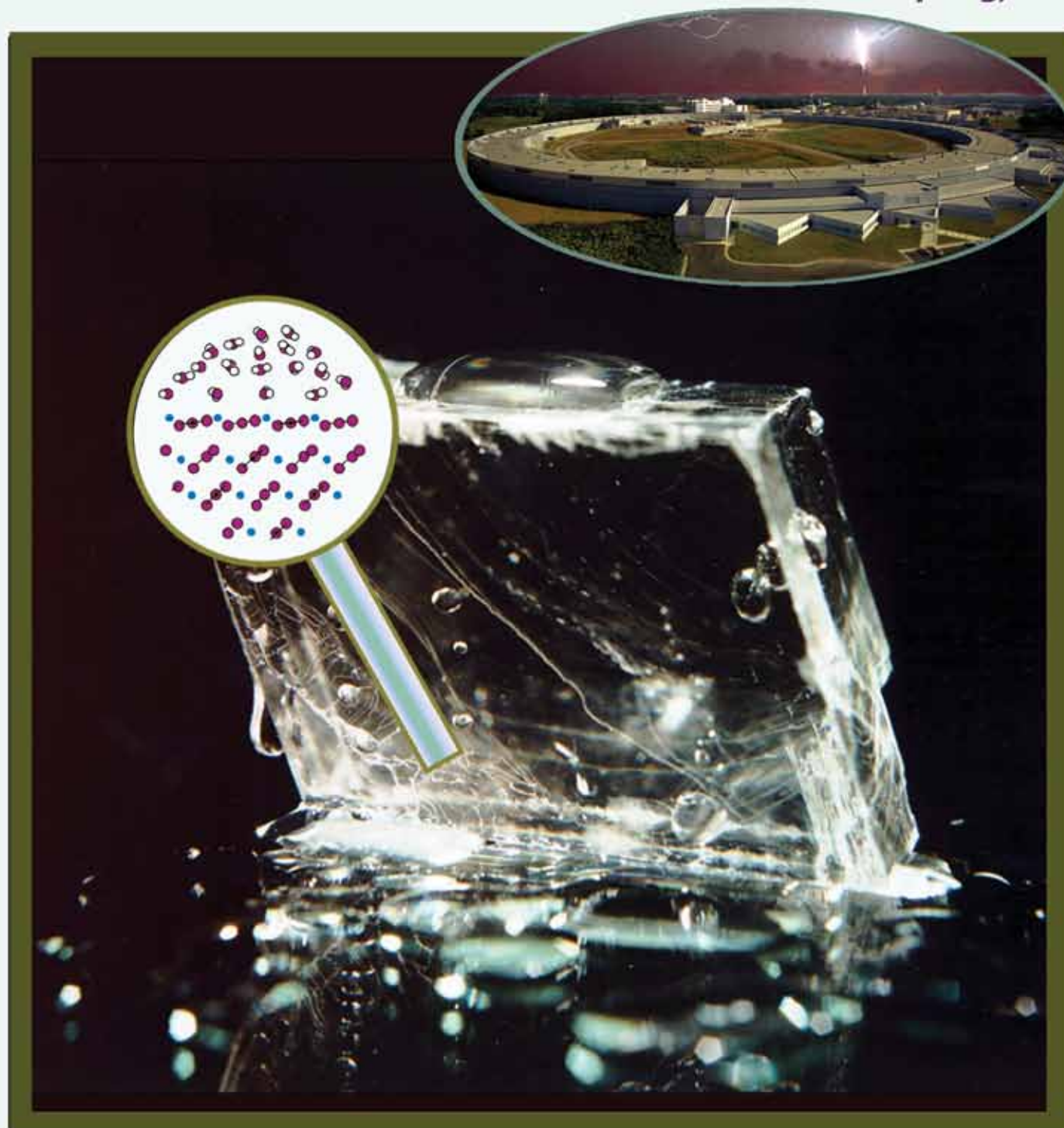


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American Crystallographic
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Number 1
Spring, 2012



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Cover: Paul Fenter will receive the Warren Award at the 2012 ACA meeting in Boston. See On the Cover, page 30.



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Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)

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Innovation with Integrity

Crystallography



It's an exciting time to be a crystallographer! For a discipline often thought to be mature, in the sense of being highly evolved and complete, there are tremendous new vistas in our field. Crystallography has long been interdisciplinary, drawing from mathematics, physics, chemistry and the biological sciences. Let me

highlight some of the recent developments that have helped generate the excitement that I feel for our field.

I'm writing this while attending a Keystone Symposium that combines two meetings into one. One is called *High-Throughput Structural Biology* and the other *Structural Biology of Cellular Processes: From Atoms to Cells*. The conference has physicists, chemists, biochemists, and cell biologists all in the same setting. Folks from both meetings go back and forth between the sessions, learning about new structural technologies and seeing how applications of these technologies answer questions in biochemistry, neurobiology, developmental biology and other domains. The multidisciplinary aspect of structural science is apparent.

The physics types are exploring new frontiers that will dramatically impact crystallography. New x-ray sources will fundamentally change atomic-level structural science. Third generation synchrotrons and new linear accelerators are changing the way macromolecular crystallography and structural science are being done. Today, a microscopic but visible crystal is needed to determine atomic positions. Soon, it seems that streams of nanocrystals will be paraded in front of an x-ray laser and their diffraction patterns merged and phased based on anomalous scattering from native atoms. These advances are driven in no small part by the longtime desire of biologists and chemists to formulate atomic level structure-based hypotheses that connect phenotype to genotype and to apply these hypotheses to biomedicine. Similar advances in chemistry, materials science and nanotechnology are facilitated by new structural science provided by the crystallography community.

ACA 2012 Call for Papers Featured Award Winning Artwork

First place in the 2005 ACA *Art in Crystallography* contest was awarded to *Blood 2,000,000X* by **David Goodsell** (Scripps Institute). This watercolor illustration shows a cross-section through the blood, with blood serum in the upper half and a red blood cell in the lower half. In the serum, look for Y-shaped antibodies, long thin fibrinogen molecules (in light red) and many small albumin proteins. The large UFO-shaped objects are low density lipoprotein and the six-armed protein is complement C1. The red blood cell is filled with hemoglobin, in red. The cell wall, in purple, is braced on the inner surface by long spectrin chains connected at one end to a small segment of actin filament. David (mgl.scripps.edu/people/goodsell) has created many exciting artworks based on molecular science. He is the author of the web-based educational series Molecule of the Month at the RCSB PDB (www.rcsb.org) and the featured systems series at the PSI Structural Genomics Knowledgebase (www.sbk.org).

The *Call for Papers* with 2012 meeting logo designed by Peter Müller is now on the ACA website: www.AmerCrystalAssn.org.

What is the ACA up to? Glad you asked. 2012 brings a new meeting format, shortened a bit by popular demand and presented to you in Boston, July 28th to August 1st. You will hear our award winners describe their exemplary work: **John Spence** has earned our **Buerger Award**, **Paul Fenter** the **Warren Award**, and **Ron Hamlin** the **Supper Instrument Award**; the **Etter Early Career Award** goes to **Emmanuel Skordalakes**. See our fine web site www.AmerCrystalAssn.org for more information on these awards and awardees. We also have a special treat planned just before the banquet. **Don Caspar**, one of the founders of the field of structural biology, has been tapped to talk us through a bit of history.

The site for the 2013 meeting has been set for Hawaii. The previous meeting there was a huge success and we are looking forward to this one also. Our Buffalo office, with Marcia Colquhoun, Crystal Towns and Kristina Vitale, are doing a great job on our meetings, as always. Don't forget about the IUCR meeting in 2014 either. It will be held in North America for the first time in quite awhile and will be well led by our ACA Canadian Division members.

In 2012 we welcome two new members to the ACA Council. Cheryl Stevens joins us as Vice-President and Patrick Loll as Secretary. The ACA could not function without the continual supply of volunteer officers. Thanks to all who came before us and to those of you yet to serve.

The year 2012 brings a special celebration commemorating the 100th year anniversary of the game changing work of Max von Laue and the father-son team of Sir William Bragg and Sir William Lawrence Bragg. From their work crystallography was born. Let's celebrate our roots and how far we have come and continue to push crystallography on with, (quoting from an anonymous source here at Wisconsin), "*sifting and winnowing by which alone the truth can be found.*"

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We would also welcome volunteers for
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& Copy Editor.
Please contact either of us
- see email addresses above.*

Errata: Thanks to Helen McDonnell at the ICDD for pointing out that on page 15 of the winter RefleXions the picture supposed to be of Richard Bostwick was instead ICDD Chair Tom Blanton.



Richard Bostwick is at left above, accepting the ICDD Distinguished Fellow Award; Tom Blanton is on the right.

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Peter Müller, in addition to his work as RefleXions Staff Photographer, designed both the logo for the Boston ACA Meeting and the promotional pages 38-39.

The crystallographic community was saddened to hear today that David Sayre, Department of Physics, State University of New York, winner of the 8th Ewald Award, and a past president of ACA has died.

A full appreciation will be published in the summer ACA RefleXions. Please send remembrances of David to either Judy: acareflexions@gmail.com or Connie: conniechidester@earthlink.net

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Cartoon courtesy of Nick D. Kim. Nick Kim is an analytical environmental chemist currently working for the Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand.

M

Motheematics

The group of sciences that deal with the quantities, magnitudes, geometries, algebra and calculi of moths.

Illustration: a motheematician.



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belong to the IUCr. The governance of the IUCr is done at triennial Assemblies (held at the Congresses). During these wonderful long evenings, delegates from each of the Adhering Bodies meet, shmooze, bicker, select future Congress sites, elect the Executive Committee (officers) of the IUCr, pass or reject motions and vote on bylaw changes. Between Congresses, the Executive Committee makes decisions and tasks the staff of the IUCr (in Chester, UK) to do all the heavy lifting. The IUCr views scientists as affiliated with the country where they work, independent of their country of origin or citizenship.

All crystallographers living or working in a country that has an Adhering Body are thus affiliated with the IUCr.

The IUCr recognizes the ACA, the European Crystallographic Association and the Asian Crystallographic Association as regional affiliates, and there are considerable informal interactions between the IUCr and the three regional affiliates. For example, the Executive Committee of the IUCr will meet this year during the Boston ACA meeting. In 2011, the IUCr amended its bylaws to ensure that its Executive Committee will have at least one representative from each of the three geographical regions. In fact, at the 2011 General Assembly two IUCr Executive Committee members were elected from our region: Marv Hackert (University of Texas) and Hanna Dabkowska, (McMaster University in Canada). However, the ACA is not a member of the IUCr and has no formal representation in the union.

The Adhering Body to the IUCr for the United States is the National Academy of Sciences (NAS). The NAS organizes the USNCCr, which interacts with both the IUCr and the U.S. scientific community. The Canadian National Committee for Crystallography (CNCC) is a comparable organization interacting with Canadian scientists (see www.canadiancrystallography.ca). The National Science Foundation (NSF) provides funding for the USNCCr and US dues to the IUCr and also pays dues for ~17 other scientific organizations (chemists will be familiar with IUPAC).

Each Adhering Body selects their category of membership based on the level of dues they are able to pay, and this determines the number of votes the country receives. The least expensive option is Category I, with one vote. Costs go up in a greater than linear fashion up to Category V, with the maximum five votes. The US is a Category V member, and Canada is a Category III member.

So -in conclusion, the role of the USNCCr (see sites.nationalacademies.org/PGA/biso/IUCr) is to represent the interests of US crystallographers and to coordinate those interests with the IUCr. We interact heavily with the ACA, but each organization has a separate outlook and role. In future issues of *Reflexions*, I will write about how the membership of the USNCCr is chosen and also cover what the committee does and what we are planning.

Brian Toby


About the USNCCr

The membership of the US National Committee for Crystallography (USNCCr) is shown above and on the preceding page. While readers will likely know a fair amount about the ACA, many people may wonder -*what is this USNCCr and what does it have to do with the ACA?* Also, - *what is the International Union of Crystallography (IUCr) and how does it relate to the ACA?* The *Reflexions* editors have charged me to explain all these mysteries and more to their readers.

You are most likely reading *RefleXions* because you are a member of the ACA (www.amerocrystalassn.org/) - or should be. I would hope that it is clear from looking at the rest of this issue that *American* in this context refers to the hemisphere, not any particular county, since the ACA is very well represented in Canada and is working to improve Latin American involvement. In fact, the ACA is populated by members from ~60 countries. The ACA holds an annual crystallography meeting, publishes *RefleXions*, runs educational programs, gives awards and does many other fine things (which is why you should be a member).

The IUCr, (www.iucr.org/) is the umbrella organization for crystallography. An international crystallography meeting (the IUCr Congress) is held every three years - the next will be August 5-12, 2014 in Montréal, during the 2014 **International Year of Crystallography**, also a major project for the IUCr. The IUCr publishes the *Acta Crystallographica* family of journals, books, the *International Tables for Crystallography* series, the *IUCr Newsletter*, and the *World Directory of Crystallographers* (please check that you are listed and that your listing is accurate!). The Ewald Award is presented at the IUCr Congresses.

How does one join the IUCr? Well, individuals do not. The IUCr membership is comprised of national Adhering Bodies, usually national academies of science or national funding agencies. Currently 38 countries plus 3 groups of countries

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Council Renames Two Pauling Poster Awards

The ACA Council has decided to rename two of the ACA Pauling Poster Prize Awards to recognize the contributions of two highly respected crystallographers. The **Pauling-Branson Award** recognizes the contributions of **Herman Russell Branson**, (1914-1995), one of the first African American physicists to make crystallography the focus of his research. The **Pauling-Sundaralingam Award** recognizes the ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids done by **Muttaiya Sundaralingam**, (1931-2004), and his colleagues.

Branson was born in Pocahontas, VA and received his BS from Virginia State College in 1936, and his PhD in physics in 1939 from the University of Cincinnati, under the direction of Boris Padowski. After a stint at Dillard University, he joined Howard University in 1941 as an assistant professor of physics and chemistry. He remained at Howard for 27 years, achieving increasingly important positions. He chaired the Department of Physics, directed a program in experimental science and mathematics, and worked on Office of Naval Research and Atomic Energy Commission projects in physics while at Howard University.



In 1948, Branson took a leave and spent time in Linus Pauling's lab at Caltech. There he was assigned work on the structure of proteins; specifically he used his mathematical abilities to determine possible helical structures that would fit both the available x-ray data and a set of chemical restrictions outlined by Pauling. After some months Branson handed in a report narrowing the possible structures to two helices, a tighter coil Pauling termed **alpha**, and a looser helix called **gamma**. Branson then returned to Howard to work on other projects but the work was ultimately published in a paper with Pauling and his assistant Robert Corey (Pauling, Corey and Branson (1951) *PNAS*, **37**, 205-211). This was the only paper on the topic that included Branson as a co-author and he later felt that he did not receive enough credit for his contributions. At Howard Branson organized cross-disciplinary research teams of physicians, engineers, mathematicians, biologists, chemists, and physicists. After more than two decades of trailblazing research, he went on to serve as president at two historically black colleges, Central State University in Ohio (1968-1970) and Lincoln University in Pennsylvania (1970-1985).

Muttaiya Sundaralingam, known as Sunda, was born in Taiping, Malaysia. He came to the US in 1959 and received a PhD in Chemistry / Crystallography with George Jeffrey (U Pittsburgh). After doing a postdoc with Lyle Jensen (U Washington) he held positions at Harvard, Case Western Reserve and Oxford University. From 1969-1989, he served as Professor of Biochemistry and Steenbock Professor of Biomolecular Structure at U Wisconsin. After retiring in 1989,



he accepted a position as Ohio Regents Eminent Scholar and Professor of Chemistry and Biochemistry at Ohio State University. He retired from that position in 2002. He then continued his research interests as an emeritus professor.

Sunda had an abiding interest in nucleic acid structure. His work had implications for the structural principles governing the folding of nucleic acids, about which little was known at the time of his research. Sunda and his many students identified the critical role played by the sugar moiety in determining the conformation of the nucleotide repeating unit and, ultimately, the sugar-phosphate backbone of nucleic acids. His work is so often cited in the literature and in textbooks of biochemistry and biophysics that he was among the top 300 of the 1,000 most cited scientists for work published from 1965-1978.

Sunda, and his wife Indrani, died together the morning of December 26, 2004 when their hotel on the beach in Nilaveli, a small village just north of Trincomalee, Sri Lanka was struck by the tsunami.

Centennial Anniversary of XRD

This year marks the 100th anniversary of the discovery of x-ray diffraction and its use as a probe of the structure of matter. Sixteen years after Wilhelm Conrad Röntgen announced in 1895 his discovery of "X" rays that can penetrate the body and photograph its bones, **Max von Laue**, a professor of physics at the University of Munich in Germany, worked on a theory of the interference of light in plane parallel plates.

In 1911, von Laue suggested to one of his research assistants, **Walter Friedrich**, and a doctoral student, **Paul Knipping**, that they try out x-rays on crystals. His reasoning was that x-rays have a wavelength similar to the interatomic distances in crystals, and as a result the crystal should act as a diffraction grating.

By April 1912, von Laue, Friedrich and Knipping had performed their pioneering experiment on copper sulfate. They found that if the interatomic distances in the crystal are known, then the wavelength of the x-rays can be measured, and alternatively, if the wavelength is known, then x-ray diffraction experiments can be used to determine the interplanar spacings of a crystal. The three were awarded a Nobel Prize in Physics for their discoveries. Hats off to all of you for advancing the study and application of x-ray analysis these past 100 years. Happy birthday, XRD!

From Bruker's FIRST Newsletter, Jan 25th 2012

Free Equipment

Two-tube x-ray generator (Enraf-Nonius Diffractis 582) with four x-ray cameras (two precession, two Weissenberg), a dual water pump and heat exchanger and other single-crystal equipment. Both of the x-ray tubes are Cu radiation, but two different tubes could be installed for flexibility. One of the cameras is relatively new, a Huber 205 precession/rotation camera with telescope and internal light source for observing crystal faces (uses conventional film or polaroid cassette). Available now, free of charge, if either transportation or cost of shipping is provided. For further details, contact **Karl J. Feierabend**, Dept of Chemistry, The College of Wooster, Wooster, OH, 330-263-2613, kfeierabend@wooster.edu.

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Ross Angel to Receive Dana Medal



Ross J. Angel, a former Postdoctoral Fellow at the Geophysical Laboratory, will receive the **Dana Medal** of the **Mineralogical Society of America** at the Goldschmidt Conference in Prague, Czech Republic on August 14-19. The award will be presented during a special session organized in his honor entitled: *Structure, Elasticity and Thermodynamics of Minerals*. The scientific content of the symposium will "...reflect [Ross'] general interests in the link between elastic properties, structure and other properties of minerals." Ross is currently Research

Professor of Crystallography at the Virginia Polytechnic Institute & State University in Blacksburg, Virginia. He was a Carnegie Fellow 1987 -1988.

IUCr Sponsors Serah Kimani's PhD Work in Africa

As part of the IUCr's Crystallography in Africa initiative, the Executive Committee has established a PhD program in crystallography to enable African PhD students to work in a South African university.

We are pleased to report that the second student to benefit from this support, **Serah Kimani**, has recently received a PhD from the Dept of Molecular and Cell Biology at the University of Cape Town.

Serah Wangari Kimani was born and raised in Gacharage, a small village in central Kenya. She has a BSc (Hons) in Biomedical Sciences and Technology from Egerton U., Kenya. She was recruited to the joint Masters Program in Structural Biology at the U of Cape Town / U of Western Cape, from which she graduated with distinction in 2007. Serah did postdoctoral work at the U of British Columbia in a graduate exchange program. She has numerous awards and prizes to her credit and has presented her research in both local and international conferences. Serah has co-authored several publications in international peer-reviewed journals.

Her graduate advisor, Trevor Sewell, reports that Serah is returning to Kenya but intends to come back to South Africa in 2012 for a postdoc appointment at the U of Cape Town. So far her thesis work has generated 3 papers that are in an advanced stage of preparation and there may well be more.

Her graduate thesis was entitled *Catalysis, Substrate Binding and Specificity in the Amidase from Nesterenkonkia Species*. The citation in the graduation program states *this was a formidable work, involving the determination of some forty crystal structures which establishes her as one of the leading structural biologists on the African continent*. The IUCr is delighted to congratulate Serah on her achievements.



New Publishing Partnership Will Produce Powder Diffraction

The International Centre for Diffraction Data (ICDD) and Cambridge University Press announced on the 11th of January that they have formed a new publishing partnership to produce ICDD's flagship journal. *Powder Diffraction* will be published by Cambridge University Press in partnership with ICDD, a non-profit scientific organization dedicated to publishing powder diffraction data for materials identification.

Powder Diffraction is a quarterly journal that brings cutting edge research and new advances to a global community of scientists on behalf of the ICDD. The journal has been consistently recognized as the international materials science journal most frequently used to aid identification and analysis. Due to the interdisciplinary nature of its papers, *Powder Diffraction* has wide appeal not only to materials scientists, but also chemists, geologists, environmental scientists, and biologists. Although practice is emphasized, theory is not neglected, especially as its discussion relates to better understanding of technique. The editorial focus will remain on a diverse selection of practical applications: diffraction methods, standard reference materials, search/match methods, indexing of powder data, and structure solutions from powders.

CERN Higgs Update

Geneva, 7th February, 2012: the standard model Higgs search analyses presented at CERN by the ATLAS and CMS collaborations at a seminar in December, 2011 have been submitted for publication in the journal *Physics Letters B*. After further analysis, the statistical significance of the measurements remains close to that presented at the seminar, underlining the conclusion that the standard model Higgs boson, if it exists, is most likely to have a mass constrained to the range 116-131 GeV by the ATLAS experiment, and 115-127 GeV by CMS. Tantalizing hints were seen in both experiments in the region 124-126 GeV; however these are not strong enough to claim a discovery.



Trevor Sewell (center) flanked by his doctoral graduates Serah Kimani (left) and Jeremy Woodward (right).

2011 AAAS Fellows

Last November, the AAAS Council elected 539 members as Fellows of AAAS. The new Fellows were recognized for their contributions to science and technology at the Fellows Forum during the AAAS Annual Meeting in February 2012 in Vancouver, British Columbia. The new Fellows received certificates and a blue and gold rosette to symbolize their distinguished accomplishments. ACA members elected are, left to right:

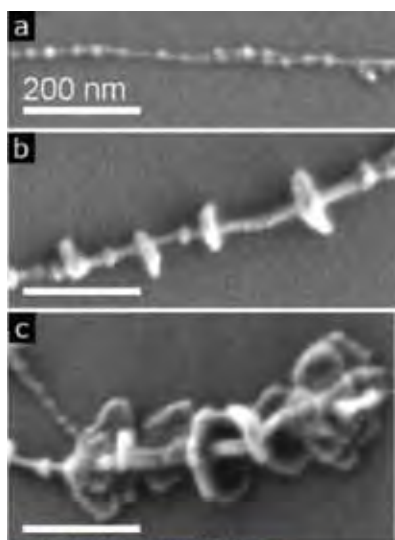


ACA members elected are, left to right: **Lukasz Lebioda**, Dept. Chem & Biol Chem, U. South Carolina, **Robin D. Rogers**, Dept. Chemistry, U. Alabama and **Peter W. Stephens**, Dept Physics & Astronomy, Stony Brook U.



2011 ACS Fellows

Three ACA members were among the 125 chemists elected to the 2011 class of Fellows. They are, left to right: **James A. Ibers**, Northwestern University, **Stephen J. Lippard**, Massachusetts Institute of Technology and **Arnold Rheingold**, University of California, San Diego.



Credit: American Chemical Society

'Shish Kebab' Structure, a New Form of Buckypaper

Scientists are reporting development of a new form of buckypaper which eliminates a major drawback of these sheets of carbon nanotubes. The new nanotubes are 50,000 x thinner than a human hair and 10 x lighter than steel, but are ~ 250 x stronger. Potential uses range from body armor to next-generation batteries. The report *Polymer Single Crystal-Decorated Superhydrophobic Buckypaper with Controlled Wetting and Conductivity* was published in the journal *ACS Nano*. Authors Christopher Y. Li et al. explain that there are several ways of making buckypaper, (named for Buckminsterfullerene, or

carbon 60, the basis for the 1996 Nobel Prize in Chemistry). In addition to being extremely strong, buckypaper conducts heat and electricity better than most known materials. This space age material is formed by depositing a very thin layer of entangled carbon nanotubes to create a fiber mat akin to office paper. Noting that no existing post-processing method allowed researchers to increase the size of the tiny holes, or pores, between the carbon nanotubes after they form the buckypaper, Li and his colleagues looked for a way to do just that. They experimented with additives to buckypapers that could make them more useful in electronics or as sensors. To control pore size, the team grew single crystals of polymers around the nanotubes, describing the result as "shish kebab" structures, where the nanotubes are the skewers and the flat crystals are the kebabs. As the buckypaper formed these crystals held the nanotubes apart. Li et al. demonstrated that the crystals permit control of pore sizes and change the conductivity, surface roughness and ability to shed water of buckypaper.

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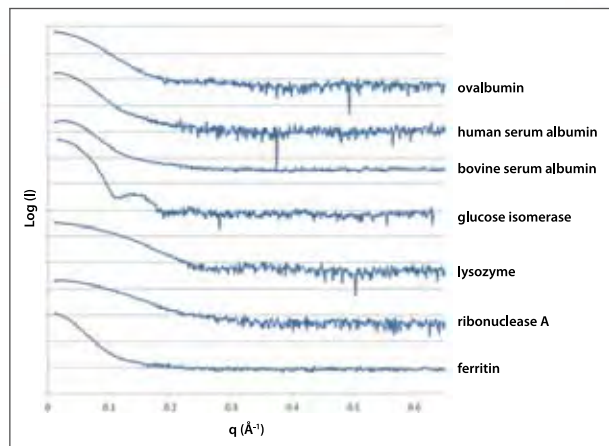
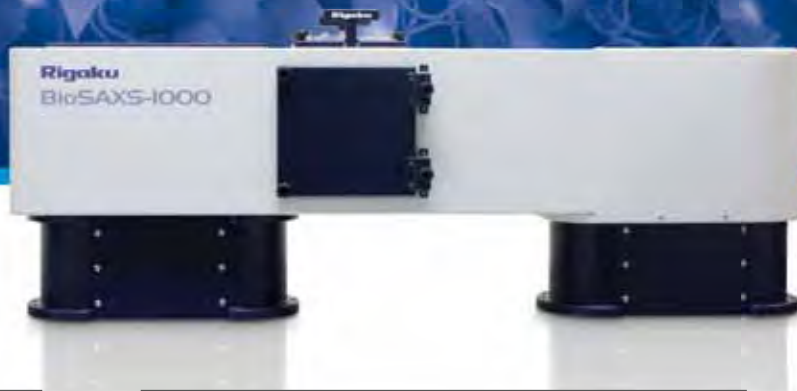
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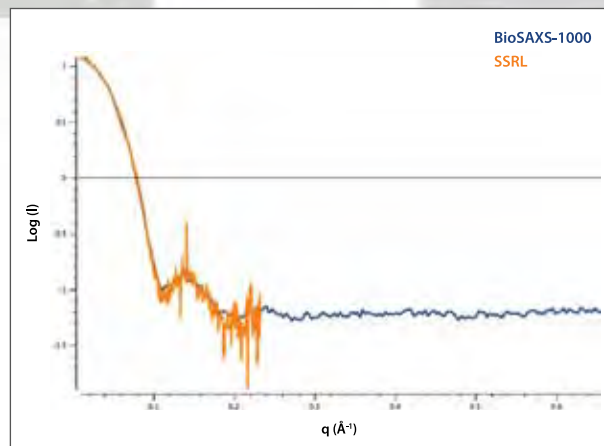
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2012 Ludo Frevel Scholarships

Thirteen recipients were selected to receive **ICDD Ludo Frevel Crystallography Scholarships**. These recipients were selected, on a competitive basis, from fifty-two commendable applications received by the ICDD Scholarship Committee. Each will receive \$2,500 to assist in the continuation of studies in their selected fields of crystallographic research.

The recipients are:

Gokhan Barin, Northwestern University, for: *Functional Metal-Complexed Building Blocks for Solid-State Structures*. **Gokhan is an ACA Member.**

Ercan Cakmak, University of Tennessee, for: *A Synchrotron X-ray Diffraction Study of Martensitic Phase Transformation Kinetics and Texture Evolution in a TRIP Steel under Torsional and Multi-Axial Deformation Conditions*.

Honghan Fei, University of California, Santa Cruz, for: *Solvo-thermal Synthesis of Cationic Inorganic Materials and Cationic Metal-organic Frameworks for Anion Pollutant Trapping*.

Sudipto Guha, University of Illinois at Urbana-Champaign, for: *X-ray Compatible Microfluidic Platforms for Protein Crystallization Screening and De Novo Structure Determination*.

Sun Woo Kim, University of Houston, for: *Investigation of New Mixed Valence Iron Fluorides: Crystal Structure and Physical Property Relationships*.

Eduard Levin, Moscow State University, Russia, for: *Influence of Structural Effects in Metallic Systems on Electrocatalytic and Charge-accumulating Properties*.

Jia-Sheng Lu, Queen's University, Canada, for: *BODIPY Functionalized PbS Nanocrystals for Solar Cell Applications*.

Gregory McCandless, Louisiana State University, for: *Chemical Crystallography at the Interface of Physics, Chemistry, and Engineering: Structure Determination of Highly Correlated Extended Solids, Main Group Compounds, Coordination Complexes, and Bioceramics*. **Gregory is an ACA Member.**

Gift Mehlana, University of Cape Town, South Africa, for: *Crystal Engineering of Some Pyridyl Carboxylic Acids*.

Sarah Spisak, SUNY-Albany, for: *Multi-Electron Reduction of Fullerene Fragments: Structural Studies*.

Vedran (Nick) Vukotic, University of Windsor, Canada, for: *Utilizing Molecular Machines in the Construction of Dynamic Solid State Materials*. **Nick is an ACA Member.**

Shuao Wang, University of Notre Dame, for: *New Insights in Actinide Borate Chemistry*.

Julie Wilkerson, University of Texas-Austin, for: *Electroluminescent Materials Based on Lanthanide-Containing Conducting Metallopolymers*.



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X-ray Crystallography. Is the Gold Standard becoming Tarnished?

The citation for the Fankuchen Award mentions my contribution to the teaching of crystallography, and my stewardship of the program CRYSTALS. Both of these fields of interest arose by chance rather than design. If I have been any good as a teacher, it was because I found the work of great crystallographers difficult to understand, and having worked to understand it, have tried to simplify it for other folk like myself. The success of CRYSTALS is entirely due to the many people who contributed to the infra-structure and the crystallographic utilities.

A Short Biography. By happy coincidence, I was invited to give the 2011 Fankuchen lecture in the year I was due to retire. This gave me the idea that the talk could be a kind of retrospective, a look back at how x-ray crystallography

had changed during the 47 years since I started work in 1964 with Tom Hamor, for my PhD in the Chemistry Department of Birmingham University. Tom was newly appointed that year, and I was his first student. The equipment he inherited was an old Leeds Weissenberg camera and a Phillips generator. Later he purchased a Stöe precession camera and an Enraf-Nonius Integrating Weissenberg. For my thesis I solved just three structures, two by visual estimation of intensities, and one using a Joyce-Loebl microdensitometer with the integrated films. At that time it would take months to collect multiple film packs for a 'full' two-axis set of Weissenberg data. Luckily I never had to use Beevers-Lipson strips because the university had recently acquired an English Electric Leo Marconi KDF9 digital computer. Tom and I were major users of the machine, running it over-night using a Fourier/isotropic least squares Autocode program written by John Rollett and his students in Oxford, or an Algol anisotropic refinement program written by Durward Cruickshank's group in Glasgow. At that time NMR and the optical spectroscopies were immature techniques, and x-ray crystallography was the Gold Standard for structure analysis.



Tom Hamor with Janet Cheatham, Univ. of Birmingham.

In 1967 I went to work in Oxford for one year as H. M. (Tiny) Powell's last post doc. My task was to get data out of the Hilger and Watts Royal Institution Y190 Linear Diffractometer. This machine was a mechanical implementation of the Ewald construction, and a great aid in making the reciprocal lattice very real. The crystal had to be aligned to the instrument axes, adjustments being made to the goniometer head with the shutter open. I still have all my fingers. Data collection times were directly proportional to the number of unique reflections (except for special zones, equivalent were almost never measured) and so could take weeks.

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Keith Prout with Pete Symmonds ~2002, Oxford Univ.

When Tiny retired, in about 1972, Keith Prout became head of the Chemical Crystallography laboratory. Like Tom and Tiny, he was a very serious and knowledgeable crystallographer, with a real enthusiasm for encouraging and teaching. In fact, his passion for helping others led to his own career being neglected, and he never got the international recognition he deserved. The Linear H&W Y190 was later replaced by a Hilger and Watts Y290 four circle diffractometer, controlled by a PDP8 computer built from printed circuit boards with discrete transistors and a ferrite core memory. This, in its turn, was replaced by Enraf-Nonius CAD4 diffractometers, which brought data collection times down to a few days, and later, in 2000, by the truly brilliant Nonius Kappa CCD machines. The xCCD machines are still working side by side with dual microsource Oxford Diffraction (Agilent) instruments. In the 47 years since I took my first Weissenberg photographs, data collection times have dropped perhaps three orders of magnitude - from months to just hours, or even minutes.



David Watkin and 'Tiny' Powell, Oxford Univ.

Of course, during this same time computers and software also evolved. By 1967 Jeff Ford and John Rollett had replaced the old Oxford Autocode programs with a FORTRAN version. At that time every crystallographer had some programming skills so that Bob Carruthers, having come across a twinned crystal during his PhD

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work, was able to convert an existing program to deal with the data. Later, he went to work with Ricardo Spagna in Rome, helping write the code that later became Caos. Returning to Oxford, Bob and John began creating CRYSTALS, with the meticulous attention to detailed infra-structure that has enabled the program to evolve until the present day.

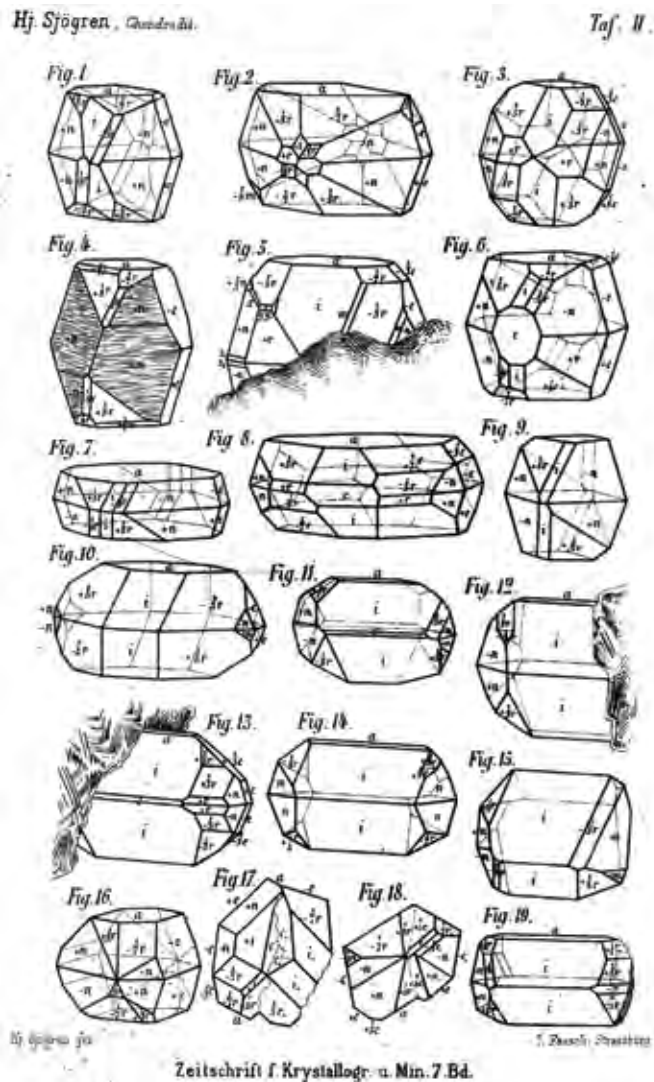
In about 1975 Bob announced that he was leaving Oxford to work with the super computer company Control Data Corporation, so that I found myself looking after not only the diffraction equipment, but also CRYSTALS. Keith Prout had always encouraged chemists to take a hands-on approach to crystallography, and visitors to the laboratory were often astonished to see project students using the instruments themselves. This endless stream of beginners led to my interest in teaching, and in trying to make our programs effective both as research and as teaching tools. During the VAX era, Stan Cameron sent Bev Vincent to work with us for a few months. Bev built our first *Interrogative User Interface*, which was later developed by Paul Betteridge into a sophisticated reprogrammable user interface. Also during this, time we tried to turn CRYSTALS into a fully automatic structure solution and refinement system. Then, as now, the automation ground to a halt whenever disorder turned up, and by 1995 Richard Cooper decided that it was probably easier to teach a chemist crystallography than to teach a computer chemistry, and he devised our first reprogrammable *Graphical User Interface*. Richard was much influenced by a close collaboration with Lachlan Cranswick, whose ideas for “eye candy” have now even found their way into programs like Olex2.

In 1976 Bob Sparks published a short program simulating refinement and useful for benchmarking computers in a crystallographic context, which was programmed into CRYSTALS. Sadly, we didn't record results from computers of that period, but we can compare a Microvax 3800 (1989) with a 3.0 Ghz Intel Duo (2010). We can now do in one day what would have taken three days in 2010, and almost five years in 1989. In high resolution (small molecule) crystallography, getting a reliable trial structure is no longer a serious issue. SHELXS soldiers on with the reliability of the Old Guard, new versions of SIRware bring new facilities, and Superflip has made charge flipping a standard technique. However, no really new ideas have emerged for working up structures, and we are still using methods which were readily available by the 1970s.

X-ray Crystal Structure Analysis in 2011. In 2011 we have diffractometers of great sensitivity, we have brilliant laboratory sources and we have immensely powerful synchrotron sources. Work at 100°K is routine, and at 10°K reasonably feasible. Diamond Anvil Cells enable samples to be examined at pressures up to 10 GPa. Computers work at breath-taking speeds.

In effect, we have amazing technology available. What science can we do with it?

"The age of intramolecular structural chemistry is declining for small molecules. There is very little that can be added to the average intramolecular geometrical data collected by use of the Cambridge Structural Database; anything at variance with these well-established averages is most probably wrong." (Gavezzotti & Flack, 2005, www.iucr.org/iucr-top/comm/cteach/pamphlets/21/21.html). Has small molecule crystallography become just stamp collecting?



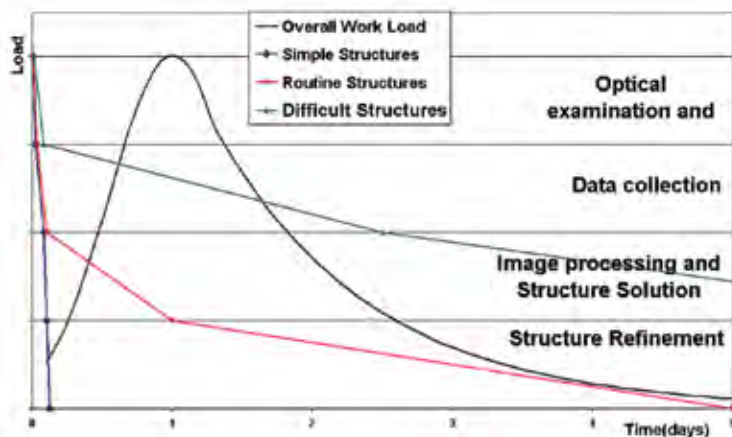
Indexing faces and measuring interfacial angles was legitimate research in Victorian times. Reproduced from Fig 2, Zeitschrift für Kristallographie, 1883.

Zeitschrift für Kristallographie, for the declining years of the 19th Century, contains page after page of beautiful drawing of crystalline minerals, and tables of the interfacial angles measured with improbable precision. With hindsight, we know that these measurements added nothing to our understanding of the Natural World, since the Law of Constancy of Interfacial Angles was already well established. Is *Acta Crystallographica E* just another repository for more irrelevant structures: the *Journal of Squeaky-Clean Structures*? Perhaps more interesting would be the *Journal of Rotten Structures*. To publish here authors would need a track record of ‘good’ structures to demonstrate their skills, but working up structures would be stubbornly intractable. The deposited material would include the author’s attempts, and all the diffraction data, including images. Keith Prout once said that there is no such thing as Bad Data, only Bad Models. This is perhaps an educational exaggeration (since a misaligned instrument will inevitably yield bad data) but the underlying thesis is that the solid state is probably more complicated than the analysts wish to admit. The truly troublesome structures are the ones which yield new insights.

On a one-by-one basis, “perfect” structures probably have a very limited crystallographic interest, but taken en masse they inform us about the physical world. At first sight the Cambridge Crystallographic Data Base might be seen as a grave yard for structures, but the software developed by the CDC turns data into knowledge, and the data base is now an arbiter of normality. It is well established that interatomic distances and bond lengths,

are influenced by the local environment. The program MOGUL enables an analyst to compare every bond in his current structure with those in the same environment in the data base. It provides a robust chemical yardstick by which to assess analyses, and should be made a mandatory part of the IUCr checkCIF process.

Structure Analyses - where next? Fully automatic structure analysis is just as far out of reach as it was in 1976, when Rollett thought it was just round the corner. Failure to correctly identify the type of every atom in the structure, and correctly insert or locate all hydrogen atoms means that the analysis has failed, and that the opinion of a human analyst is needed. Finishing anything but a trivial structure still requires a structure analyst to use his time and experience. The diagram below summarizes experience with the Analytical Ser-



Schematic time profiles for Simple, Routine and Difficult structures. The Poisson-like curve represents the numbers of structures brought to a publishable condition as a function of time taken for the analysis. Courtesy of Amber Thompson.

vice in Oxford. There are three bands, reading from the top. Initial evaluation of a sample requires human experience, but is relatively quick. The second band, data collection, may take from hours to days and is fairly predictable once initial diffraction images have been obtained. It is the bottom band, working up the data to a publishable conclusion, which is least predictable.

Direct methods and charge flipping are now very powerful procedures for phasing a Fourier map to the level that the atomic skeleton of the structure can be seen. However, physics alone cannot always make automatic unambiguous assignment of atomic sites. Worse than that, some molecules refuse to fit into normal space groups - they are disordered. Disorder is a bottomless

pit into which crystallographers throw time, effort and money. When disorder is eventually resolved, it is often clear that the resolution has added nothing significant to the scientific value of the structure. Was it worth the effort?

From time to time our administration asks us to provide a “Cost for a Structure Analysis”, expecting a simple answer. Of course, there is no simple answer. One way to evaluate the cost is:

$$COST = (\text{instrument cost}) / \text{write-off period} + \text{space charge} + \text{salary \& overheads} + \text{consumables}$$

The first three terms in this expression have to be paid even if the equipment is turned off so, in part, the cost of no structures is the same as the cost of some structures. The only saving which can be made by turning away a structure is that of the consumables – perhaps just \$30! Administrators don’t like this calculation, and so ask how many structures are done in a year (to try to get an average cost). Does “done” mean published, completed to a publishable standard and then left to rot on a hard disk, or completed just enough to confirm the identity, and, does it include work started but then abandoned for whatever reason? However ‘done’ is measured, a few things are possible to bring down the unit cost.

1. Put more samples on the instruments each day. This increases the burden on the analyst, and may even require additional analysts unless the data processing can be distributed over the end users, in much the same way that NMR data is.
2. Provide better automation for working up the data, and in particular for the treatment of disorder. It is a sad indictment that, in an age when

car registration plates are automatically read by computers at every garage, when OCR of old documents is routine and Immigration can automatically check passport holders against their photographs, we still have no software to automatically resolve structures. This will need a new approach to codifying chemical knowledge – it has been my experience that the best service crystallographers we have had in Oxford have also been first-class chemists.

3. Have a clear strategy to limit the amount of time spent on each structure.

Item 3 in this list is one which many analysts shy away from, yet in financially difficult times it is perhaps the most important. In the UK, research funding is not so generous that we can be wasteful of resources. Before starting an analysis it is important for the customer to declare what the analysis will be used for, for example if or how the work will be published. The

experiment and data processing can then be tailored to those aims. For example, don’t collect 10 equivalent reflections when just a few will do. Occasionally an analysis proves to be much more important than was foreseen. In general, re-measuring a few data sets is a better use of resources than collecting everything to the highest standards first time around. Joe Reibenspies, in an earlier session of the 2011 ACA meeting, declared himself unhappy with this approach, saying that while he was working on a structure it was “his”, but when he published it, it was “ours”. A seductive argument, but I believe that when I do work, it is for the Chancellor, Masters and Scholars of the University of Oxford, who may agree to share their results through publication. The old mineralogists measured interfacial angles with great care, ‘just in case’. You can be reasonably sure that this accuracy was rarely needed, and if careful measurements were needed, the material was reexamined.

The Gold Standard.

Few people regularly eat from a golden platter; we don't measure the timber for a chicken hut with a micrometer. Crystallography can still be the Gold Standard, but a gold standard is not needed for all work. The analyst simply needs to demonstrate fitness-for-purpose. If the customer changes the purpose later, that is a separate issue. The problem for journals is to understand the purpose of the work, and see if it is satisfied. The purpose cannot be evident from the information currently included in a CIF, and it is therefore unlikely that a program can make this decision. However, checkCIF may help the referee decide if the analysis is 'good enough' for the purpose described in the text. In the future, CIFs may also need to record what the analysis was 'good enough' for. If someone has a different purpose, they may need to re-measure the data.

Small Molecule Crystallography – Where Next?

For over half a century small molecule crystallography has been driven (and funded) by the chemist's interest in molecular structure. Chemistry can still be crystallographically challenging, for example the study of excited states. However, for the professional crystallographer, the molecular solid state has become interesting in its own right. We understand quite a lot about strong interatomic interactions - those which form 'bonds', but very little is known about the weaker interactions - the ones which enable molecules to form solids. Structure prediction is scarcely feasible, morphology prediction even less reliable, and we can only rarely predict the conditions needed to grow decent crystals of a novel material. If a proper amount of effort were expended in automating the final stages of analyses, we could say that structure analysis was 'Done and Dusted', and crystallographers could turn their attention away from determining molecular geometry, and towards developing an understanding of the solid state. This is a period of renaissance for crystallography, with new horizons wide open for adventurous young scientists.



David Watkin

Cartoon courtesy of Nick D. Kim. See page 10.

What Is the Future for Crystallography?



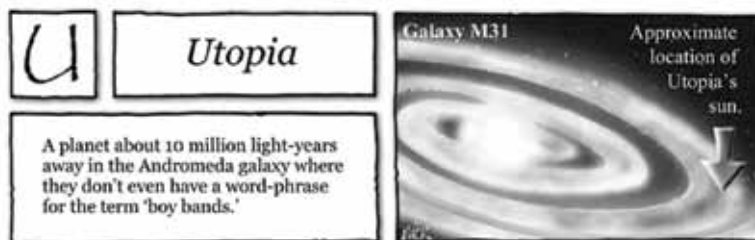
With all the hoopla surrounding the primary and national elections, are there any things we can be reasonably sure of regarding the prospects for crystallographers? I hope so and I think so. Whenever you start talking about where the US needs to make progress in education it always comes down to STEM (science, technology, engineering, math). Crystallographers certainly exercise their skills in all of these areas and have graduate students adept in one or another of these disciplines. Admittedly we no longer lead the way in usage of 3D graphics, having yielded that position long ago to the "gamers", but we continue to push useful graphical applications. We use many different display options and have tools for figure creation in applications, e.g. docking simulations based on multiple structures. Computer coding, whether it's for structure solution and refinement packages, robotic control software, or edge detection for crystallization imaging is based on fundamental mathematics. Other aspects of what we do are founded on practicing science, from biology through chemistry and physics to material science and geology. Our field relies on and enhances STEM.

While NASA may shudder at questions about the relevance of the space program in these tight fiscal times, crystallography remains the primary means of determining the atomic structure of materials all the way from small molecules to viruses and structural complexes. And the solutions of these structures are highly relevant to the real problems that we face today. From the structure of an iridium bromide complex with potential for hydrogen storage to elucidating the mechanism of plant response to stress as well as the structures with relevance to the biomedical fields, *crystallography really matters*. Our ACA SIGs range from highly applied to highly theoretical, from problem solving to problem proposing, but all share in their dependence on density from Fourier transforms of diffraction. Wouldn't the early pioneers of crystallography be amazed by how far we have come, not to mention how diverse we are?

As a university professor who teaches experimental physics, I often wonder about the new generation of students coming through my classes. They don't even know how to use an Abstract Index (I haven't seen one in awhile, now that I think about it.) They're much less likely to know constants, remember formulae, or even, in some cases, own their own textbooks. In 10 more years their bookshelves will likely be filled with Ipads, Kindles, Nooks or simply drive space in the "cloud" (for which I have little trust). The things they excel at are searching, finding, and concatenating. It surprises them that I know integration techniques other than Maple or Mathematica and sometimes get a simple answer where theirs are hopelessly complex. But nevertheless, the imagination and creativity of this generation, the perseverance when interest is captured and the curiosity for unknown things still runs strong. Our students may come from farther away but they will continue to advance the field, innovate, and produce both our software and our hardware.

So, looking forward, whether the blue states overwhelm the red or vice-versa, I'm sure there will be difficulty with funding. And there may be scarcity of resources as more is asked for and less provided. However, I am equally certain that our field will continue to advance, engage new minds, and provide a basis for solving many of the truly important, non-political problems that arise.

Ross Reynolds



Quasicrystal History

In 1984 Dan Shechtman, Ilan Blech, Denis Gratias, and John W. Cahn published *Metallic Phase with Long-Range Orientational Order and No Translational Symmetry* in *Phys. Rev. Lett.*, **53**, pp 1951-53.

In 2011 Dan Shechtman was awarded the Nobel Prize for “the discovery of quasicrystals.”

In preparation for writing the *News & Awards* section in the winter issue of *RefleXions*, I corresponded with **Marjorie Senechal**, who offered to help with the part about Dan Shechtman winning the Nobel prize. She noted that: *I had met them (Dan Shechtman and John Cahn) before, the first time in Paris (or rather Bures-sur-Yvette, just outside of Paris) in January 1985, at the Institut des Hautes Etudes Scientifiques, a mathematics and physics (and now biology too) research paradise modeled on the Institute for Advanced Study in Princeton. With my colleague, Louis Michel, a permanent member of the IHES, I had organized a month-long workshop on mathematical crystallography for January 1985. When I arrived in Paris at the beginning of the month, Louis immediately showed me the just-published paper by Shechtman, Cahn, Gratias and Blech. By our great good fortune, the first three authors happened to be in Paris just then, so we invited them to join us. We changed gears and devoted most of the workshop to the mathematical aspects of quasicrystals; and I changed research directions on the spot.*

I wrote to Marjorie because of fond memories of talking with her at ACA meetings. I bought her fine book *Patterns in Symmetry* when I saw it at Polycrystal Book Service (remember them?) She was a speaker at several ACA meetings, and may even have chaired sessions. At one point she asked me if I thought she should host an ACA meeting at Smith College, but, alas, that was not to be because about that time the Council became concerned that exhibitors needed a large space that could be locked and was handy to the sessions.

Our History Editor **Virginia Pett** has informed me that Marjorie agreed to write an autobiography for the crystallography archives later this year that we can publish in *RefleXions* (preview of coming attractions!).

From *What is . . . a Quasicrystal* by **Marjorie Senechal**, *Notices of the American Mathematical Society*, 2006, **53**, number 8.

The long answer is: no one is sure. But the short answer is straightforward: a quasicrystal is a crystal with forbidden symmetry. Forbidden, that is, by *The Crystallographic Restriction*, a theorem that confines the rotational symmetries of translation lattices in two- and three-dimensional Euclidean space to orders 2, 3, 4, and 6. This bedrock of theoretical solid-state science, i.e. the impossibility of five-fold symmetry in crystals, can be traced in the mineralogical literature back to 1801. It crumbled in 1984

when Dany Shechtman, a materials scientist working at what is now the National Institute of Standards and Technology, synthesized aluminium-manganese crystals with icosahedral symmetry. The term “quasicrystal”, hastily coined to label such theretofore unthinkable objects, suggests the confusions that Shechtman’s discovery sowed. What’s “quasi” about them? Are they sort-of-but-not-quite crystals? Solids with some sort of quasiperiodic structures? For that matter, what is a crystal? Since the discovery of x-ray diffraction in 1912, a crystal’s identifying signature has been sharp bright spots in its diffraction pattern; that’s how Shechtman knew his were special. If it looks like a duck and quacks like a duck, it’s a duck. Charged in 1992 with formulating a suitably inclusive definition, the IUCr’s newly-formed *Commission on Aperiodic Crystals* decreed a crystal to be “any solid having an essentially discrete diffraction diagram.” In the special case that “three dimensional lattice periodicity can be considered to be absent,” the crystal is “aperiodic” (www.iucr.org/iucr-top/iucr/cac.html).

I was a member of the commission when this definition was hammered out, and I argued strongly in favor of it. It wasn’t a cop-out; it was designed to stimulate research. Which atomic structures or, more abstractly, point sets, have essentially discrete diffraction diagrams? The set of vertices of a Penrose tiling does - that was known before Shechtman’s discovery. But what other objects do, and how can we tell? The question was wide open at that time, and I thought it unwise to replace one inadequate definition (the lattice) with another. That the commission still retains this definition today suggests the difficulty of the question we deliberately but implicitly posed. By now a great many kinds of aperiodic crystals have been grown in laboratories around the world; most of them are metals or alloys of two or three kinds of atoms with binary or ternary metallic phases. (For a survey of current research on real aperiodic crystals see, for example, the website of the international conference ICQ9, www.icq9.ameslab.gov/index.html/.)

Marjorie Senechal is Louise Wolff Kahn Professor Emerita in Mathematics and History of Science and Technology at Smith College. She Co-Edits *The Mathematical Intelligencer*. Her home page is: www.math.smith.edu/~senechal/.

Books she has written that are relevant to crystallography are: M. Senechal and G. Fleck, editors (and contributors), *Patterns of Symmetry*, U Massachusetts Press, Amherst, 1977, hardcover, 152 pp. ISBN: 978-0870232329. Paperback: U of Massachusetts Press, 1981. ISBN: 978-0870233456.

M. Senechal, ed., *Structure of Matter and Patterns in Science: inspired by the work and life of Dorothy Wrinch, 1894-1976: proceedings of a symposium held at Smith*. Schenkman Books Inc., 1980, paperback, 200 pp. ISBN: 978-0870739095.

M. Senechal and G. Fleck, editors (and contributors). *Shaping Space: a polyhedral approach*. Birkhauser, Boston, 1987, hardcover, 284 pp. ISBN: 978-0817633516.

M. Senechal, *Crystalline Symmetries: an informal mathematical introduction*, Taylor & Francis, 1990, hardcover, 152 pp. ISBN: 978-0750300414.

M. Senechal, *Quasicrystals and Geometry*, Cambridge University Press, 1995; paperback, 308 pp., 1996. ISBN: 978-0521575416.



From **Brian Toby**: I was intrigued by quasicrystals in the mid-1980s and when I left my industrial job to work for Takeshi Egami as a glorified postdoc, it was with the intent to do PDF studies of quasicrystals. Although high-Tc superconductors intervened, I did attend conference sessions on structural studies of quasicrystals whenever I could. Two such sessions were quite memorable. In one Takeshi presented some early PDF studies on quasicrystals, and after that session I found myself called into a huddle with Takeshi and Linus Pauling. Linus had seen a slide from Takeshi's talk with a glass/liquid structure factor, $S(Q)$, for a quasicrystalline material. Linus wanted to get the original data and I was called in to mediate the electronic format discussion and (as is a postdoc's lot) do the work and prepare the floppy disk. We presumed that Linus's goal was to show that the powder pattern could be explained by a conventional structure, which both Takeshi and I were convinced was not possible, but it was still quite a thrill for both of us to meet such a living legend. I did supply the data, but never heard any results back. Perhaps that might have helped motivate my decade of travail on pdCIF, so that now we have a standardized format for powder diffraction data.



The second session was on icosahedral approximants to quasicrystals and was most likely at an American Physical Society meeting. One talk was mistakenly placed into the session that involved theoretical spectroscopic computations on a hypothetical molecule. As I recall either the title or abstract mentioned something about icosahedral symmetry so at a quick glance it might have seemed that the topics overlapped. The speaker was apologetic in her introduction, since it was clear that in a structural analysis session not too many people would be interested in normal mode analysis, but she explained that this molecule had been predicted to exist and there was some evidence for it occurring in interstellar space. I was both impressed and embarrassed by my fellow (gender reference intentional) scientists. A few listened and made a point to ask questions of the speaker despite the large gap in fields and interests, but others carried out normal-voiced conversations where they sat in the meeting room during the talk, showing a shocking level of disrespect. I note with irony that, not too many years later, a surprising percentage of the people in that room were busy studying that same truncated icosahedral molecule, later to be named a buckyball.

Brian is one of several crystallographers who responded to my request in the winter issue of *RefleXions* for material for a historical article on 5-fold symmetry and quasicrystals. Virginia Pett and Carol Brock kindly provided many references. Carol especially remembers one session at the 1986 ACA meeting (McMaster) in which Pauling, Cahn and others spoke about the newly discovered quasicrystals. Pauling kept asking where the atoms could be located and the physicists kept asserting that his question was not especially important. It seemed that they were talking past each other.



Carolyn Brock

I (Connie), remember being fascinated by 5-fold symmetry and Penrose tiles. Another favorite book in my library is *Tilings and Patterns*, an almost 700 page tome by Branko Grünbaum (U Washington) and G.C. Shepard (U of East Anglia, UK), W.H. Freeman & Company, NY, 1987. Marjorie Senechal is referenced in the first chapter on *Basic Notions* as well as in Chapter 2 on *Tilings by Regular Polygons and Star Polygons* and Chapter 4 on *The Topology of Tilings*. She is referenced in 4 sections of Chapter 8 on *Colored Patterns and Tilings: Color Symmetries, Color Groups, Perfect Colorings of Tilings, and Notes & References*. Alan Mackay is also referenced in several chapters including his 1982 paper, (*Physica*, 114A, pp 609-613: *Crystallography and the Penrose Pattern*). In Chapter 10 on Aperiodic Tilings the authors refer to the 1984 Shechtman et al. paper *Metallic Phase with Long-Range Orientational Order and No Translational Symmetry*.

In 1985 Linus Pauling published a note in the Letters section of *Nature*, 317, pp 512-514: *Apparent icosahedral symmetry is due to directed multiple twinning of cubic crystals*. This was followed in 1986 by *Nature* Letters section responses by several people: Cahn, Gratias, & Shechtman; Mackay; Bancel, Heiney, Stephens, & Goldman, and Berezin under the heading *Pauling's model not universally accepted*.

At the conference held at Oregon State University February 26th-March 2nd, 1995: *The Life and Work of Linus Pauling (1901-1994): A Discourse on the Art of Biography*, - from the talk in Session 3 on March 1st by **David Shoemaker**: *My Memories and Impressions of Linus Pauling*:

... The last decade of our relationship with Linus Pauling was the era of quasicrystals, those strange materials which seemed to violate well-established crystallographic principles by possessing five-fold symmetry in single crystal electron diffraction patterns. Indeed, the materials seemed to possess in most cases the full symmetry of the icosahedron. One day Pauling showed up at our house in Corvallis, and as we were drinking tea on our patio he astounded us by expressing his strong disbelief in the quasicrystal hypothesis. The so-called quasicrystals, he said, were really multiple twins of a probably cubic crystal, with a twinning angle of 72 degrees, the supplement of which, 108 degrees, was close to the tetrahedral angle of 109.5 degrees. Shortly afterwards he voiced this hypothesis at an ACA meeting, and it was accepted overwhelmingly. What stimulated his thinking was a statement by Shechtman that the x-ray powder pattern obtained from this material could not be indexed by any Bravais lattice, . . . *a statement I knew to be wrong*. Most of the materials under discussion had approximate formulae $MnAl_4$ - $MnAl_6$. For the face-centered cubic structure that Pauling proposed to be twinned, he borrowed from the gas hydrate structures investigated by W.F. Claussen, and Sten Samson's structure of $NaCd_2$. He arrived at a unit cell length a_0 of 26.73 Å. The predicted powder pattern seemed to fit Shechtman's data except for a scale factor which Pauling thought was 15 percent off, but Shechtman and Leo Bendersky succeeded in persuading Pauling that the error was in his unit cell, so Pauling reluctantly reduced a_0 to 23.36 Å, corresponding to 820 atoms per unit cell.

Quasicrystal History, cont'd Meanwhile I programmed my personal computer to calculate powder diagrams for various values of the unit cell length, and to plot the deviation of observed values of the reciprocal spacing against unit cell length over a wide range of values. I was pleased to inform Dr. Pauling that I got a very close fit to his value of 26.73 Å. Soon afterwards Pauling had to change his value to 23.36 Å, and I was unable to get any support for that value from my computer. Pauling attempted to find support for his twinned hypothesis in the electron diffraction patterns, but I am obliged to say that our own examination of these patterns left us skeptical of his interpretations. More recently Clara and I have come to believe that the quasicrystals are very closely related to our tetrahedrally close-packed structures, or to a closely related family of structures containing aluminum, possessing in common with them the same kinds of coordination polyhedra, especially icosahedra. Clara determined the structure of a so-called μ phase $MnAl_4$ with a hexagonal structure and a very large unit cell. This she examined closely in various orientations in comparison with features of a postulated quasicrystal with decagonal symmetry, and found striking similarities. These results were sent to Linus Pauling, who expressed his interest in his reply. Meanwhile, new quasicrystal phases continue to be found in many systems, including some that appear to be thermodynamically stable. Work on icosahedral and decagonal phases has reached the point of actually assigning atomic positions in those phases. The reality of these phases can no longer be seriously doubted. However, the structures derived or postulated for these materials were not without the mark of Linus Pauling, especially as regards the linkage and clustering of icosahedra, in particular the 104-atom complex found in $Mg_{32}(Al, Zn)_{49}$, the structure of which was derived by Pauling by the stochastic method.

In sum, Linus Pauling is the most remarkable person I have ever known, for his intellectual brilliance and for his bold willingness to risk being wrong. His strategy of generating lots of ideas and throwing out the bad ones was overall extremely successful, and the bad ones that did get through have not significantly detracted from his genius. In addition, he had a wonderful sense of humor, and a warm regard for his students and colleagues. We will all miss him.

Recommended reading (with Amazon.com book descriptions): *Useful Quasicrystals* by Jean-Marie Dubois, World Scientific Publishing Co, Ptc. Ltd, 2005, paperback, 504 pp. ISBN: 978-9812561886.

The aim of this book is to acquaint the reader with what the author regards as the most basic characteristics of quasicrystals: structure, formation and stability, as well as the properties related to applications of quasicrystalline materials. Quasicrystals are fascinating substances that form a family of specific structures with strange physical and mechanical properties compared to those of metallic alloys. This has both stimulated research to understand them within the framework of generalized crystallography, and opened the way to technological applications, especially energy savings.

Aperiodic Crystals: From Modulated Phases to Quasicrystals (IUCr Monographs on Crystallography) by Ted Janssen, Gervais Chapuis, & Marc de Boissieu, 2007, hardcover, \$153. ISBN: 978-0198567776.

Since 1970 efforts to determine and understand the class of crystals deemed aperiodic intensified. Aperiodic crystals are long range ordered structures that lack lattice periodicity in at least one dimension. They are found in organic and inorganic compounds, minerals, and metallic alloys under various pressures and temperatures. Because the usual techniques for studying physical properties no longer worked for structures lacking periodicity, new techniques had to be developed. This book discusses structure characterization, structure determination, and physical properties of aperiodic crystals, especially their dynamical and electronic properties, and uses superspace (greater than 3 dimensions) to generalize standard crystallography and to look differently at dynamics. The three main classes of aperiodic crystals: modulated phases, incommensurate composites and quasicrystals are treated from a unified point of view which stresses similarities of the various systems.

Quasicrystals: Structure and Physical Properties, Hans-Rainer Trebin, Ed., 2003, 668 pp., hardcover, \$232. ISBN: 978-3527403998.

The authors are in a research program on quasicrystals sponsored by the German Research Society and managed by Hans-Rainer Trebin. Most of their latest results are presented, including interesting new solid state structures.

Quasicrystals: An Introduction to Structure, Physical Properties and Applications (Springer Series in Materials Science), J.-B. Suck, M. Schreiber, & P. Häussler, Eds., 2010, 579 pp, paperback, \$158. ISBN: 978-3642083907.

This book provides an introduction to all aspects of the physics of quasicrystals. The chapters, each written by an expert in the field, cover quasiperiodic tilings and modeling of the atomic structure of quasicrystals. The electronic density of states, the calculation of electronic structure, and atomic dynamics play key roles. Important applications of aperiodic crystals include the study of defects in quasicrystals by high resolution electron microscopy and computer simulations of defects in decorated tilings.

Crystallography of Quasicrystals: Concepts, Methods and Structures by Walter Steurer and Sofia Deloudi, Springer Series in Materials Sciences, 2009, 398 pp., hardcover, \$140. ISBN: 978-3642018985.

From tilings to quasicrystal structures and from surfaces to the n-dimensional approach, this book gives a full, self contained, in depth description of the crystallography of quasicrystals. It not only conveys concepts and provides precise pictures of the structures of quasicrystals, but also enables the interested reader to enter the field of quasicrystal structure analysis. Going beyond metallic quasicrystals, it describes the new, dynamically growing field of photonic quasicrystals.

Readers who wish to know more about the history of Dan Shechtman's Nobel Prize winning discovery should see I. Hargittai's 2011 essay in *Isr. J. Chem.*, **51**, 1144-1152.

Connie Rajnak



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Puzzle Corner: On the page opposite, write the appropriate answer in the numbered spaces below each clue. Then copy the letter from the same-numbered box above the clues into the grid above. This will spell out a quote. Words in the grid are separated by black spaces. The first letters of each answer, read in order, will spell the name of the author of the quote.

This puzzle submitted by **Charlene Lawrence**.

Answers to the puzzles in the winter ACA RefleXions:

DISORDERED word puzzle: ALANINE FOLDING MYOGLOBIN SUBSTRATE SHEETS

What the vampire saw in the glide plane: ONLY THE TRANSLATION

What poem ends with the Law of Constancy of Interfacial Angles (Steno's Law)?

John Updike's *Ode to Crystallization* begins:

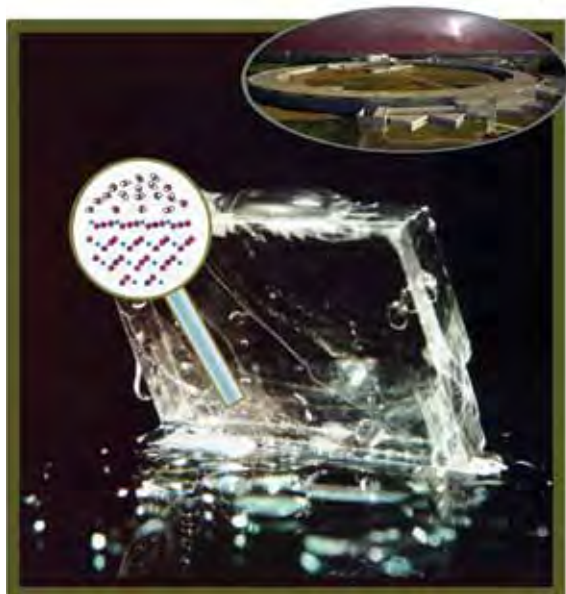
*The atom is a crystal
of a sort; the lattices
its interlockings form
lend a planarity most pleasing...*

and ends:

*Steno's Law, crystallography's first:
the form of crystal admits no angle but its own.*

Published in the *New Yorker* magazine Jan. 21, 1985.

The full poem can be found at: <http://cims.nyu.edu/~almgren/fun/crystal.html>



The ACA 2012 **Warren Award** will be given to **Paul Fenter** at the ACA meeting in Boston for understanding the structure of interfaces, particularly those involving liquids or soft matter. His relentless and creative pursuit of the mechanisms underlying otherwise routine scattering methods has led to substantial breakthroughs. By making use of the concept that robust knowledge of the scattering phase effectively transforms scattering techniques into imaging tools, Paul was able to image interfaces with x-rays. Paul and coworkers used for the first time an interfacial microscopy technique that they developed, as well as various x-ray scattering techniques that had been developed to implement phase sensitive imaging capability.

Images from Paul Fenter, Chemical Sciences and Engineering Division, Argonne National Laboratory. An overview of the Advanced Photon Source is at top right¹. The calcite crystal (~2 inches across) has water droplets that illustrate the calcite-water interface.² Inside the magnifying glass is a schematic of the molecular-scale structure of the calcite-water interface.³ These images illustrate the ability to image molecular-scale structures at solid-liquid interfaces through the use of a range of phase-sensitive x-ray scattering techniques. Approaches included imaging interfacial density

profiles at interfaces by recovering the phase from x-ray reflectivity data⁴, using resonant reflectivity to image element-specific profiles at interfaces,⁵ and using phase contrast with x-ray reflection microscopy⁶ as x-ray lenses to image elementary (sub-nm high) topography at interfaces. These approaches have opened up new avenues for understanding processes at complex solid-liquid interfaces ranging from low-temperature geochemistry to lithium ion batteries.

1. Photo from the APS photo gallery www.flickr.com/photos/advanced-photonsource/. © APS.

2. Photo made by the photography staff at Argonne.

3. P. Fenter, P. Geissbühler, E. DiMasi, G. Srajer, L. B. Sorensen, & N. C. Sturchio, "Surface Speciation of Calcite Observed In Situ by High Resolution X-ray Reflectivity", 2000, *Geochimica et Cosmochimica Acta* **64**, 1221-1228.

4. P. Fenter & Z. Zhang, "Model-Independent One-Dimensional Imaging of Interfacial Structures at < 1 Å resolution", 2005, *Phys. Rev. B, Rapid Communications*, **72** 081401(R,1-4); also in *Virtual Journal of Nanoscience and Technology*, 2005, **12**(7).

5. C. Park & P. A. Fenter, "Phasing of Resonant Anomalous X-ray Reflectivity Spectra and Direct Fourier Synthesis of Element-Specific Partial Structures at Buried Interfaces", 2007, *J. Applied Crystallography*, **40**, 290-301.

6. P. Fenter, C. Park, Z. Zhang & Y. Wang "Observation of Sub-nanometre-high Surface Topography with X-ray Reflection Phase-Contrast Microscopy", 2006, *Nature Physics*, **2**(10) 700-704, and P. Fenter, C. Park, V. Kohli & Z. Zhang, "Image Contrast in X-ray Reflection Interface Microscopy: Comparison of Data with Model Calculations and Simulations", 2008, *Journal of Synchrotron Radiation*, **15**, 558-571.

1	T	B		3	E	4	I		5	G	6	E	7	L	8	T		9	M	10	U		11	R	12	N	13	G	14	J		15	B	16	O	17	K	18	C		19	B	20	P	21	F			
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43	F	44	J	45	C		46	I	47	T	48	C		49	O	50	G	51	L	52	C	53	B	54	U	55	H		56	H	57	O	58	U		59	S	60	A	61	M	62	T	63	J	64	F	65	G
66	F	67	K	68	D		69	T		70	F	71	T	72	O	73	B	74	S	75	N	76	U		77	P	78	B	79	G	80	J		81	D	82	Q		83	M	84	N		85	D	86	Q		
87	S	88	O	89	H	90	N		91	Q	92	K		93	R	94	A		95	J		96	K	97	G	98	J	99	A	100	U	101	P	102	O	103	B		104	N	105	Q	106	G		107	F		
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129	O	130	S	131	R	132	M	133	F	134	A		135	S	136	Q		137	T		138	M	139	Q	140	K	141	O	142	B	143	N	144	U		145	I	146	F	147	E	148	P	149	O	150	J		
151	T	152	J		153	Q	154	F	155	G	156	C	157	N	158	F	159	P	160	E		161	C	162	E	163	U	164	M	165	F	166	G		167	A	168	O	169	N	170	Q		171	F	172	E		
173	P	174	M	175	S	176	E		177	M	178	R	179	A	180	S	181	D		182	F		183	B	184	A	185	U	186	T	187	P	188	Q		189	N	190	P	191	K	192	M	193	I	194	A		
195	A	196	R		197	U	198	A	199	B	200	B		201	B	202	H	203	T	204	J	205	Q	206	L	207	N	208	P	209	C	210	G		211	R	212	R	213	H	214	F	215	I	216	E	217	P	

- A. Turns light just right? 25 198 60 120 194 195 128 94 179 184 167 117 99 134
- B. Fish people 73 201 103 142 78 116 2 183 19 53 29 199 15 200
- C. How Pauling often solved problems; he _____ 27 123 118 156 45 126 18 52 161 209 48
- D. Kind of vacuum 125 81 181 85 68 E. Threatened soap use 147 172 6 216 112 3 162 160 176
- F. Curing phthisis 43 66 171 64 107 146 70 165 21 158 214 133 182 154
- G. Smashed Iceland spar fragments 13 50 40 5 106 155 97 65 210 166 79
- H. Theophrastus wrote on them: 36 55 202 56 89 213 I. State capital in Lewis & Clark county: 108 4 215 193 145 46
- J. Passages at the end of a book: 95 152 80 14 44 122 98 150 63 204
- K. AB - BA if A, B are operators; slip ring wired to act as rotary switch: 67 121 140 191 37 96 17 28 92 124
- L. The molecule _____ a conformation ... Acta Cryst B29, 1611: 109 206 51 22 115 7
- M. What scholarship isn't in JACS: 61 174 9 138 83 114 164 177 192 132 33
- N. Restores to youthfulness: 90 157 104 12 75 143 189 169 31 207 84
- O. A good place to reach 72 (two words): 149 141 102 168 88 129 119 110 49 32 16 57 72 35
- P. Set of atoms in a unit cell with simpler pattern than the whole: 30 190 148 217 77 208 20 42 159 101 173 187
- Q. The filling in of intermediate values: 139 170 91 86 188 153 24 38 127 82 205 105 136
- R. Those unlikely to succeed at clue 'O': 93 131 178 196 212 211 11
- S. Fete use of crawfish or shrimp dishes served over rice: 59 87 135 26 41 130 74 180 175
- T. Air broken? This will fix most of it naturally: 47 69 8 34 151 186 71 203 137 1 62
- U. [Type of] forms occur[ing] when we have a union of one-fourth of all the similar possible planes ... of any crystallographic system (Marshman Edward Wadsworth): 163 10 58 113 23 39 100 54 76 144 185 111 197

***The Hidden Reality: Parallel Universes and the Deep Laws of the Cosmos*, by Brian Greene, 2011, ISBN-13: 978-0307265630**

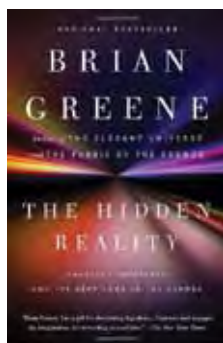
My wife has been asking me to explain string theory. I had been putting it off until I caught her watching a rerun of *The Big Bang Theory* in which the character Sheldon Cooper heckles the real Brian Greene at a sitcom-style book reading for *The Hidden Reality*. I had listened to an interview with the author on *Science Friday* a few months back and I already had the book. Now I figured I'd better read it.

Greene sets the tone with a simple introduction that allows readers to skip ahead at various points. However, unless you really know this stuff, don't - the overview is worthwhile. Greene spends the rest of the book describing in detail the current models for nine possible multiverse theories and the philosophies that might come with them. The first of these multiverses is the **Quilted Universe** - a multiverse comprised of approximately 10^{500} universes in parallel with ours. In this multiverse, some versions of me are typing this book review and some aren't.

The second multiverse is the **Inflationary Multiverse**. I came to this section just a few days after the announcement of this year's Nobel Prize in physics to Perlmutter, Schmidt and Reiss for finding experimental evidence of inflation. In this multiverse, inflation causes the popping up of new universes, outside our field of view. In Chapter 4, the author gives us a lesson in string theory. String theory is an attempt to unify all four forces of nature by invoking six extra dimensions that are so small we can't see them. This allows for a description of gravity without the singularities associated with a conventional quantum description. This sets the stage for a description of the **Brane** and **Cyclic Universes** in Chapter 5.

In Chapter 6 we learn that Einstein's biggest flop, the cosmological constant, may not have been such bad idea after all since it seems to explain dark energy. This leads the author to the **Landscape Universe**. Chapter 7 looks at the philosophy of the multiverse and explores the question: *If we can't observe them, are they there?* Chapter 8 tells the story of the thesis of Princeton graduate student Hugh Everett III. Everett asked the questions: *What is a measurement?*, and *What is the outcome of a measurement?* The answer is that at the quantum level, the act of measurement creates a new observer, and thus a new universe. This seems to be a reformulation of the idea that observing an event changes its past. You can imagine that a new universe is generated with each observation.

Chapter 9 looks at the holographic projection of the string theory universe onto a four dimensional universe producing quantum mechanics and general relativity. This one seemed to me to be most comprehensible. Chapter 10 explores the possibilities of a simulated universe (think: *The Matrix*) and the resources required to create it. It also questions the nature of sentience and from whence it derives. The **Ultimate Multiverse** is also described in this chapter - it consists of all universes that can be described by mathematics only. Looking back, it is clear that the **Quantum Multiverse** and the **Quilted Multiverse** are probably manifestations of similar objects. The same might be true of the **Brane**, **Cyclic** and **Holographic** multiverses. In fact the **Ultimate Multiverse** might describe all of them. In the final chapter, the author addresses these questions: *Which multiverse is the right one?* and *How would we know?* The answers are not known, of course. This is the beauty of science: we can ask questions and search for answers in the data we collect. Like all books of this nature, I come away feeling like a very small and insignificant part of the cosmos.



***The Better Angels of Our Nature*, by Steven Pinker, 2011, ISBN: 978-0670022953**

Pinker is a professor of psychology at Harvard University. He is the author of several books including *The Blank Slate* and *The Stuff of Thought*. I started reading this right after I heard an interview with Pinker on *Science Friday*. Since then it



has been discussed in *Nature*, *The New York Times*, and *Scientific American*. Like his other books, *The Better Angels of Our Nature* is long but well written and very well referenced.

Pinker proposes the hypothesis that we are living in a time when we are less likely to die at the hands of another human than at any other time in history. He spends several hundred pages providing copious evidence to support why he thinks this is true. When you consider that certain warring tribes have kill rates as high as 25%, this is an astounding turn of events. You are thirty times less likely to die a violent death in Europe than 500 years ago. You can cheat and read the *Nature* summary by Pinker but you will miss all the data that help support his hypothesis.

Pinker suggests that there are five changes in human culture responsible: **the formation of states, gentle commerce, feminization, humanization and reason**. Considering **the formation of states**, *The Leviathan* from Hobbes' book of the same name, is important because the state gains a monopoly on violence. This can be detrimental, as in the case of a totalitarian regime, but beneficial in a democracy. The state has the ability to make the punishment for the crime harsher than the crime itself. The return on the crime is diluted and, therefore, no longer as appealing.

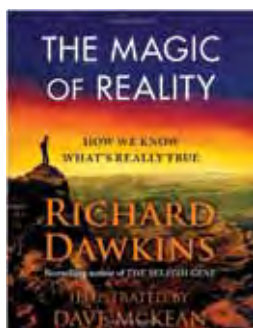
Pinker believes **gentle commerce** is important because it is more costly to take that which does not belong to you than it is to trade equitably for it. In other words, you are more likely to die in the process of taking something than while trading for it. If you have something to live for, let's say a family, it makes sense to trade rather than take. The next notable change is the **feminization** of society. This is important because women are less prone to engaging in violent behavior. Pinker lists a number of reasons for this related to the large investment women have to make in ensuring their genes are passed down. Also important is the fact that since women have gained control of their reproductive faculties they can contribute to society at much higher levels - reducing violence. The author suggests that the development

of **humanization** is important but could not have happened until the printing press became available. The ready availability of books allowed the people who had time, usually those in the upper class, to begin to think about what life was like for others. This empathy allowed for changes in attitude about oneself and others. Also included in humanization are self-control and morality. Although, like *The Leviathan*, morality can be misused, resulting in more violence rather than less.

Finally, Pinker suggests we are getting smarter as a race. He uses the **Flynn effect** as an example; that is, that IQ tests have had to be renormalized in order to maintain a mean of 100. We are learning to reason better and faster, and this reduces violence. Pinker is optimistic that violence will continue to decrease. I am not so optimistic because in order for violence to keep reducing we, as a species, would need to keep improving our ability to reason, and the forces of fundamentalism and conservatism clearly work against us.

The Magic of Reality: How We Know What's Real
by **Richard Dawkins**, 2011, ISBN: 978-1439192818

In keeping with the theme of reality in the *The Hidden Reality* review, I decided to read Dawkins' latest, *The Magic of Reality*. This is the kind of book you might give a neighbor who is not a scientist, though perhaps not in Texas. The text is easy to read and there are many illustrations to provide historical and scientific context. Dawkins avoids the militant atheism he has advocated in the past and takes a less provocative approach to debunking myths.



He starts off by defining reality as that which is around us, regardless of whether or not we can observe it. Next he discusses how we describe that which is around us through the process of defining a model of a phenomenon and then using it to reliably predict future phenomena. He goes on to define three types of magic: supernatural, stage and poetic magic. This book attempts to convert what might appear to be supernatural into poetic magic.

In a pattern followed throughout the book, Dawkins begins with various myths associated with a topic, reviews the information that has been observed, and concludes that the scientific answer does a better job of explaining the myths. He starts with what is arguably his favorite topic: evolution. Here he provides a very elegant argument *for* evolution: while there are many inconsistent stories associated with the variety of species on the planet, the fossil record spanning hundreds of millions of years provides for a completely consistent explanation and so debunks the myths.

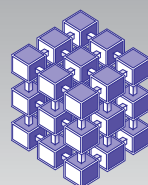
Other topics covered include the nature of matter; molecular biology; night, day and the seasons; the sun and rainbows; the origin of the universe; the possibilities for extraterrestrial life; earthquakes; good and bad; and miracles. Dawkins concludes that to understand the world in which we live is magical, in the poetic sense.

Joseph D. Ferrara.

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Knocking on Heaven's Door, by Lisa Randall,



2011, ISBN: 978-0061723728

Lisa Randall provides an illuminating and enthusiastic argument in defense of the importance of scientific exploration and discovery in the modern world in her new book, *Knocking on Heaven's Door*. She emphasizes the importance of scaling and methodology in particle and modern physics as she explains the history of the Large Hadron Collider (LHC) at CERN in Switzerland; she details her predictions

for potential discoveries at the LHC, and also manages to debunk a number of myths currently circulating in the non-academic community concerning science and its effects on modern society. Randall begins by discussing the significance of scaling in particle physics. The principles and "laws" of modern physics do not necessarily apply at the quantum level. Developing and maintaining a comprehensive understanding of the universe and its structural composition requires an acceptance of the dynamic nature of scientific discovery. Since many phenomena may not be or are difficult to observe directly, models are frequently used to postulate and test hypotheses about the machinations of the said phenomena. This is not only true for the microsphere of particle physics, but also for the macrosphere of astrophysics. The examination and interpretation of phenomena that are, quite literally, out of this world, requires a broadened perspective on the applicability of classical laws and theories.

The LHC is the pinnacle of modern experimentation and exploration in the world of particle physics; it is the world's largest and highest-energy particle accelerator. An international scientific community dedicated to solving the mysteries of the quantum world and filling in the current gaps in the Standard Model of particle physics has high hopes for this accelerator. Located near the Alps outside of Geneva, Switzerland, the LHC is an incredible feat of engineering, architecture and science. The inaugural run was conducted on September 10, 2008, with great success and tremendous publicity. An unfortunate setback occurred a little over a week later, and repairs took more than a year, but the system is back on line and has delivered some incredible results in the past two years. Randall expresses her enthusiastic hopes that over the next few years, further research and experimentation will result in advances concerning the postulated Higgs boson, a somewhat elusive particle in quantum physics. She also debunks a number of myths and fears voiced by the public about the project, including the apprehension that should something disastrous occur at the LHC, a black hole would be formed that would envelop Earth and all of its inhabitants.

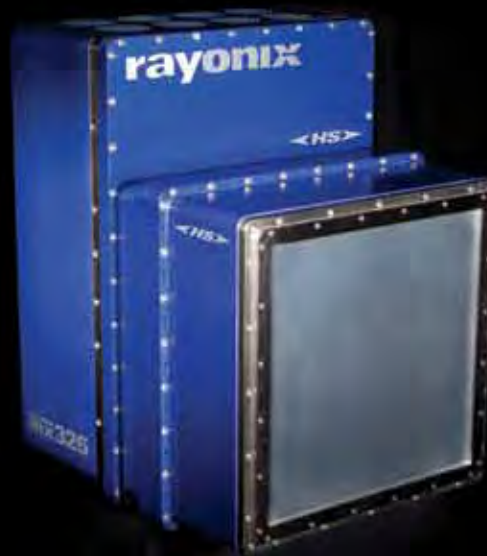
Randall's newest work is a fast-paced and enjoyable read. As someone with a very limited understanding of the complex arena of quantum mechanics, I was able to comprehend a sizable portion of the science and the history was fascinating and addressed in a manner that was neither dry nor drawn-out. I highly recommend this book to anyone who wants to brush up on current developments in the world of particle physics or be reassured that scientific discovery is still important in the modern world.

Jeanette S. Ferrara, Princeton, Class of 2015

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Notes of a Protein Crystallographer: Crystallographer's tour of La Alhambra

There was a unique event after the 26th IUCr Congress that made the exhausting meeting days well worthwhile. The Commission of Crystallography, Art and Cultural Heritage (CrysAC) organized a tour of the Palace of the Alhambra in the southern city of Granada. This promised to be no ordinary visit to this shrine of Islamic Art. From the flier for the workshop: *The palace complex of the Alhambra in Granada (Andalusia) holds a comprehensive collection of Hispano-Islamic ornamental art at its peak development and offers examples that span a wide range from plane groups of symmetry to quasilattices. The 2 1/2-day excursion from Madrid will present and analyze ornamental patterns based on simple plane groups and dichroic plane groups, give an analysis of the Islamic approach to polychromatic patterns, the use of layer groups and 1-D groups, the conscious combination of different symmetry principles in one pattern and, finally, two-dimensional decagonal and octagonal quasicrystalline patterns. An afternoon session with presentations and discussion will precede the in situ study of the ornamental art the following day.*

The organizers and tour guides of this event were two specialists in Hispano-Islamic ornamental art: Purificación Fenoll Hach-Alí (Dept. Mineralogy and Petrology, Universidad de Granada, Inst. Andaluz of Earth Sci.) and Emil Makovicky (Dept. of Mineralogy, Geological Inst., U Copenhagen). Together they have published more than twenty papers on the mathematical analysis of some of the most beautiful and intriguing decorative patterns in the treasure trove of symmetrical patterns at the Alhambra.^{1,2} Emil Makovicky has also investigated very extensively the quasiperiodic decagonal¹ and dodecagonal tiling patterns in Islamic architecture.³ Incidentally, Fenoll Hach-Alí was the person who first introduced me to Bragg's Law in a graduate course in crystallography in Salamanca, Spain. I had not seen her since the early 1970s. My motivation to participate in this excursion was irresistible both personally and professionally.

Emil Makovicky and the 14 participants were transported in a comfortable minibus from Madrid to Granada. During the five hour journey we passed the spectacular quartzite rock formations of the pass of 'Despeñaperros' which marks the boundary of the southern limit of the castilian plateau and is the gateway to Andalusia. The Sierra Morena mountain range extends for 500 km, and this narrow pass is at the eastern end of the range. This part of Spain has been the theater for many historical battles, among them Navas de Tolosa (1212) against the Arab invaders, and Bailén (1808) against the Napoleonic troops that occupied Spain. When the mountains gave way to the open plateau we saw the extensive and beautiful olive groves so characteristic of the landscape of this part of Spain.

Although small, our minibus was too big to crawl along the narrow streets of the historical section of Granada and we had to abandon our bus in the center of town and catch a smaller one in order to get to the Carmen de la Victoria, where we were staying. The 'Carmen' is an amazing place, right across from the palace of the Alhambra in the part of Granada called 'El Albaicín'. The view from the windows was breathtaking both day and night. Our secluded and superb accommodations were courtesy of U Granada and Fenoll Hach-Alí.

View of the Alhambra from the window of one of the rooms at the Carmen de la Victoria.



But we had also come to Granada to work. Emil gave an excellent introduction to plane group symmetry, layer group symmetry, color groups and polychromatic patterns as well as quasiperiodic patterns. All of this was condensed in a concise and beautifully illustrated booklet edited by him, entitled *Crystallographer's Alhambra*, a remarkable and unique compendium of crystallographic and symmetrical patterns in the Alhambra. I will treasure my copy. Dinner at the Carmen was a collegial and friendly event where we had the opportunity to learn more about the interests of the other participants in the tour: there were young artists, established university professors, mineralogists and materials scientists. Several of the participants had used diffraction and spectroscopy to authenticate works of art or archeological artifacts.

The climax of our excursion was the visit to the Alhambra palace with our distinguished experts in the decorative patterns of Islamic Art and other experienced guides. We walked along the different gates, halls, rooms, and courtyards of the palace as Emil and the other guides described the historical aspects of the palace. Hundreds of photographs were taken by workshop participants. I will describe the different parts of the Alhambra and the main architectural and decorative landmarks in an attempt to entice you to visit whenever you have the chance.

The Alhambra or Alcazaba (an Arab word) refers to a set of buildings consisting of an old fortress and the palaces that extend away from it. Several palaces were built in Roman times, but the incomplete renaissance style palace across from the Alcazaba was started ~1562 by the Christian king, Charles V. (In 1492 the Alhambra had fallen to the Spanish Catholic monarchs Isabella of Castile and Ferdinand of Aragon, leaving the recently unified Spanish kingdom in a position to send the Columbus expedition to the West.)

We entered through the ~1348 Gate of Justice and continued on into the Court of the Mexuar itself. Around the Court of Myrtles (Patio de los Arrayanes) we visited the Palace of Comares, Sala de la Barca and the Hall of Ambassadors (Salon de Comares). We stopped

often to hear about a special ornamental or decorative element of which the corresponding symmetry was explained in detail by our guides. The mathematical features described by Emil were augmented by historical anecdotes or insights by the other guides.

One of the gems of the Alhambra is the Court of Lions with the Hall of Mocarabes and Hall of the Two Sisters around it. Unfortunately, the beautiful fountain of the lions was under extensive restoration and was not open for visitors, but we did visit some of the surrounding galleries (see below). Along the way we saw the Gardens of Generalife and the Torre de las Infantas (Tower of the Infantas).



The group of participants mesmerized by Emil Makovicky's explanation of the symmetrical patterns in one of the galleries around the Courtyard of the Lions. Photo courtesy of P. Fenoll Hach-Alí.

On the other hand, some of their creations also represent pinnacles of applied geometry, several centuries ahead of the modern geometric and physical concepts of quasiperiodicity as we know them today.

All in all, the excursion was an unforgettable visit and an exhilarating experience. This note of appreciation is intended to recognize the efforts of the organizers and to offer sincere thanks for their friendliness and camaraderie during the visit. I do hope that this brief note entices other crystallographers to visit the Alhambra in the company of the reading materials prepared by our hosts P. Fenoll Hach-Alí and Emil Makovicky. If possible, try to stay at the Carmen de la Victoria. As it was written on a majolica tile by the famous Spanish writer M. Vazquez Montalbán: *it just seems as if these were created one for the contemplation of the other.*

1. P. Fenoll Hach-Alí, and A. López Galindo: *Simetría en la Alhambra, Ciencia, Belleza e Intuición, (Symmetry in the Alhambra, Science, Beauty and Intuition)*, 2003, Universidad de Granada, Consejo Superior de Investigaciones Científicas.

2. E. Makovicky: *Crystallographer's Alhambra. Beauty of symmetry – symmetry of beauty*, 2011, Special booklet published by University of Copenhagen and University of Granada, Dept of Mineralogy and Petrology for the participants in the visit. ISBN:978-84-931819-8-7.

3. E. Makovicky & N. Makovicky: *The first find of dodecagonal quasiperiodic tiling in historical Islamic architecture*, 2011, *J. Appl. Cryst.* **44**, 569-573.



Previous studies of the crystallographic patterns of the Alhambra^{1,2} have described how all 17 plane space groups are represented in the decorations of the different palaces, gates or residences of the Alhambra; one of the major achievements of the artisans. However, the workshop at the Carmen de la Victoria and the detailed tour by Emil Makovicky made clear that the complexity of symmetrical patterns goes far beyond that simple observation. A rigorous description of the ornamental patterns in the Alhambra has to include also: i) layer patterns and layer groups of symmetry; ii) dichroic and polychromatic symmetry groups (see above); iii) geometric theory of octagonal and decagonal quasilattices and quasiperiodic patterns; and iv) even twinning patterns. A separate study would be required to describe and annotate properly within the context of crystallographic symmetry the structure of ceilings, domes (for instance in the Salón de Comares) and muqarnas (large stalactite vaults) as well as the plaster/stucco ornaments. The following quote is from Emil Makovicky's booklet, page 49: *Islamic art was created to admire and analyze or, alternatively, to analyze and admire. [...]. On the one hand, the workshops of the Alhambra and Nasrid Granada created some of the most beautiful examples of mosaic and ornamental art of the World of Islam, constructed in agreement with classical plane, dichroic and layer groups.*

Cele Abad-Zapatero

Logo by P. Mueller & C. Landolt



Boston 2012
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

ACA 2012 Jul. 28 - Aug. 1
Westin Boston Waterfront Hotel

Abstract Deadline: March 31, 2012

Student & Young Scientist Travel Grant Applications: March 31, 2012

Advance Registration Deadline: May 31, 2012

Hotel Registration for Conference Rates: July 5, 2012

Meeting website: <http://www.amerCrystalAssn.org/2012-meeting-homepage>

Exhibits website: <http://www.amerCrystalAssn.org/2012-exhibits>

Submit abstracts, register, make reservations at www.AmerCrystalAssn.org



Downtown Boston seen from the Cambridge side of the Charles River.

Program Chairs



Bruce Foxman
foxman1@brandeis.edu



Bruce Noll
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Peter Mueller
pmueller@mit.edu

Local Chair

The 2012 Meeting will have a new 4-day, 5 concurrent session pattern. The meeting will start with workshops on Saturday, July 28, and scientific sessions on Sunday, July 29. The meeting will end on Wednesday, August 1 after the Awards Banquet. Join us for the opening and closing plenary lectures by Eric Mazur and Don Caspar.



Downtown Boston



Zakim Bridge



Downtown Boston

Workshops

Refmac / Coot
Organizers: P. Emsley, G. Murshudov

OLEX2
Organizer: I. Guzei

Refinement of Nanoparticle Structures
Organizers: T. Proffen, K. Page, R. Neder

Crystallography: World of Wonders
Organizers: C. Lind, C. Rawn

Note: this is an outreach workshop for K-12 teachers, not for ACA members.

Transactions Symposium

Transformations and Structural Oddities in Molecular Crystals. In Honor of Bruce Foxman
Organizers: K. Wheeler, M. Hickey, G. D. de Delgado

Awards Symposia

Buerger Award to **John Spence**
Warren Award to **Paul Fenter**
Margaret Etter Early Career Award* to **Emmanuel Skordalakes**
Supper Award to **Ron Hamlin**
Wood Award to **Daniel Norcera**

* Young scientists are encouraged to submit abstracts for the Etter symposium to Eric Montemayor (montemayor.eric@gmail.com).

Plenary Lectures

Saturday: Eric Mazur, Confessions of a Converted Lecturer
Wednesday: Donald Caspar, The History of Structural Biology

Vendor Exhibition 2012

An exhibition of the latest instruments and techniques for sample isolation, purification and preparation, crystal growth and data collection, computer software for data storage, retrieval, analysis, graphics systems, databases, and books, journals and other materials essential to modern crystallography is scheduled to begin on the evening of Saturday, July 28 in conjunction with the Opening Reception. The exhibition will run through the evening of Tuesday July 31.

Discounts for first-time and not-for-profit exhibitors apply. For further information see:

<http://www.amerocrystalassn.org/2012-exhibits>



New England Aquarium



Boston's North End "Little Italy"

Poster Chair

Session Photos Chief



Ilia Guzei
iguzei@chem.wisc.edu



Jeff Deschamps
deschamps@nrl.navy.mil

All photographs © P. Mueller

Staying Green: The full set of abstracts will be distributed only on CDs with a hard-copy Program Schedule. We will provide note pad portfolios but no meeting bags. If you would like a bag, you should bring one from an earlier meeting.



USS Constitution, Boston Harbor

Financial support for young scientists will be available through the ACA and the IUCr. Applications for this support should be made by the abstract deadline on the meeting web site. The Organizing Committee will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Union.

Student Accommodations: The ACA has secured a limited number of rooms for students and postdoctoral associates at a reduced rate at the Westin Boston Waterfront Hotel. Online reservations are available through the meeting web site. Room sharing can make the student room rates even more reasonable - use the **Room Sharing** feature under accommodations on the meeting web site.



Stata Center on MIT Campus



DURGIN-PARK MARKET DINING ROOMS

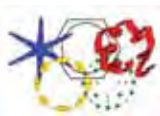
Panoramic view of Downtown Boston

APRIL 2012

2-3 **5th Proteins Congress**, Radisson Blu Portman Hotel, London, UK. www.proteins-congress.com.



16-19 **British Crystallographic Association Spring Meeting**, Warwick University, UK. Chair: **Kirsten E. Christensen**, kirsten.christensen@chem.ox.ac.uk.



MAY 2012

23-25 **9th Canadian Powder Diffraction Workshop**, Dept. Geological Sciences, U. Saskatchewan, Saskatchewan, Canada, www.cins.ca/cpdw/.



JULY 2012

28-2 **ACA2012**, Westin Boston Waterfront Hotel, Boston, MA. See pp 38-39. www.amerocrystalassn.org.



AUGUST 2012

5-8 **26th Annual Symposium of the Protein Society**, San Diego, CA, www.ProteinSociety.org.



7-11 **ECM27 27th European Crystallography Meeting**, Bergen, Norway. ecm27.ecanews.org/.



SEPTEMBER 2012

9-13 **EMC 2012, European Mineralogical Conference**, Johann Wolfgang Goethe-University, Frankfurt, Germany.



NOVEMBER 2012

18-23 **15th International Small-Angle Scattering Conference**, Sydney Convention & Exhibition Centre. www.sas2012.com. Contact: **ICMS Australasia** info@sas2012.com.



DECEMBER 2012

2-5 **AsCA'12**, joint meeting with SCANZ, Adelaide Convention Centre, Adelaide, Australia. Contact: crystal2012@sapmea.asn.au.



6 **The Bragg Symposium**, Elder Hall, University of Adelaide.

JULY 2013

20-24 **ACA 2013 will be back in Hawaii at the Sheraton Waikiki.**

AUGUST 2014

5-12 **XXIII Congress and General Assembly of the IUCr**, Montreal, Quebec, Canada. www.iucr2014.org/.



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