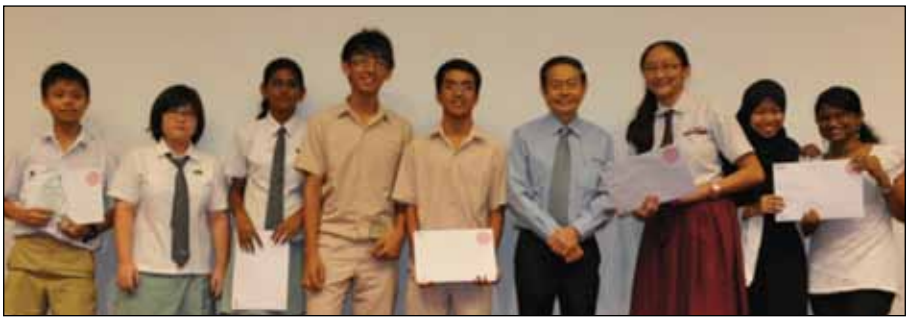


Prize winners from Open Category with the guest of honour Professor Leo Tan, President of Singapore National Academy of Science (SNAS) and director of Special Projects, NUS (4th from Right).

dents), Senior (Junior College and Polytechnic students) and Open levels. For each category, there were first, second, third and two meritorious prizes carrying cash awards $400, 300, 200 and 50 (x 2) respectively in addition to trophies for the top three winners. Junior level student grew colored sugar crystals. Senior level students grew Rochelle salt, Na,K (Tartrate)·4H_2O. Open level students were challenged to grow the longest single crystal they could to exercise their creativity, individuality and scientific knowledge.

The students displayed their posters and crystals in the morning of October 6. The award ceremony, held that afternoon, was attended by more than 300 guests, students and teachers. Jagadese J Vittal, the founder of the competition described its history since its inception in 1997. The guest speaker Ms Sadow Tanja, Dean of the Jewellery Design and Management International School (JDMIS) in Singapore discussed natural gems and minerals and how they differ from the synthetically made crystals.

The guest of honor, Leo Tan, President of Singapore National Academy of Science (SNAS) and Director of Special Projects, presented tokens of appreciation to the judges and the guest speaker and presented prizes to the winners of all the categories including the best display and creativity, and the biggest single crystal. This year's competition was sponsored by Bruker Singapore Pte Ltd, the Material Research Society of Singapore (MRS-S) and World Scientific Publishing, Singapore. In fact, Bruker Singapore Pte Ltd has been a constant sponsor since this event began in 1997. The details of this challenge are available at the website: www.chemistry.nus.edu.sg/events/CommunityOutreach/ncgc/announce.htm.

The next crystal growing competition in Singapore will be held as a special event in conjunction with the International Year of Crystallography in 2014. ❖

Bragg Centennial Symposium

Adelaide, Australia, December 2012

The 12th Asian Crystallographic Meeting and the Bragg Centennial Symposium were held in Adelaide, December 2-6, 2012. At the Bragg Symposium fifteen speakers presented lectures on the life and work of the Braggs, and their remarkable impact on the science of the last 100 years. W.L. Bragg is still the youngest person to have received a Nobel prize. In 1915, at the age of 24 he shared the prize with his father. The Bragg equation was entirely the work of the son reported in a paper read at the Cambridge Philosophical Society in November of 1912. Working together the father and son determined the crystal structure of sodium chloride. This structure determination not only confirmed the power of the equation and the accuracy of Bragg's theories but unequivocally demonstrated that sodium chloride was a salt composed of separate ions and not a molecule as was widely "believed" at the time. As late as 1927, the President of the Royal Society of England continued to disparage the crystallographic finding and dismiss the absurd notion that sodium chloride was not a molecule.

Bragg Symposium lecturers. Front row(l to r): Gautam Desiraju, Anthony Kelly, Patience Thomson, Steve Wilkins, Brian Matthews. Second row: Sir Colin Humphreys, John Jenkins, Anthony Klein, Peter Colman, David Thomson, Anders Liljas. Back row: Tony Cheetham, Wayne Hendrickson.

Nevertheless the significance of the new science of crystallography was immediately recognized with a Nobel Prize to the Braggs. Over the past 100 years more crystallographers have been awarded Nobel prizes than people working in any other scientific discipline. After making early applications of crystallography to the structures of metallic and organic structures Bragg went on to nurture the beginnings of macromolecular structure determination and analysis. Many speakers in the session reviewed the highlights of the past century of crystallography and expanded on recent technological advances that are opening the way to analysis of larger and more complex systems as well as single molecules. These new developments promise to keep crystallographic analysis powerful and pertinent well into the next century.

Lawrence Bragg's youngest daughter Patience Thomson presented a wonderful lecture describing her fathers gentle, kind and delightful personality and the audience of over 350 people were able to view films of his lucid and lively explanations of structural biology for the layman that were broadcast on BBC television in the 1950s. That evening in the former Bragg home in Adelaide (designed by and for them) Lawrence Bragg's granddaughter and grandson described their memories of a caring grandfather and the menu was composed of what Patience remembered as her father's favourite dishes. Articles by the lecturers at the Symposium are available in the Bragg Centennial Issue of *Acta Crystallographica A* (January 2013 issue).

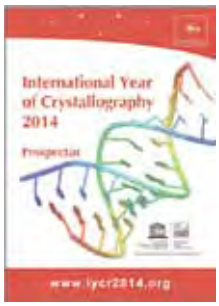
Steve Wilkins and W.L. Duax

IYCr2014

The International Year of Crystallography website is now live at www.iycr2014.org/.

This website will provide an opportunity for organizations worldwide to coordinate their activities and initiatives.

The website has a list of events planned around IYCr. If you have an event being planned, please send early notification to the site Webmaster.

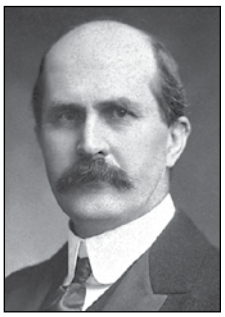


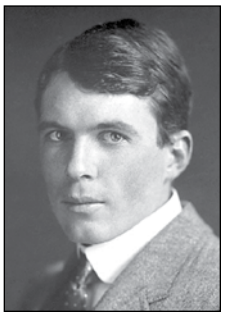
A 12-page booklet outlining the scope of the International Year of Crystallography is now available for download at www.iycr2014.org/about).

"The Two Braggs" Exhibition

from *News*, by Northern Networking Events, Oct. 23, 2012

Approximately 100 years ago in Germany Max Theodor Felix von Laue (1879-1960), Paul Karl Moritz Knipping (1883-1935), and Walter Friedrich (1883–1968) showed that X-rays could be diffracted by crystals. Laue was subsequently awarded the Nobel Prize in Physics in 1914. Following this discovery, the unique partnership, father and son, William Henry Bragg (1862-1942) and William Lawrence Bragg (1890-1971) in England, successfully showed how X-ray diffraction could lend itself to the solution of crystal structures, for which they shared the Nobel Prize in Physics in 1915. A major exhibition is planned to coincide with the ECM28 at the U. of Warwick to celebrate their lives: for the first time it will be possible to view historic equipment, notebooks, honors, letters, films and artwork. The exhibition will be open to all participants and to the public at large.


W.H. Bragg


W.L. Bragg

We were saddened to hear that Guy Dodson passed away on December 24, 2012.

Guy Dodson (right) with Peter Murray-Rust at the 2011 IUCr Congress.

An article will appear in a future issue.

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A selection of future meetings. A more complete list is available at www.iucr.org. Corrections and new listings are invited by the Editor.

MAY 2013

30-8 ♦ Int'l School of Crystallography 46th Course: "The Future of Dynamic Structural Science". Erice, Italy. www.crystalerice.org.

JUNE 2013

12-16 ♦ 22nd Cro-Slo Cryst Meeting (CSCM22). Biograd, Croatia. spopovic@phy.hr, or ivan.leban@fkkt.uni-lj.si.

JULY 2013

20-24 ♦ ACA 2013. Honolulu, HI, USA. www.amercrystalassn.org/.

AUGUST 2013

4-10 ♦ 15th Int'l Summer School on Crystal Growth (ISSCG-15). Gdansk Poland. http://science24.com/event/isscg15/.

6-11 ♦ ECM28. Coventry, UK. http://ecm28.org/. See Back Cover.

11-16 ♦ 17th Int'l Conf. on Crystal Growth and Epitaxy (ICCGE-17). Warsaw Poland. http://science24.com/event/iccge17/.

SEPTEMBER 2013

1-6 ♦ 12th Int'l Conf. on Quasicrystals. Kraków Poland. www.icq12.fis.agh.edu.pl/.

OCTOBER 2013

14-29 ♦ X-ray Methods in Structural Biology Cold Spring Harbor, NY, USA. http://meetings.cshl.edu/courses/2013/c-crys13.shtml.

DECEMBER 2013

1-4 ♦ AsCA 2013. Dhaka, Bangladesh. www.asca2013.org/.

MAY 2014

24-28 ♦ ACA 2014. Albquerque, NM, USA. www.amercrystalassn.org/.

AUGUST 2014

5-12 ♦ 23rd IUCr Congress and General Assembly. Montreal, Quebec, Canada. http://www.iucr2014.org/. See Page 22

SEPTEMBER 2014

14-20 ♦ 15th Int'l Conf. on the Crystallisation of Biological Macromolecules (ICCBM15). Hamburg Germany. www.iccbm15.org/.

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