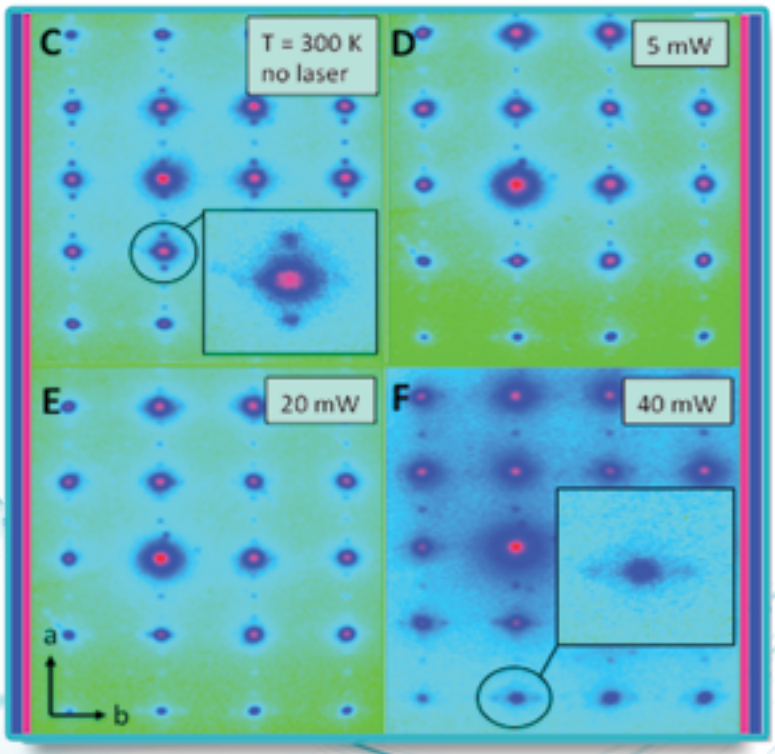
ACA RefleXions

ACA
Structure Matters
Number 4
Winter, 2013

Structural Dynamics



Structural Dynamics
Issue 1, January, 2014

Electron Diffraction Pattern
from a Laser-excited Manganite

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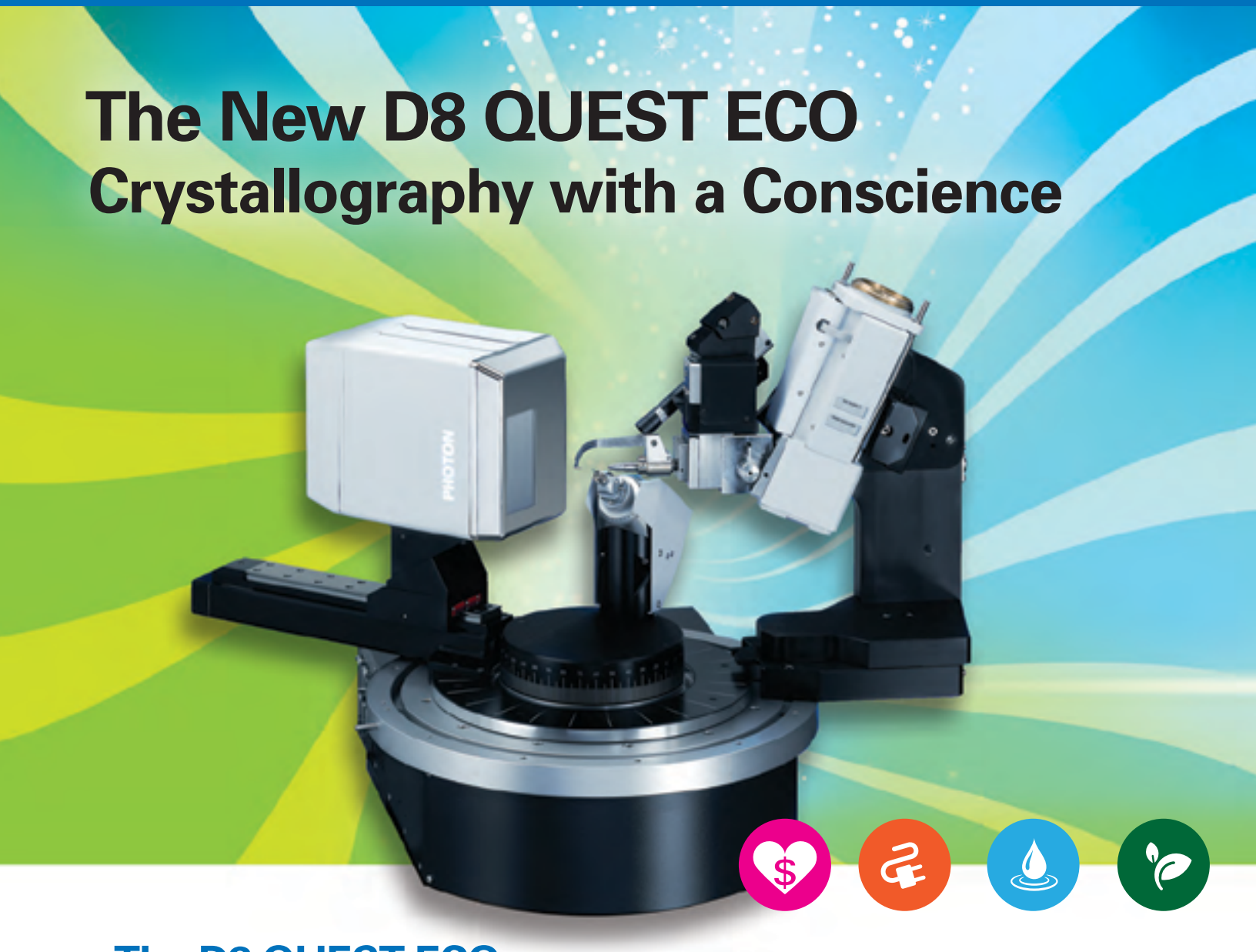
Crystallography with a Conscience



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What's on the Cover
Page 43

Table of Contents

Election Results

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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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President's Column

This is my last President's column, and as I reflect back on the last year I think that we have accomplished a good bit. Highlights include forming the partnership for the new ACA/AIP journal, *Structural Dynamics*, and beginning a strategic planning process for the ACA. By the time you read this column, the journal website will have been open for a few months and the first published articles will have been posted.

As you scan the Table of Contents for this issue you will notice a change in the staffing of *RefleXions*. Starting with the spring issue in 2014 Tom Koetzle will be taking over from Connie Rajnak as co-editor and Connie will become the cover editor. Connie was sole editor of the then ACA *Newsletter* from the second half of 1990, following Jenny Glusker, through the end of 1992. She talked Judy Flippen-Anderson into joining her in 1993 and the two of them co-opted Ron Stenkamp to replace Connie when she needed a break. Ron shared the co-editor respsonsibilties with Judy until Connie returned in the spring of 2002 after completing her term on Council. The ACA has been, and continues to be extremely fortunate to have a cadre of long-standing loyal volunteers and Connie stands out as one of the best. I know I speak for the entire membership in extending my appreication for all she has done to help *RefleXions* evolve into the magazine it is today.

As part of the strategic planning process, the committee has identified the reevaluation of the Mission Statement and development of an ACA tagline as a priority. The following statement was taken directly from the original ACA Articles of Incorporation written in 1947. *The mission of the American Crystallographic Association is to promote the study of the arrangement of the atoms in matter, its causes, its nature and its consequences, and of the tools and methods used in such studies*.The Strategic Planning Committee (SPC) believes that this statement is just as relevant today as it was then. It reaffirms the original roots of the organization yet allows for the breadth that has evolved in technique and application. We also propose the following tagline. ***ACA - Structure Matters*** We propose to place this tagline at the top of the ACA webpage, on marketing materials, in *RefleXions*, and on ACA letterhead. We envision this tagline becoming broadly recognizable and representative of our passion and commitment to our mission. I encourage you to give me some constructive feedback. Let me know if you like the mission statement and/or the tagline. This is your professional organization and we want your input. If you have other ideas or suggestions, please let me know. The SPC (and the ACA Council) represent you. We need you to give us feedback. Thank you for allowing me the opportunity to serve as the President of the ACA. I have enjoyed getting to know so many of you. I will continue to serve on the SPC. See you in Albuquerque.

Cheryl Stevens

From the Editor's Desk

Once again the winter issue of *RefleXions* carries the notes written by the recipients of our travel grants. It's obvious from their remarks that most of them would not have been able to come to meeting without the grant. This underscores the value of the program. What impressed me this year was the recurring theme: how much they enjoyed being able to learn about research, outside their own current interests, from the wide world encompassed by ACA members. There was also widespread appreciation of the workshops and the networking opportunities provided to our young scientists. We can all feel good about supporting the student travel program and should encourage program chairs to select more abstracts from young researchers for oral presentations.

I am also excited that in this issue of *RefleXions* we are announcing both the first issue of *Structural Dynamics* (***sd.aip.org)*** and the debut of the *ACA History Portal* (***www.amercrystalassn.org***). The *Portal* would not have been possible without the dedicated volunteerism of both Virginia Pett and her husband Dick Bromund. The ACA is very fortunate to have such volunteers, but the site itself is being designed and maintained by a professional and that costs money. If you think this is a project worth doing and preserving for the long term you can help support it with a donation to the *History Fund*. You can do it at the same time you renew your membership or whenever the mood strikes using the ***'DONATE NOW'*** button that can be found under the Awards tab on the ACA home page.

Dave Rognlie (1934-2013)

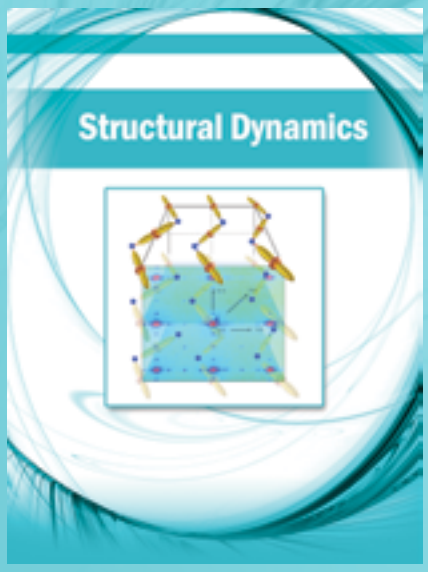
And, speaking of ACA history, as I wandered through the exhibit hall in Hawaii this summer something did not seem just right, and then it struck me; the Blake Industries 'vintage' booth was nowhere in sight nor was Dave Rognlie. Instead, in the slot reserved for Dave there was a display and representative from Huber. In response to my query he told me that all he knew was that Dave was in the hospital. Then, a couple of weeks later we heard that Dave had passed away on July 29th. Dave and Blake were part of the ACA corporate family as far back as I can remember. He was one of the good guys that are representative of our entire corporate family, and he will be truly missed by many of us. I always took every opportunity to 'rag' Dave at the meeting about his 20th century booth, to which he would respond with his usual shrug and a smile. Oddly, I now find myself hoping that whoever takes over Blake Industries will show up in Albquerque with that same booth. So long Dave - it was great to know you.

Judith Flippen-Anderson

Structural Dynamics

sd.aip.org

FIRST ISSUE
JANUARY
2014



Structural Dynamics is a new open access and online-only journal which is now accepting submissions. Co-published by ACA and AIP Publishing, it will highlight research articles on structural determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies.

http:/sd-peerx-press.org

TOPICS INCLUDE:

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  - o Materials
  - o Biological Systems
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- *Letters to the Editor:*
  - o Errata
  - o Comments on papers
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News from Canada

In many ways, the 2013 ACA Meeting was one of the most successful ever from a Canadian perspective. There were over 50 attendees from Canada, forming a visible presence in most of the sessions. In view of the large contingent from Asia at the meeting, this was disproportionate compared to US attendance. But it wasn't just the numbers that were positive. I was involved in judging for the Pauling poster prizes. Of the seven winners and three honorable mentions, five were from Canada, one from Korea, and four from the US. Several of my fellow judges commented on the high quality of the Canadian contingent. We have a lot to be proud of both among our trainees and the quality of their supervision. It is most certainly noticed by the whole organization.

This will be my last *News from Canada* article as we have just elected Mike James to be the new Canadian Representative on Council. Together with the soon to be elected new Chair of the Canadian Division of the ACA, Mike will continue to feature Canadian participation in the ACA.

In recent meetings, the Canadian Division has been jointly sponsoring 4-6 sessions, meaning that there are Canadian Co-Chairs helping to choose abstracts for oral presentations. At the Albuquerque meeting, we will be co-sponsoring sessions with the BioMac, YSSIG, Synchrotron and Small Molecule SIGs. We also sponsor the Delbaere Pauling Prize to recognize the top Canadian poster from a student. Canadians are also well represented in leadership positions among the various SIGs. More general initiatives include the emphasis on submitted abstracts as a source of oral presentations. In addition, largely facilitated by the YSSIG, there have been a growing number of *Blackboard* sessions, where advances in technology, both software and hardware, are discussed by those doing the development. This was the best-attended session of the whole meeting this year. All of these initiatives contribute to making the ACA a logical home for scientists from across the continent, who use crystallography as a focus for their research. Finally, the ACA is always looking for appealing (and cost-effective) venues for our meetings. With fond memories of the Montreal and Toronto meetings, suggestions for sites in Canada are always welcome. Send any ideas to Marcia at the ACA. I look forward to continuing to see all my Canadian colleagues at future ACA meetings.

Speaking of IUCr, 2014 has been designated the International Year of Crystallography (IYCr). With the Congress in Montreal, this is a great opportunity to show off Canada's deep history in this field. Our representative on the IYCr task force is Louise Dawe at Wilfrid Laurier University (***ldawe@wlu.ca***). Louise is on the lookout for local educational, historical or outreach events that feature crystallography, culminating in the IUCr Congress in Montreal in August. Please contact Louise with any plans or ideas you might have.

David Rose

The 22nd annual BHT (Southern Ontario/Western New York) Regional Crystallography Symposium, McMaster University, November 8, 2013

This year's symposium featured special guest André Hoelz from CalTech, who was invited to talk about how to approach structures of huge macromolecular complexes. André's description of the assembly of the structure of the nuclear core complex highlighted this astonishing accomplishment combining crystal structures of individual components of the complex with electron micrographs, small-angle scattering, and other solution techniques. His take home messages were that even beginning students can play important roles in such a project, that there is no substitute for persistence in screening of constructs and crystallizations, and, when confronted with an obstacle, "go bigger"; that is, often larger domains or complexes work better.

Dan Yang, Doug Kuntz and Leanne Wybenga-Groot

By tradition, the afternoon session featured talks by trainees from the participating laboratories, including Agnesa Shala (Audette lab, York University), Takefumi Morizumi (Ernst lab, Toronto), Francis Wolfram (Howell lab, Sick Children's), Monica Pillon (Guarné lab, McMaster), Vikash Iha (Ling lab, Western), Michael Lee (Jia lab, Queen's), Shuaiqi Guo (Davies lab, Queen's), Kritica Arora (Allingham lab, Queen's), Alan Ji (Privé lab, UHN), and Leanne Wybenga-Groot (McGlade lab, Sick Children's). As always, the quality of not just the research but also the presentations reminded us how active this area is in structural studies. The afternoon ended with a lavish wine and cheese reception sponsored by Rigaku and Art Robbins.

John Allingham and André Hoelz

The symposium would nothave been possible without the sponsorship of Art Robbins, Bruker, ForteBio, Infinity Biochemicals, Molecular Dimensions, Norton, Rigaku and ttplabtech. We are extremely fortunate to have such generous support for our community from our loyal vendors. Finally, the local organizers at Mac (Murray Junop's group and others) deserve thanks, as well as Lynne Howell for keeping the whole operation on track. If you are in the neighborhood next November 7th, please come to BHT'23!

David Rose

First Latin American Crystallography Meeting, Córdoba, Argentina, October 29 - November 1, 2013.

The *Primera Reunión Latinoamericana de Cristalografía* was held in conjunction with the Ninth Annual Meeting of the Argentinean Crystallographic Association (AACr) at the Universidad Nacional de Córdoba (UNC), Córdoba, Argentina. The meeting was preceded by the second workshop of the AACr dedicated to *Neutron Diffraction Techniques for Materials Characterization*. Alberto Podjarny (IGBMC, France), Gabriel Cuello, Mónica Jiménez-Ruiz (ILL, France), and Javier Campos (ICMA, Spain) participated as instructors. The fifth school of the AACr followed the meeting from November 4 to 8. The theme of the school was *Structure Solution and Microstructural Analysis from Powder Diffraction Data,* and it was led by Jordi Rius and Carlos Frontera (ICMB, Spain) and Ernesto Estévez-Rams (ICTM, Cuba). Raúl Carbonio (UNC, Argentina) coordinated the local organizing committee. The scientific program included 11 plenaries, 8 semi-plenaries, 13 short presentations, and about 130 poster presentations. Participants came from Latin American countries (Argentina, Brazil, México, Chile, Colombia, Cuba, Perú, Uruguay, and Venezuela) and from the US, Canada, Spain, France, Italy, Germany, UK, United Arab Emirates, South Africa, and India. Invited speakers included Joel Bernstein, Claude Lecomte, Robert Dinnebier, Mino Caira, and Bill Duax. An Honorary Doctorate from Universidad Nacional de Córdoba was conferred on Gautam Desiraju, IUCr President. Major equipment manufacturers (Agilent, Bruker, and Rigaku) as well as the ICDD were represented at the exhibit. Financial support for the event was provided by CONICET (Argentina), Universidad Nacional de Córdoba, IUCr, and ICDD, among others. At the Latin American assembly it was decided to hold the Latin American meetings every year, except in the same year as an IUCr congress. Brazil will host the 2015 meeting, and for 2016 it will be decided between Venezuela and Cuba.

Latin American Crystallographic Association (LACA)

A major accomplishment during the meeting in Córdoba was the formation of the *Asociación Latinoamericana de Cristalografía* (Latin American Crystallographic Association, LACA). A committee composed of representatives from each Latin American country with active crystallographers will work on the proposal to become a Regional Associate of the IUCr. J. Sabino (Brazil), D. Lamas (Argentina), and L. Bucio (Mexico) were elected as provisional President, Vice-President, and Secretary, respectively. The newly formed LACA will encourage collaboration within the American continent and the formation of crystallographic societies and committees in Latin America.

Graciela Díaz de DelGado

Top left: Front: Alexander Briceño and Mauricio Fuentealba, Middle: Viviana Dabbene and Raúl Carbonio, Back: Daniel Vega, Aldo Craievich, Edilso Reguero and Oscar Piro. Top right: Silvia Cuffini, Natalia De Vincentis, Iris Torriani, Aldo Craievich, Miguel Delgado, José Solís and J.R. Santisteban. Middle left: Front: Iris Torriani and Mario Suwalsky, Back: Claude Lecomte, Joel Bernstein, Hugo Monaco and Jordi Rius. Middle right: Diego Lamas, Raúl Crbonio and Gautam Desiraju. Bottom left: Graciela Punte, Daniel Vega and Diego Lamas. Bottom right: Raúl Carbonio. Background: Jacaranda trees blooming on campus.

7th Max Perutz Prize, August 2013

The European Crystallographic Association has awarded ***Randy J. Read*** the 7th ***Max Perutz Prize*** for his contribution to the development and application of advanced statistical approaches to all stages of protein structure solution.

The main research focus of his group at the Dept. of Hematology of Cambridge University, UK, is to develop new methods based on the maximum likelihood principle that can be applied to solve macromolecular structures. He also investigates the structural biology of medically relevant proteins, such as serpins (**ser**in-**p**rotease **in**hibitors), enzymes involved in hereditary metabolic disorders, and bacterial toxins. Using x-ray crystallography, he determined the structures of Shiga-like *E.coli* toxins and used them to design inhibitors. One of the molecules he designed, a five-armed polysaccharide named the "starfish" molecule, holds promise as therapeutic for *E. coli* food poisoning, also known as "hamburger disease" in the US.

2013 ICDD J. D. Hanawalt Award

ACA member ***Robert Von Dreele***, from Argonne National Laboratory, received the 2013 ***ICDD Hanawalt Award*** for his insight, courage and creativity in bringing powder diffraction to the macromolecular community. The award was presented at the 62nd Annual Denver X-Ray Conference, held in Westminster, Colorado. Von Dreele presented a lecture appropriately entitled *Protein Polycrystallography*.

Von Dreele has authored more than 150 publications, most of them related to the development of methods for the analysis of powder diffraction data based on Rietveld refinement. He adopted this technique, the first allowing structure determination from powder materials rather than single crystals, in 1972, three years after the publication of the fully implemented method. Foreseeing its potential in structural biology, he pioneered its use for the analysis of powder diffraction data obtained from biological samples. He called this approach *protein polycrystallography*. Using high resolution synchrotron radiation and Rietveld refinement, Von Dreele showed for the first time that powder diffraction data can be used to refine and solve the crystal structure of proteins and to investigate the formation of protein-ligand complexes.

Among his many achievements, he developed the General Structure Analysis System (***GSAS***) program suite used to refine structural data derived from x-ray and neutron scattering of crystalline or powder samples. Currently he focuses on scientific problems related to protein powder diffraction, such as crystal growth, phase transformation and radiation damage, and on possible pathways to determine *de novo* protein structure from powder data.

Before moving to Argonne in 2003, he was a staff scientist at Los Alamos National Laboratory (1987-2003) and a professor of chemistry at Arizona State University (1971-1987). Von Dreele was president of the ACA in 2009 and co-organizer of the GSAS-II workshop at the 2013 ACA meeting in Hawaii.

Suzanne Fortier Installed as Principal and Vice-Chancellor of McGill University, September, 2013

ACA member ***Suzanne Fortier*** has started her five-year mandate as ***Principal and Vice-Chancellor of McGill University***. Her election, announced last March, closes a circle that began more than 40 years ago, at the same university. Here Fortier carried out her undergraduate and graduate studies in crystallography, and began her journey into the academic world as a research scientist. After completing her PhD in 1976, she moved to Buffalo to work at the Medical Foundation of Buffalo, Inc. (now the Hauptman-Woodward Research Institute) with Herbert Hauptman, a pioneer in the development of mathematical methods for the analysis of protein x-ray diffraction data. In 1982 she became the first woman to be appointed associate professor of chemistry at Queen's University in Kingston, Ontario, and in 1992 she received a cross-appointment as associate professor in the Computing Department at Queens's. She became full professor both in chemistry and computing in 1993.

Her research focused on developing and integrating mathematical and artificial intelligence strategies for protein structure determination using x-ray diffraction data. Her studies included implementation of routines for automatic interpretation of protein electron density maps; construction of a protein knowledge database; and development of machine learning systems to facilitate crystallographic data interpretation. She was also interested in crystallographic structure determination of organic and organometallic compounds.

While at Queen's, she cut her teeth on academic administration, occupying several executive positions within the university in the years 1991-2006. In 2006 she was elected president of the Natural Sciences and Engineering Research Council, the division of the Canadian government that provides funding for research in natural science and engineering, where she remained until McGill summoned her.

Suzanne Fortier has authored more than 80 scientific publications and is a Fellow of the American Association for the Advancement of Science. She has received several recognitions for her services to research and administration. Among them: the Clara Benson Award for distinguished contributions to chemistry by a woman (1997); the Queen's University Distinguished Service Award (2005); and the Honorary Doctor of Letters degree from Thompson Rivers University in British Columbia for her scientific achievements and administrative gifts (2006).

2014 Gregori Aminoff Prize

The Royal Swedish Academy of Science will bestow the 2014 ***Gregori Aminoff Prize*** on ***Yingong Shi.*** He won the prestigious prize of 100,000 SEK, a little more than $15,700, because of his crystallographic studies of protein complexes involved in programmed cell death, or apoptosis. Shi investigates the molecular details of the apoptotic pathways in *D. Melanogaster*, in *C. Elegans* and in humans. His elegant crystallographic studies reveal how caspases (**c**ysteine-dependent **asp**artate-directed prote**ases**) are activated to promote cell death at the atomic level.

Shi has been dean and professor at Tsinghua University, in Beijing, since 2008. He received his bachelor's degree from the same institution, and then pursued his PhD in the US at Johns Hopkins University School of Medicine. After a short post-doctoral experience at Memorial Sloan Kettering Cancer Center in NYC, he became assistant professor and then full professor in the Department of Molecular Biology at Princeton University, where he remained until 2008.

Shi will receive the prize at the Royal Swedish Academy of Science's Annual Meeting, on 31 March 2014.

2013 Nobel Prizes in Chemistry

On October 9, 2013, the Royal Swedish Academy of Sciences awarded the ***Nobel Prize in Chemistry*** to Martin Karplus (top), Michael Levitt (center) and Arieh Warshel (bottom), for *the development of multiscale models for complex chemical systems*. The Prize honors the ever-growing importance that theoretical models play in today's scientific world. In structural biology the link between experiments and models is especially strong. In a continuous feedback loop, computational scientists need protein structures to develop their models and structural biologists rely on models for the calculation and optimization of their structures. In fact the software they use produces the lowest energy structure ("the" protein structure) after iterative rounds of computation and comparison of empirical and theoretical potentials for selected atomic distributions.

The three Nobel awardees, all born overseas but working at American institutions, researched on similar problems in the 1970s, and overlapped in different places and times, with fruitful collaborations and exchange of ideas. The challenge to describe what happens when two molecules react with one another, with particular reference to biological molecules, and the possibility of predicting the behaviors of these molecules, pushed them to develop simple computational methods that could serve these tasks. In Arieh Warshel's words: "… what we developed is a way, which requires a computer, to take the structure of a protein and then to eventually understand how exactly it does what it does".

The "way" is a hybrid quantum mechanics/molecular mechanics approach ("QM/MM"), computationally light yet extremely accurate, that allows simulation of complex enzymatic reactions. It uses quantum mechanics to describe the movements of the electrons involved in the reaction and classical molecular mechanics to treat the atomic rearrangements occurring in other parts of the molecules. Since its first application to study the lysozyme reaction, published in 1976, QM/MM has been applied to a diverse variety of phenomena such as protein folding, electron transfer, and drug and material design. It has remained a fundamental tool to uncover the mechanistic aspects of enzymatic catalysis.

QM/MM allows us to see proteins moving and breathing, as they naturally would, complementing structural biology studies and offering guidelines for downstream biochemical and functional studies. It animates molecules, otherwise essentially rigid in their crystal structures, giving them back the flexibility and the capability to interact with their environment in a dynamic way. And it makes us marvel at the beauty of the perfectly choreographed dance of the proteins with their substrates, and at those movements increasingly refined by millions of years of evolution that, ultimately, govern life.

Credit for Levitt photo: Linda A. Cicero / Stanford News Service. .

Index of Advertisers

2014 ACA Wood Award to Dan Rabinovich

The ACA will bestow the 2014 ***Elizabeth A. Wood Science Writing Award*** on ***Daniel Rabinovich***, from the University of North Carolina, Charlotte, during its upcoming annual meeting in Albuquerque, NM. The Wood Award is presented every Three years to science communicators who engage in activities aimed at promoting science to a broad audience.

Dan Rabinovich is a Peruvian inorganic chemistry professor with Ukrainian ancestry and a keen interest in the history of chemistry and philately. He combines the two passions in his column in the IUPAC bimonthly newsmagazine *Chemistry International*, where he recounts science journeys by means of images and words. Starting from the chemistry celebratory images that appear on stamps from around the world, Rabinovich narrates enticing stories on the discovery of Vitamin C, on Lavoisier's wife, on the giant sulfur bacteria of Namibia or on the newest addition to the periodic table, Flerovium, just to mention a few. The miniature images are fascinating; some have the vintage flavor of black and white photos and sepia portraits, others are sleek and modern. Like kids in a candy store, readers are drawn from one image to another and from one story to another. Rabinovich's catchy titles offer perfect entry points to his informative and easily digestible descriptions of complex molecules and "genius" scientists and of how they ended up on a stamp.

Rabinovich obtained his BS degree from the Catholic University in Lima, Peru (1990) and his PhD from Columbia University, NY, (1994). He then moved to Los Alamos National Lab for a two-year post-doc, and since 1996 has been a professor at UNC Charlotte. Here he specializes in synthetic and structural inorganic, bioinorganic and organometallic chemistry; his research has resulted in some 60 peer-reviewed publications. He was featured several times in *Chemical and Engineering News* and his letters appeared in the *Journal of Chemical Education*. He also edits the quarterly publication *Philatelia Chimica et Physica*, dedicated to the study of postage stamps related to chemistry and physics. Passionate about education and science communication, he has mentored almost 110 undergraduate students from UNC Charlotte and other institutions, 19 high school students, and 29 graduate (MS) students.

All award articles written by Chiara Pastore

ACA History

In January 2014 the ACA will launch its new History webpage, accessible from the ACA Home page, which will provide crystallographers, historians and curious science-enthusiasts alike easy access to multimedia historical material gathered throughout the years by the Association.

The History webpage will be a sort of magician's hat, from which interested readers will be able to pull out fascinating, absorbing and inspirational stories of great men and women that contributed to the development of the science of x-ray crystallography. The webpage will also contain audio and video recordings from the ACA meetings and conferences.

The video documentations consist of the awardees' talks at the ACA meetings, interwoven with the slides from their presentations. The first video was filmed in 2010, while the first audio files of award speakers were recorded four years earlier, in 2006.

Ron Hamlin (left) and Don Caspar (right) speaking at the Boston ACA meeting (2012).

The written documents that will be included in the webpage are currently part of "Living History", the section of *RefleXions* that collects personal stories from ACA crystallographers. The series was conceived by Judy Flippen-Anderson and was developed by Virginia Pett in 2010. Judy is co-editor of *RefleXions* and Virginia is a longtime member of the ACA and a retired faculty member at The College of Wooster, a small liberal arts college in Wooster, Ohio.

In the *RefleXions* articles and on the "Living History" website, scientists who played an important role in our history share their experiences with the ACA community. Participation in the project is voluntary, and anyone interested in presenting his/her memoir is encouraged to write to Virginia. Stories from individuals working in government, industry, and academia are welcome, as well as stories coming from research groups or organizations such as the ACA or the PDB.

The first contributor to "Living History" was James M. Stewart, with his article published in the summer 2010 issue. Since then, a total of 10 authors have submitted their memoirs. Each article within the series is unique in its structure and style, and represents a very personal account of its author's journey in science. The result is a lively collection of scientific experiences and discoveries, often accompanied by photographs and graphics. Many of the contributions are spiced up with behind-the-scenes anecdotes and recollections, such as the one by Jack Dunitz, which appeared in the Summer 2013 issue and revealed how we came really close to having a "DNA double spiral" rather than a "DNA double helix".

The full accounts of the narratives — only extracts are published in *RefleXions* — and the recordings are archived at the Niels Bohr Library and Archives in College Park, MD. The Library and the Archives are divisions of the American Institute of Physics (AIP) and are devoted to the preservation of the history of physics and affiliated sciences. The documents, stored on CD-ROMs and DVDs, are available for the public to consult onsite or by mail upon request.

The History webpage will provide an alternative, more convenient path to the information: popping up with a simple Google search, it will contain the complete online versions of the personal memoirs, plus links to the videos hosted on the YouTube website. This will guarantee that a broader audience will enjoy instant access to the documents.

The creation of the webpage was possible thanks to the kind donations of the ACA members, and to the work and passion of Virginia, Judy, and Patricia Potter. Patricia is the production manager for the *IUCr News* and is also in charge of updating the ACA website.

Timing could not be more perfect for its implementation: the History webpage's debut will coincide with the start of the International Year of Crystallography.

Chiara Pastore

Banner Photos, left to right: William Lipscomb and Herbert Hauptman at an IUCr Congress (year unknown); Dorothy Hodgkin and J.D. Bernal on her left (third person, time and place unknown); Walter Hamilton, Helen Berman and Tom Koetzle on their way to a meeting in Aarhus in 1972; Richard E. Marsh and Linus Pauling at Caltech during Pauling's 85th birthday celebration in 1986. (Help with filling in the "unknowns" would be appreciated - pett@wooster.edu)..

GSAS-II: The Workshop - ACA - Hawaii

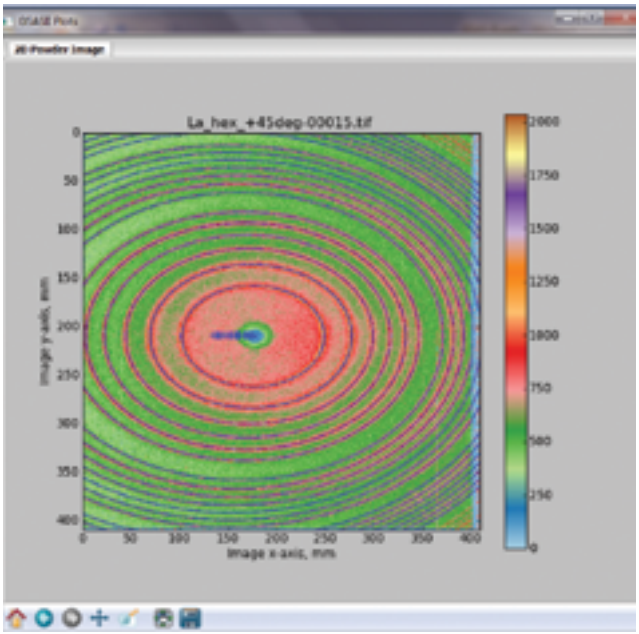
GSAS-II is a new crystallographic data analysis software package planned to handle all types of structural analysis problems, including both powder diffraction and single-crystal data. Synchrotron and lab x-ray data as well as neutron diffraction data are used. The package features constraints and restraints needed for problems ranging from complex mixtures of simple materials to structural analysis of proteins. An all-new program that is highly graphically oriented, GSAS-II is open-source and is largely written in the modern language Python, but inherits much from the design of the very widely utilized GSAS/EXPGUI codes that are reaching the end of their life cycle.

Brian Toby holds up an apocryphal (at least to those under age 40) computer input-output device he alleges was commonly used at one time in crystallography. None were harmed in the creation of GSAS-II. Photo courtesy of Peter Müller.

While some aspects of GSAS-II have not been completed (for example, fitting of TOF data and magnetic scattering), the code can be used for many types of problems and offers many capabilities that GSAS does not, for example powder diffraction area detector data reduction, PDF computation, and structure solution. Even though development of GSAS-II is ongoing, with new features being added regularly and some changes in the program operation anticipated, the developers are interested in seeing the software be deployed by experienced scientists, since it already has unique abilities and user feedback aids the development process. For this reason, the developers braved the harsh climes of the 2013 ACA meeting to instruct ~25 potential users in how to use GSAS-II.

The rather energetic "mascot" molecule of GSAS-II (PETN), showing off the program's 3D graphics capabilities.

The workshop started with assistance in the installation of GSAS-II on windows, linux and mac laptops (no cellphone version is yet planned) and then continued with alternating presentations and hands-on exercises in data reduction, structure solution and model refinement. It culminated



One feature of GSAS-II is its ability to handle all types of diffraction data and, for powder diffraction, handle data analysis from start (data reduction) through structure solution, refinement and completion (CIF preparation). Here GSAS-II determines detector alignment calibration for a detector set approximately 45 degrees from oblique to be used in data integration.

with a description of the constraint and restraint capabilities of the program. While one or two less-than-hardy (or beach-loving) crystallographers bailed out early, almost all of the remaining participants hung in through, and in some cases past, the end of the workshop, avidly turning electricity into heat as they plugged away at test data and their own structural problems. The advantage of open source software was brought home by the observation that two different workshop attendees were able to make small changes to the GSAS-II software during the workshop to allow them to use data from their home institutions. The advantage of Python is that as soon as the code is changed, it can be used with no compilation needed. The developers also gained from seeing where users stumbled, such as the self-upgrading feature (now rewritten) that failed under certain circumstances on an obscure OS called Windows-7.

All present would like to thank Marcia and the rest of the ACA staff for making arrangements for this workshop and Argonne National Lab for covering the audio-visual costs, allowing the workshop registration fee to be returned to participants in the form of a box lunch.

Brian H. Toby and Robert B. Von Dreele

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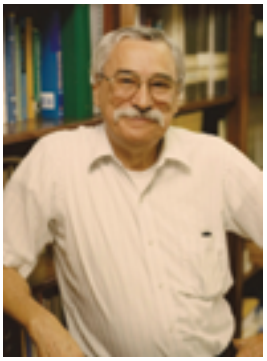
A Life in Crystallography – Abe Clearfield



The author of over 600 scientific papers and several books, Abe Clearfield's career spans over five decades of crystallographic science. Throughout his career he has utilized powder diffraction to study a wide variety of inorganic compounds. He and his group at Texas A & M developed techniques to solve crystal structures from powder diffraction data and applied these methods to solid state and materials chemistry.

My parents were born in Ukraine, then a part of Russia. My family lived in Romanivka, a small town near Kiev. My father had a horse and wagon with which he collected produce from local farmers to sell in Kiev, ten kilometers away. He slept under the wagon, even in winter, to sell the produce in the morning. My father emigrated to the US in 1912. However, because of WWI and the subsequent revolution and upheavals it took my mother nine years before they were reunited, having lost three children in the interim. My mother was able to bring out only one child, Sam, who was 15 years my senior. The two girls died from the flu in a refugee camp on the Romanian-Ukraine border. The boy, Tevia, was killed in a bandit raid. I am not sure but think he was trying to protect the girls. My mother substituted her nephew using Tevia's passport. So in all there were three boys, Sam, Ted and me, the baby. The nephew, Harry, went off on his own. My brother Ted and I were born in Philadelphia, PA.

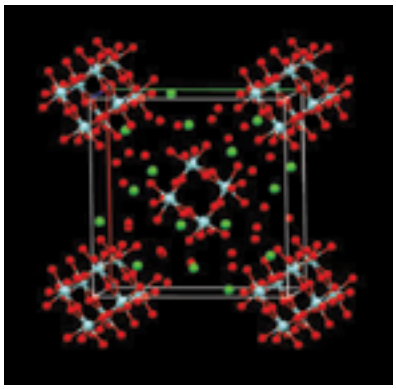
Shortly thereafter the great depression arrived, and we along with others were hard hit. My father had a pushcart stand in a market selling fruit and vegetables. Our part of South Philadelphia was divided into sections. The Irish lived from the Delaware River to Fourth Street. The Jewish neighborhood extended from Fourth to Eighth Street, and beyond that for as far as the eye could see was the Italian section. There was some overlap so we had two Italian families and one Irish whose boys were readily accepted into our gang. White people lived in the broad streets while the narrow streets were mainly African American.

When I was 12 years old my brother Ted gave me a Chemcraft Chemistry set for my birthday. It was the best possible gift and started me on the road to being a chemist. A very poor high school chemistry course did not dissuade me. My high school, Southern High, was an all boys' school that reflected the mix of nationalities and religions. Race or religion did not bother me; I made friends with all groups. I was elected secretary-treasurer of my graduating class, a post I held later in the US National Committee for Crystallography, 1995-97. Although I finished 12th in a class of 400 I did not get a scholarship as there were very few in those days. However, Ted came to the rescue. He was in the Navy and stationed in the South Pacific. Every month he sent me part of his pay, and together with money I earned in a variety of jobs in high school it was enough to see me through to a BA from Temple University. The chemistry department offered me a position to run the physical chemistry lab in their night school and earn an MA with free tuition and a monthly stipend. Half way through my MA, I married Ruth and after some reflection she convinced me to go on for a PhD. I was accepted at Rutgers University and did so well in the entrance exams that I was offered a fellowship with Philip A. Vaughan. Thus, began my career in crystallography.

Phil had received his PhD at Caltech under Linus Pauling. My project was to determine the structures of zirconyl chloride, $ZrOCl_2 \cdot 8H_2O$. This compound was important because pure zirconium metal was required for cladding of nuclear reactors but very little zirconium chemistry was known at that time. The zirconyl compound was the major source of a soluble zirconium compound.

We had no automated equipment and no computers. We used a Weissenberg camera to obtain films of the individual layers, read the spots by eye and calculated structure factors by hand. Pauling punch cards were used for electron-density calculations. If that were not stressful enough, the crystals lost water in air with destruction of the crystals. They had to be kept in sealed capillary tubes with some mother liquor in the tube. I solved the structures of the chloride and the bromide and they are nothing like what had been predicted.

The compounds are tetramers with the eight-coordinate Zr^{4+} ions at the corners of a square. There are four OH^- groups bridging Zr ions. The coordination is completed by four water



A 3-D representation of the structure of zirconyl chloride, $[Zr_4(OH)_8 \cdot 16H_2O]^{8+} \cdot 8Cl^-$. Color code: Zr, white; Cl, green; Oxygen, red.

molecules bonded to each Zr. The eight halide ions surround the tetramer yielding the formula $[Zr_4(OH)_8 \cdot 16H_2O]^{8+} 8Cl^-$. This study showed that there were no ZrO^{2+} ions in the solid, and this has proved to be the case for the solutions also. Interestingly, a group at Argonne National Lab and Northwestern University has recently begun a study of the structure of zirconium ions in solutions containing sulfate ions. They have used an array of the latest scattering techniques to attempt to determine the nature of the ions in solution as opposed to the structures that crystallize from those solutions. This paper referred to our work on the zirconium tetramer and my subsequent studies on the zirconium sulfates. So my 1956 paper in *Acta Crystallographica* is still of interest more than 50 years later.

Phil wanted me to present my study at the upcoming ACA conference at the University of Michigan (in June, 1953). Lucky me, this was the meeting where Hauptman and Karle presented

their "direct methods" procedure. Everybody who was anybody in crystallography stood up to criticize the presentation but Phil leaned over and whispered to me, "These guys really have something." He even solved a structure using direct methods and after some editorial problems was able to publish it.

Upon graduation I took a job with the Army Quartermaster Corp., in Natick, Mass. My job was to develop x-ray data of stretched fibers. I had an old G.E. generator with a rabbit ears tube. The tube needed adjustment, so when the technician came he showed me how to correct the problem. He held the tube by the rabbit ears, loosened the screws and made the adjustment. Then he said, "Make sure all the screws are tight before you let go." Then he let go and you guessed it, it struck bottom and smashed into a thousand pieces. With no tubes available and no possibility for a new x-ray generator I left for an industrial job with Magnesium Electron in Niagara Falls. Among their major products were semiconductor powders $BaTiO_3$ and $SrTiO_3$ prepared for the transistor industry. Often they made a batch that did not function properly. I convinced the physics group to purchase a powder x-ray unit so we could examine the powders during preparation and ensure the correctness of every batch based on crystallographic principles. As a side issue I solved the structure of $BaTiS_3$ and the Ca and Sr sulfides using x-ray powder data.

Somewhat later I taught a course in crystallography in the evening at Niagara University. I drew about 15 students working in industry and was astonished to find that none of the companies had x-ray equipment even though they made solid products based on clays and cement. I tried to teach them what could be learned using x-ray powder diffraction. A student, Jim Stynes, who worked in our analytical division obtained permission to use me as his research director at Niagara University so he could qualify for a master's degree. Working together we synthesized crystalline zirconium phosphate, $Zr(O_3POH)_2{\cdot}H_2O$ (α-ZrP) a layered compound that behaved as an ion exchanger. Although the company patented this compound, they were not going to develop it further. I had acquired a liking for teaching and wanted to further develop this class of layered compounds. Of course the key was structure so I wanted a place where I could have an x-ray lab.

I obtained a position with Ohio University in Athens, Ohio where I was able to buy an x-ray generator and Weissenberg camera. In short order, two students, G. David Smith and Robert H. Blessing, who wanted to study crystallography, joined my research group. I instituted a course in X-ray Diffraction and Crystallography with lab sessions on use of the equipment. Dave solved the structure of α-zirconium phosphate, and Bob worked on new Zr phases and structure studies. Then Bill Duax joined my group as my first post-doc. With these three jokesters, every day was a happening. Bill did his usual acrobatics to the delight of the females in our group. Yes, I encouraged women to be a part of the group in 1964.

Dave loved to catch a fly and paste a tail on its rear. The fly would lift off and remain suspended in air unable to fly freely and the boys would try to knock it down with a squirt bottle from five paces back. Our initial labs were in the basement of the chemistry building. One morning I entered the lab to see Dave standing on a box looking out at girls walking past our parking lot. Bob was at the air hose on the lab bench. At Dave's signal he opened the air jet to blow air but where? They hooked up tubing to the rear of a parked car and aimed at the passing girls. They took turns changing places.

Bill and I tried to solve structures from powder data by cutting out the printed peaks and weighing them for intensity data. We did find the heavy atoms but without digital equipment and computers we could not do any meaningful refinement. Bill did produce a major paper on the ion exchange mechanism of Na^+ exchange of zirconium phosphate.

During this time Sir William L. Bragg came to speak at Georgia Tech in Atlanta. This was an event not to be missed. Bob, Dave and I drove over the hills of West Virginia to hear this founder of x-ray crystallography and shake his hand. I still remember the great man's final statement. "I have no doubt that someday we will solve the structures of proteins routinely and this will revolutionize our understanding of biological processes."

Jobs were very difficult to obtain at this time so when Bill was invited to an interview at the Medical Foundation of Buffalo I urged him to go even though he was skeptical. Well, he took the job and the rest is history. Imagine my pride when Bill became President of the ACA and later Chief Executive Officer from unheralded Ohio University. Bill to me was a kindred soul; the care of his family and his devotion to teaching young students pleased me no end. Some years later, when I was awarded an endowed lectureship for my service as Associate Dean of the College of Science at Texas A&M, and after having two Nobel Laureates and several world-renowned chemists as speakers, I invited Bill to visit us at A&M. His talk was eclectic as expected. In true fashion he used the honorarium for science mentoring of high school students. What better thanks could a teacher have?

My next student who was crystallographically inclined was Jan Marshall Troup. He learned to do crystal structures with me but then went to Texas A&M to work for Frank Albert Cotton. Cotton's lab contained a completely automated x-ray unit that allowed Jan to solve all the problems Cotton had brought unfinished from MIT. Jan won the award for the best dissertation from the College of Science upon graduation. Then Jan and Bert Frenz founded Molecular Structure Corporation, the first company to do crystal structures for toll. I was on the Board of Directors for about ten years.

You see, Al Cotton and I had been classmates at Temple University. So just after Jan graduated I was invited to apply for a position at Texas A&M and accepted their offer. This was 1976, and I am still here. Meantime Bob and Dave had obtained post-docs, and as fate would have it they eventually both joined Bill at the Medical Foundation of Buffalo. A few years later Herbert Hauptman was made Director of Research of the Medical Foundation and the name was changed to the Hauptman Woodward Medical Research Institute. So I was invited to present a lecture at the Institute and Herb and I became good friends as did Ruth and Edie. Ruth liked the ACA the best of all the meetings we attended. She had a large cadre of friends who every year looked forward to enjoying each other's company at these conferences.

Abe and Ruth at the Buffalo ACA meeting (1999).

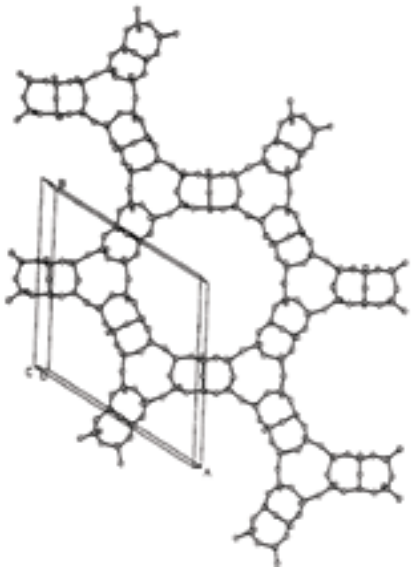
At Texas A&M I was able to build a major x-ray diffraction laboratory and I was instrumental in hiring Joe Reibenspies and later Nattamai Bhuvanesh to manage this lab. We also rekindled our interest in solving crystal structures from x-ray powder data and this time we were successful. Shown below left is an example of the type of structures we were able to solve. This was a 50-atom problem that held the record for size! A notable success was to unravel the structures of the largest (at that time) zeolite pore structures. They were designated H1 and VPI-5 and could not be differentiated. Both compounds had space group $P6_3cm$ with very similar unit-cell dimensions. We found that in H1 the six membered rings are disordered, so have special arrangements whereas the VPI-5 has ordered six membered rings. Incidentally my former student synthesized these compounds as a post-doc at VPI (Virginia Polytechnic Institute and State University).

In conclusion it should be noted that we did crystal structures for students in foreign countries like India, Iran and Nigeria as a goodwill gesture. I also received an honorary Ph.D. (*Honoris Causa*) from the University of Oviedo, Spain, March 18, 1998 for introducing their chemistry department to the intricacies of metal phosphonate chemistry.

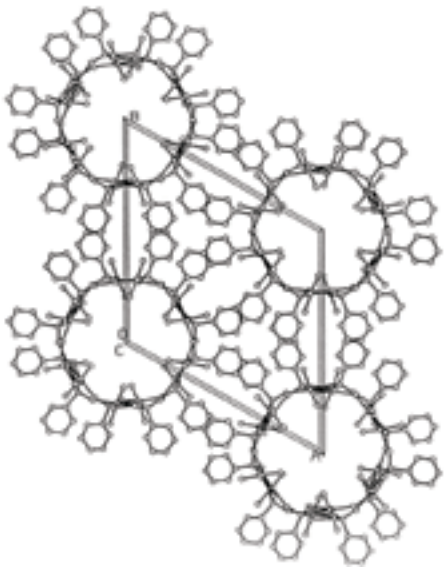
In recent years the teaching of crystallography has changed. With the advent of a Materials Science Program, which I recommended as Associate Dean for Research in the 1980s, but has only become a reality at Texas A&M in the past three years, the emphasis is on powder diffraction rather than structure solutions. I still give advice on structure solutions to the chemistry students and intense training to my graduate students but diffraction theory is now missing from the x-ray course.

It has been a highly interesting and rewarding life in chemistry and crystallography, but it has not yet ended. The zirconium phosphates have continued to interest scientists around the world with more than 10,000 papers and more each year. We are currently using them as nanoparticles for anti-cancer drug delivery. The search for knowledge and wisdom is eternal.

Abe Clearfield



The structure of a complex tubular uranyl phenylphosphonate, a 50 atom problem.



The structure of the 18-ring aluminum phosphate VPI-5.

Eventually, I was able to convince the ACA council to create an X-ray Powder Special Interest Group, which I chaired in 2004. In between I was Chairman of the Synchrotron Radiation Special Interest Group 1995-96, Secretary/Treasurer, USNCCr 1995-97, Vice President and President of the ACA 1998, 1999. I also won awards for excellence in research by the Southwest (1995) and Northeast (2008) sections of the American Chemical Society.

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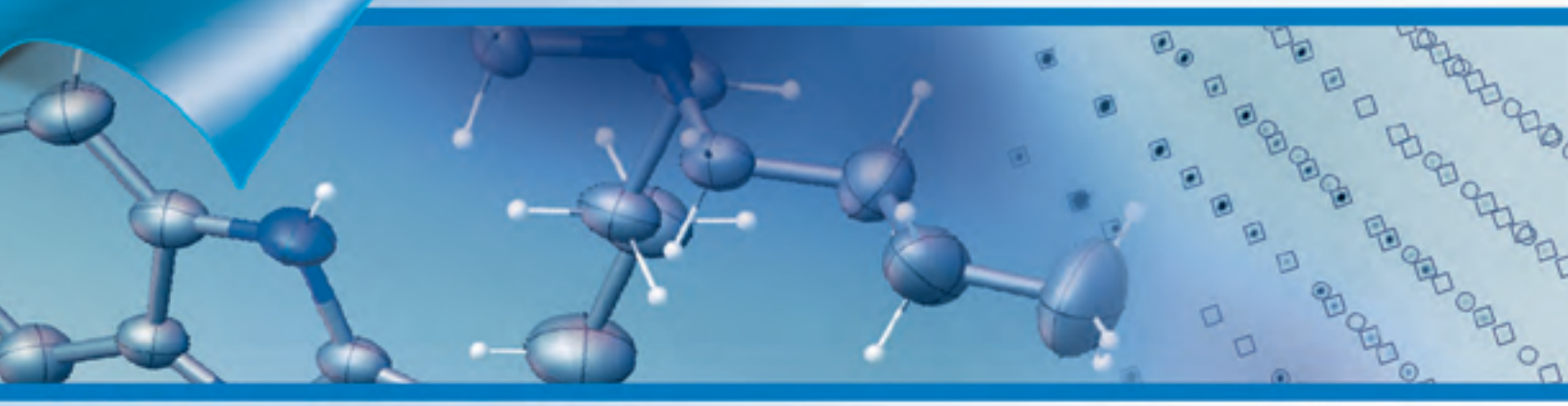
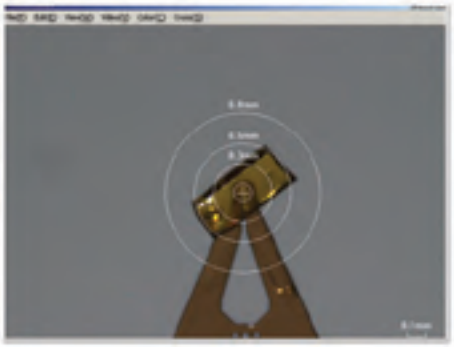


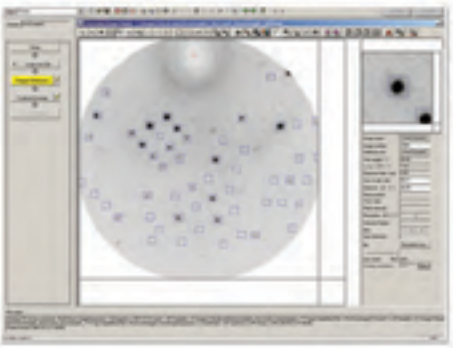
1. Walk up

2. Mount crystal

3. Align crystal



4. Collect data



5. Solve structure

6. XtaLAB mini™

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Small Angle X-ray and Neutron Scattering from Solutions of Biological Macromolecules: Dmitri I. Svergun, Michel H. J. Koch, Peter A Timmins, and Roland P. May, Oxford University Press, Oxford, 2013, ISBN 978-0-19-963953-3.

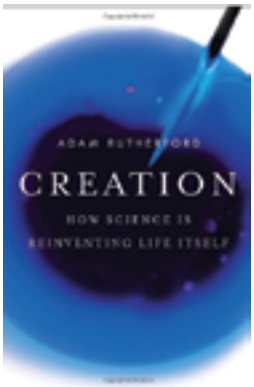
The authors set out to provide a modern textbook on the application of small angle scattering (SAS) to biological macromolecules and have succeeded. The layout allows for note-taking in the wide margins, but I did not partake since my copy was signed by one of the authors. The heavy math associated with Fourier transforms and spherical harmonics is placed in the first two appendices so crystallographers, who should be well versed in these methods, can go right to the core of the topic and neophytes can absorb all this information in one nice bundle. Throughout the book, caveats associated with the SAS technique are provided that will help prevent novice users from making fatal or dumb mistakes. The authors also provide numerous examples for the reader and supply the names of various programs in the ATSAS package that would apply to each case.

The book is divided into four major parts: *Theory and Experiment; Data Analysis Methods; Biological Applications of Solution SAS;* and *Appendices*. I've mentioned two of the four appendices already. The other two cover interactions between spherical molecules, and web resources.

Part 1 is further divided into chapters on *scattering, instrumentation* and, importantly, *experimental setup and data processing*. Part II covers *analysis of data from monodisperse and polydisperse/interacting systems*. Part III, which is the part that seems to be most needed by the community, covers *static studies, kinetic and perturbation studies, analysis of interparticle interactions, and hybrid methods*.

There is a *Conclusions and Future Prospects* section that provides a short retrospective and prospective on SAS. I hope everyone reads this section, as it also alludes to both the limitations and promise of SAS.

I received a first printing of this book, and there are a few typographical/typesetting errors. The authors have set up a web page where the community can input errata (***www.saxier.org/forum/viewtopic.php?f=12&t=2159***) so that subsequent printings will be errorless.



Creation: How Science is Reinventing Itself: Adam Rutherford, Penguin Group, NYC, 2013, ISBN 978-1-61723-005-9, 278 pg.

I listen to the podcast ***Science Talk***, produced by *Scientific American*, on a more or less monthly basis. In July and August they interviewed Adam Rutherford, author of *Creation*. Rutherford is an editor of *Nature* and I have heard him speak and have read numerous news articles written by him. The interview intrigued me so I bought a copy of the book.

The title is meant to be provocative, at least in the United States where we still seem to have issues with evolution, let alone creation. The book takes a long look at how modern biology has come to terms with both concepts.

I was a little disappointed, though, as I found a few technical errors; for example, diesel does not come from gasoline and the FAA doesn't care about trips to Mars—not yet, anyway. A few trivial errors like these call into question the correctness of the rest of the book. I can't even argue that these were related to nuances in British and American English—the book was printed in the US. One positive aspect of the book is that it presents information as current as the middle of 2012.

The book is divided into two parts: *The Origin of Life* and *The Future of Life*. The titles are self-explanatory. The author takes us through the discovery of the cell, the genetic code, and how the genetic code has allowed scientists to hypothesize when LUCA, the Last Universal Common Ancestor, may have come into being. Rutherford reviews our current understanding of how life may have come into existence at undersea vents, rather than in primordial soups activated by lightning.

The first chapter of the second part, *Created Not Begotten,* reviews the history of our understanding of DNA, culminating in the creation of Synthia by Craig Venter. Interestingly, we learn of the Easter eggs the team left in the genome, including a misquotation of Feynman. The lesson here is: don't believe everything you read on the Internet. The next chapter, *Logic in Life*, looks at how we might use DNA programs to create cancer treatments and sensors. *Remix and Revolution* discusses the BioBrick project and even touches on the intellectual property issues associated with genes. This book was printed before the Supreme Court handed down the Association for Molecular Pathology v. Myriad Genetics, Inc. decision, so it does not reflect the results of this historic case.

OS X Mountain Lion: The Missing Manual: David Poque, O'Reilly Media, 2012, ISBN-13: 978-1449330279, 888 pages.

I went to Amazon to look for a book, and my landing page displayed this title. I like what Pogue has to say about technology and this seemed like a good book to read. Actually, it is a great book. I once heard Jerry Pournelle say that the great thing about Mac OS X is the fact it takes only a few minutes to figure out whether you can do something or not, whereas with the other major desktop OS it can take much, much longer. This book demonstrates that OS X is very feature rich and contradicts Pournelle's statement because there are so many really, really useful features in OS X that are not obvious, ones that you really need once you learn about them.

The author fulfills what he set out to do, which is to provide the missing manual for OS X. Frankly, the chapter on *Spotlight* alone is worth the purchase price. After finishing the second chapter, I bought the upgrade to 10.8. After finishing the chapter on security I decided the next computer I buy for home will be a Mac. Also, the editions for *Snow Leopard* and *Mountain Lion* would have saved me a lot of money, time and grief had I known about them when I switched to Mac OS three years ago. I've bought a number of apps that I probably did not need because the functionality was buried in the OS somewhere.

I do have one critical comment. I bought this as an ebook for my Kindle and that was a mistake. The Kindle does not know how to display properly. Sometimes it is displayed, but more often than not it is replaced with a space or, worse, overlayed with the symbol to the right. I have the Kindle app on my MacBook, so I read the book there when convenient. This actually had a very positive effect. I could switch from the Kindle reader to the OS and try out whatever I was reading. I found this positive reinforcement very beneficial in committing keystrokes to memory.

Another important feature of the Kindle version is that everything is hyperlinked, so you can bounce around or use another great feature: ***www.missingmanuals.com***, where you can access ***The Missing CD-ROM*** for this book. The book's index is massive, taking up 25% of the book itself, making it easy to find specific items. There are sidebars with the titles *Gem in the Rough, Note, Tip, Power User Clinic*, and others. These provide details beyond the main text and are quite useful.

The book is divided into eight sections: *Introduction, The OS X Desktop, Programs in OS X, The Components of OS X, The Technologies of OS X, OS X Online, Appendices and Index*. As I mentioned earlier, the chapter on *Spotlight* is very illuminating and even details the query language available, which allows for intelligent searching. Here's one neat trick I learned: -space takes you to *Spotlight*. Enter a formula, for example sin(pi), and you get the answer. *Spotlight* is a basic scientific calculator. If you type a word, look down a bit and hover over the 'Look Up' entry, the dictionary entry appears.

OS X is capable of taking dictation (Chapter 5), but it requires one to upload their contact list to Apple. I haven't tried it yet, because I cringe at the thought of uploading my contacts, but I would be curious to hear about your experiences with dictation.

Chapter 11 is chock full of useful stuff. *Calendar* has a feature that will display a document at a specific time, which is great for reminding you what you should be doing right now. *Preview* is far more powerful than I realized, especially in the way it handles PDFs. In fact, I am going to see if I can jettison Acrobat and all other utilities I've acquired for handling PDFs and live with *Preview* alone. If you turn on *TimeMachine* it will make backups of critical files to your main disk when your backup drive is not connected. *TimeMachine* is so easy to use there is no longer an excuse for being among the 96% of people who don't back up their files.

Chapter 13 covers security, and Mac OS X provides plenty of that by default. However, I learned I can enhance security significantly. I have already activated *FileVault* and will add a boot password. There is one command program not described that is extremely useful: *purge*. Execute this from a terminal and your Mac's memory is cleared of rubbish. Do this once or twice a week and you won't have to reboot except for updates. Now if I can just get *Calendar* to activate this every day at 0200.

Before I close, here is another great time saver: hold down any character key for a second or so and an accented character selection dialog appears. Pick a number and you are done. I could go on and on about things I learned about OS X, but you really need to get the latest version of OS X, 10.8, and this book to take advantage of the rich features. Or you can spend all your free time poking around and figuring it out for yourself.

Joe Ferrara

The Neils Bohr Library & Archives

The Library is located within the AIP Center for the History of Physics at the AIP headquarters in College Park, MD. The Library's print holdings consist of approximately 14,000 titles. At the Library's core is a matchless collection of "primary" printed works of historical importance, including physical science monographs, textbooks, laboratory manuals, instrument catalogs, and published correspondence. About two-thirds of the collection was published between 1850 and 1950.

The collection also includes:

AIP/Member Society journals

Books and journals on the history of physics and allied sciences (astronomy, geophysics, etc.)

Biographies

Institutional histories

Philosophy of science

Social aspects of the scientific community

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CCDC in the USA - The Easy Move

Change can be unsettling for some, exciting for others. Sometimes it can leave you scratching your head, bewildered. But sometimes you just have to smile and say, "of course"..

We are proud to announce that we have established operations on the ground in North America – at the Center for Integrative Proteomics Research, at Rutgers, the State University of New Jersey. We will be alongside the RCSB Protein Data Bank and on a campus leading the way in new integrated approaches to biomedical research.

Now that we have set up operations in the US, we're in the ideal location to serve the 40% of our worldwide users that are in North America. Moreover, we're perfectly positioned to work with the RCSB PDB. Of course, the CCDC and the wwPDB partners have worked together in the past, but it's now become a whole lot easier. The Protein Data Bank in Europe is just a few miles from us in Cambridge UK. Our friends at Osaka University look after our academic users in Japan as our National Affiliated Center there and also host PDBj. We will now have the RCSB PDB just down the hallway at Rutgers. With all these relationships you should expect to see all sorts of collaboration – and you will.

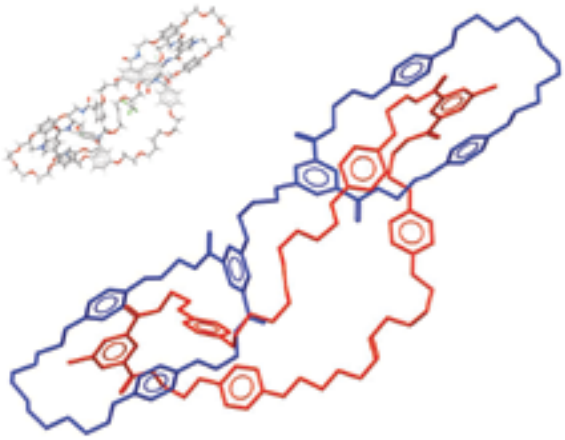
The Cambridge Structural Database was established in 1965, with the Protein Data Bank not far behind in 1971. Since then the two resources have grown enormously; there are nearly 700,000 organic and metal organic structures available and almost 100,000 macromolecular structures. Crystallography has, for many decades, been a shining example to other disciplines. The publication of a crystal structure determination without the timely deposition of structural data is simply unthinkable. That the output of almost every published crystallographic analysis, ever, is available to all is a phenomenal achievement of this research community.

The wwPDB and the CCDC have much in common; we share technology and all of us strive to deliver the most useful structural information possible to our users. However, we also have our own distinctive character and a few healthy differences!

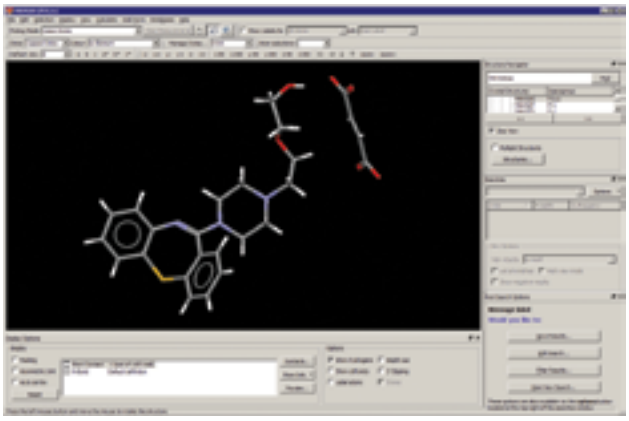
There is also scientific synergy; structures contained in the PDB teach us a great deal about the conformations and interactions of the small peptides in the CSD. Likewise, the conformations and interactions of small molecules in the CSD inform us on the binding of ligands to macromolecules. There can scarcely be a macromolecular crystallographer who hasn't turned to the CSD to get the best possible insight into small molecules bound to their target of interest. Similarly, many structural chemists turn to the PDB to give them biological insights into their molecules.

So, after a combined 90 years of serving our respective and overlapping communities, we're ideally placed (literally!) to develop even more innovative, integrated approaches to serve our users – wherever they are in the world.

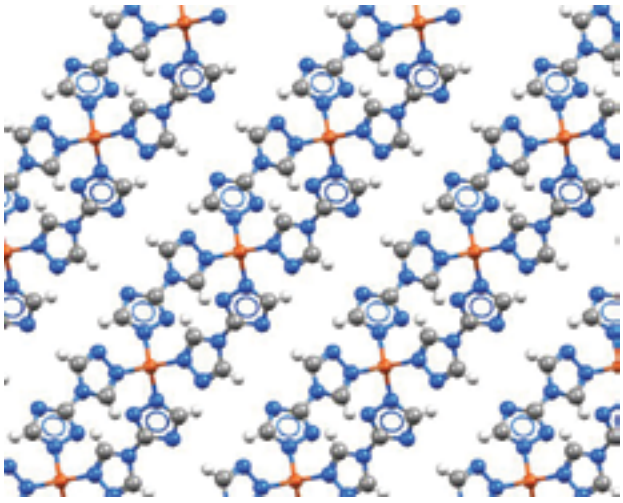
Paul Davie, General Manager, CCDC Inc.



CSD entry EMIDOU, a "handcuff" catenane. The handcuff component of the structure is shown in blue; the inset is the structure colored by element.



CSD entry MAVGAS, synonym Quetiapine, which is an antipsychotic drug - as viewed in the Mecury application.



Packing diagram of CSD entry XEMWAP, a copper triazole polymer that fluoresces blue.

Cryocool: Gas Stream Coolers

Cryogen Free
CRYOCOOL-LT

Cryo Industries of America, Inc. (CIA) has been manufacturing gas cooling systems for over 27 years.

With the CRYOCOOL family of gas stream coolers we have opened new frontiers in crystallography, allowing researchers to take advantage of a product family having the widest temperature range in the market
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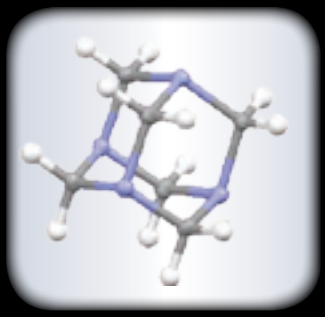
(-269°C to 227°C)



Crystal at 10 K:
CRYOCOOL-LHE

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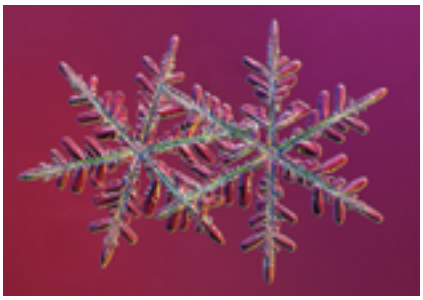
- Cryocool-LN7: 7 l/day LN2

CRYO Industries of America, Inc.

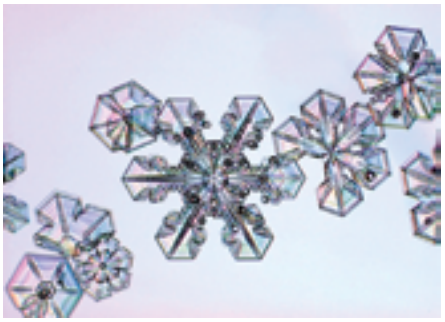
www.cryoindustries.com

NetfleXions

There's a chill in the air in my neck of the woods these days. As the Starks say, *winter is coming*. And with winter comes my favorite form of crystal – snow. I'm always looking for ways to make crystallography more accessible to friends and family who *aren't into science*. What better way to do that, than by pointing out the loveliness of those crystals so ubiquitous during winter in colder climes! Just a few snow crystals caught on a mitten are enough to show off symmetry, polymorphism, crystal growth and a whole host of other topics near and dear to our hearts. But what if it doesn't snow where you live? Or what if you just dislike the cold? Well, fear not gentle reader! There are several websites around showing off snow crystals in all their glory.

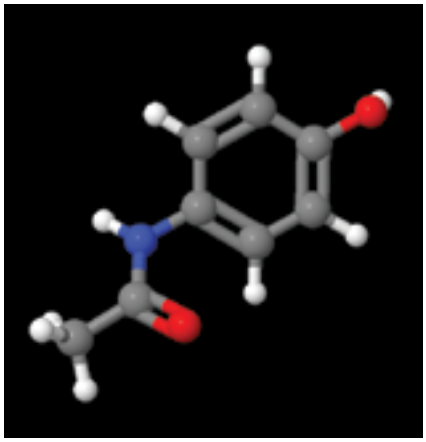


Caltech physicist Kenneth Libbrecht maintains the page at ***www.its.caltech.edu/~atomic/snowcrystals/*** which offers high-resolution, magnified images of a variety of snow crystal forms. In addition to his fantastic photography, Libbrecht explores the physics of snow crystal formation, classifies crystal morphologies and provides several useful tips for viewing snow crystals and building your own snow crystal photography kit. The *Bentley Snow Crystal Collection of the Buffalo Museum of Sciences* (***bentley.sciencebuff.org/index.htm***) contains the un-retouched images of Wilson A. Bentley, the first person to successfully capture snow crystals on film. This website offers a biography of Bentley and information about his methods, as well as links to several other snow sites. These are just two of the multitude of web resources available to anyone interested in looking at photos of snow crystals, or even creating their own.



Once you have hooked your unsuspecting audience on crystallography, it's time to wow them with your own research. After a long day of trekking through the snow, you'll want to have something handy on which to display your favorite small molecules. If you have your coordinates in PDB format, most protein structure viewers will also render small molecules. However, most of the small molecule sets deal in CIF, not PDB. There aren't many CIF readers out there for tablets, but Android users can avail themselves of *Jmol* through the free *Jmol Molecular Visualization Activity* app. The app will read in CIF files downloaded to the Android device and will pick up files from the PDB or from NIH/NCI compound libraries. Structures can be searched by compound name, InChi string, PDB code, CAS registry number, and other keys. Additionally, *Jmol* commands can be employed to enhance structure visualization with various rendering formats, symmetry operations, and Miller planes, to name a few. Android users can download the app for free from the *Google Play Store*.

For iOS users, *CrystMolPad*, developed by David Duchamp, will be available soon from the Apple *App Store*. The app will read CIF files to render small molecules (as well as macromolecules) and will come with a library of structures – including several mineral types. Duchamp says of his soon-to-be-released app, *It has a simple user interface that should allow anyone – secondary school kids through research scientists – interested in crystal [or] molecular structure to use it to explore and enjoy the wonderful world of crystal and molecular structure at the atomic level*.



Now that you have a few more crystal structure visualization apps in your toolkit, you'll never want for distractions to while away those long winter nights. Get inspired by the snow around you and spread the word about the beauty of crystallography. Grab your tablet or your laptop, curl up by the fire and tell stories of your crystallographic wonders to all who will listen. You have much work to do, gentle reader. The International Year of Crystallography – like winter – is coming!

Amy Sarjeant

Notes of a Protein Crystallographer: Honoring our Mathematical Methods Developers

International Symposium on the Frontier Between Cryo-EM and Protein Crystallography, Hotel Igeretxe, Getxo, Spain, 3-4 October 2013. Photo courtesy of Xabi Muñiz.

The most recent updates from the PDB indicate that approximately two-thirds of the structures deposited currently have been phased by Molecular Replacement methods using a related, pre-existing, structure in the database.

This is a tribute to the success of the discipline and definitively to the power of the Molecular Replacement method proposed and championed by Michael G. Rossmann and David Blow in the early sixties in parallel with the more experimentally demanding Multiple Isomorphous Replacement (MIR) method.

For the younger generations of structural biologists 'Molecular Replacement' refers to programs available in the CCP4 package that are used essentially as a 'magic black box' that either succeeds or fails in finding the structure of the known or 'related' fold inside the unknown crystal structure.

This state of affairs was not always so and many insightful crystallographers and computer scientists have developed the original idea to an extraordinary degree of effectiveness in the field. In fact, some of the 'crystallographers' who dramatically improved the performance of the mathematical tools originally proposed were not *bona fide* crystallographers but rather mathematicians such as Gerard Bricogne or physicists like R.A. Crowther, who originally proposed the Fast Rotation Function expansion in terms of spherical harmonics in 1971. In this note I would like to highlight one of them, Jorge Navaza, for several reasons. First and foremost are the impact that his contributions to crystallography and its younger sister (i.e., electron microscopy) have had in the two fields separately, and the resulting synergy that has ensued in the past decade. Second is the professional respect and personal friendship that Jorge has always inspired in the narrator. Finally, I wish to mark the momentous occasion of a modest homage that friends and colleagues of Jorge offered him on the occasion of his retirement from his latest research position at the laboratory of Structural Biology (IBS) in Grenoble, France.

The meeting honoring him on his retirement was a unique gathering of early students, colleagues, collaborators and friends of Jorge and his spouse (Alda) and his son Rafael, in the Basque town of Getxo in the outskirts of Bilbao, Spain, on October 3-4, 2013. The meeting was entitled *On the Frontier between Cryo-EM and Protein Crystallography* and was organized by Diego Guérin, Ignacio Fita, Pedro Alzari, José R. Castón and Jean Lepault with the support of several research institutions of France, Spain, and the Basque Government: Consejo Superior de Investigaciones Científicas (CSIC, Spain), Centre National de la Recherche Scientifique (CNRS, France), Gobierno Vasco/ Eusko Jaurlaritza, Institut Pasteur (France), Universidad del País Vasco (UPV/EHU) and Fundación Biofísica Bizkaia (FBB).

The meeting was brief but intense. The scientific talks centered around the collaborations that Jorge Navaza has had in the past few years related to difficult structures that were solved by the use of the AMoRE suite of programs, and also on the successful applications of his software URO, for the combination of Cryo-EM data with crystallographic data. Only the highlights are summarized; details of the different structures presented can be found in the published scientific papers.

In the first session, Félix Rey from the Institut Pasteur (Paris) described the details of the structures of regular enveloped viruses and the implications for evolution. Later, Fasselli Coulibaly (Monash University, Australia) presented the protein-induced membrane remodeling by D13, the scaffolding protein of vaccinia virus.

These lectures were followed by the impressive work of José R. Castón and collaborators (Group of Electron Microscopy of Autonomous University in Madrid, Spain) on the near atomic resolution (~ 4 Å) structure of the virus attacking the fungus *Penicillium chrysogenum* (PcV), a fungal dsRNA virus. The mechanical and dynamical properties of the vault ribonucleoprotein particle were presented by Nuria Verdaguer (IBMB-CSIC, Barcelona, Spain). This aggregate is a massive 'vault-like' structure composed of two identical subunits of 39 copies each of the component protein vault protein (MVP).

Eleanor Dodson eloquently presented the importance and impact that the first release of AMoRE had as a part of the CCP4 release in 1994. The vastly improved mathematical procedures and the distinct introduction of automation within the suite of programs facilitated enormously the program performance and effectiveness to solve difficult structures by Molecular Replacement methods.

Eleanor's presentation was followed by spirited and often hilarious presentations by two of Jorge's most brilliant students Leandro F. Strozi (Grenoble, France) and Stefano Trapani

(Montpellier, France) who played an important role in the early publications related to the mathematical improvements of AMoRe.

Xavier Gomis-Rüth presented the spectacular results of applying these methods to the intricate structure of the α2-macroglobulins later in the program.

The emotional highlight of the meeting was in the late afternoon of October 3 after the first technical sessions. Briefly introduced by the narrator describing Jorge's flirtation with Structure-Based Drug Design, Jorge presented a retrospective of his work on crystallography starting from the core of physicist friends at the University of La Plata in Argentina: E. Castellano, Alberto Podjarny, Abelardo Silva and the younger Pedro Alzari. Pedro followed with a series of photos of the younger Navaza and the group and soon thereafter appeared the surprise of the evening. A Basque dancer-player ('Dantzari-Txistulari') pair appeared in the room to perform a symbolic Basque dance named 'Aurresku' in homage to Jorge. This is a unique intricate dance based on the 5/8 meter. At the conclusion, Jorge was presented with a silver-decorated walking stick (or 'makila') as a sign of respect from his friends and peers.

Left to right:. Pedro Alzari, Jorge Navaza, Diego Guérin, Alda Navaza, José R. Castón, Ignacio Fita (behind), Cele Abad-Zapatero (Courtesy of A. Podjarni)..

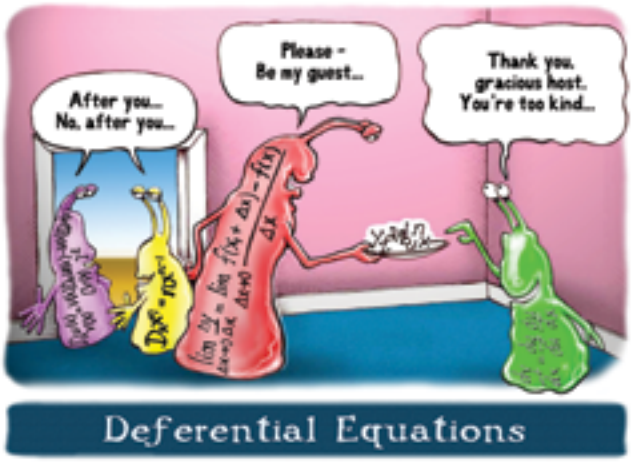
The next day the first presentations highlighted computational developments related to structure determination. Abelardo Silva (Advanced Molecular Sciences, USA) discussed his efforts to revisit and improve the issue of parameters describing the molecular geometry, and Garib Murshudov (MRC, Cambridge, UK) discussed his efforts to improve the refinement of structures at medium to low resolution.

These lectures were followed by another series of structural results. Alberto Podjarny (IGBMC, Strasbourg, France) presented his results of neutron diffraction combined with subatomic resolution x-ray diffraction (<1 Å resolution) in two systems: human aldose reductase (h-AR) and the antifreeze proteins (AFD) of artic fish. Philippe Dumas (University of Strasbourg, France) presented an intriguing lecture on the use of the classical Clayperon-Clausius Equation (CCE) and a generalized form (GCCE) to physical phenomena ranging from thermal regulation in biological systems to black holes. Vicente Rubio (IBV-CSIC, Valencia, Spain) presented his twenty-year journey studying enzymes of the urea cycle in humans in collaboration with Ignacio Fita (IBMC, Barcelona, Spain). The meeting closed with the presentation by Dino Moras of the work of his group on the structure of nuclear hormone receptors and its regulation via DNA transcription, combining SAXS, SANS and FRET to establish the architecture of heterodimers bound to DNA elements. Dino's concluding remarks impressed upon the audience the extraordinary impact of Jorge Navaza's work on the structural biology community as judged by the number of citations (~5,000 for a single paper) present in the literature. An emotional applause concluded the sessions of the meeting honoring this 'craftsman' of the mathematics behind the implementation of the Molecular Replacement method and the calculation of the Fast Rotation Function.

Collage of the location of the 'golden spike' at the base of the Lutetian stage (Eocene) in the Gorrondatxe beach, near Getxo where the meeting took place.

There were many touristic temptations to pique the curiosity of the attendees of the meeting, from the world-renowned Guggenheim Museum at the center of Bilbao to the magnificent vistas of the beaches and cliffs in the seashore. For the Geology enthusiasts, there was a special treat. The seashore of the Atlantic Coast of Spain where the Basque country is located, from Bizkaia to Bayonne in France, is a treasure trove of remarkable formations that serve as reference points for the stratigraphy of the various epochs of Earth's history. Just a few kilometers away from the meeting venue, there is a recent (Feb. 2012) 'golden spike' placed by the International Union of Geology Scientists at the Aizkorri beach to mark the base of the 'Lutetian' stage of the Eocene Epoch dated approximately 48 millions years ago.

Cele Abad Zapatero



ACA Election Results

Council Officers

Vice President
Chris Cahill

Canadian Representative
Mike James

Standing Committees

Communications
Ilia Guzei

Continuing Education
Edward Collins

Data and Standards
Peter Müller

SIGS

Biological Macromolecules
Chair-elect: Susan Buchanan
Secretary: Blaine Moors
General Interest
Chair-elect: Stacey Smith
Industrial
Chair-elect: Peter Wood
Secretary: Mark Olivera
Materials Science
Chair-elect: Simon Billinge
Neutron Scattering
Chair-elect: Anna Llobet
Powder Diffraction
Chair-elect: Craig Brown
Service Crystallography
Chair-elect: Bruce Noll
Secretary: Stacey Smith
Small Angle Scattering
Chair-elect: Shuo Qian
Secretary: Angela Criswell
At-Large: Thomas Weiss
Small Molecules
Chair-elect: Christine Beavers
Secretary: Louise Dawe
Synchrotron Radiation
Chair-elect: Marian Szebenyi
Young Scientist
Chair-elect: George Lountos

Name Change
Synchrotron SIG is now
Light Source SIG

Chris Cahill
Vice-President

Professor of Chemistry and International Affairs, Department of Chemistry, The George Washington University, Washington, DC 20052.

Statement: I am looking forward. to serving the community that has become my scientific home. I have held several positions within the community including membership on the ACA Continuing Education Committee and on the USNCCr. I have also served as Program Chair for the 2011 ACA Meeting in New Orleans. As such, I have worked closely with Council in the past and have a sound appreciation for what the position of Vice President entails. Moreover, this comes at a time in my career where I am able to give back to an organization that has provided me with invaluable inspiration and support over the years. Having established a sustainable and well-funded research program, I am excited by the prospect of a leadership position where I can leverage my experiences thus far to help guide and shape an organization about which I am passionate. One of the more intriguing aspects of the VP position of ACA is that this organization is vibrant and thriving. This might prompt an eye roll or two from some readers, but think about it: here is a relatively lean organization dedicated to its members and that operates on their input and service. This is not typical for a number of other scientific organizations. While on Council it is my intent to enhance an already strong foundation and explore opportunities for improvement. With respect to the latter, I see opportunities (and challenges!) for broadening participation across the Americas. We need to remember that the first 'A' in ACA includes North, Central and South America and accordingly, we should make sure we are doing our best to be inclusive and supportive. Further, my 13 years in Washington, DC have made me keenly aware of how intricately linked science and policy have become. How policy influences science and vice-versa is not only fascinating, but is also often grossly misunderstood from within the respective camps. My own interests in this arena have led to a recent promotion to Full Professor with a secondary appointment in the Elliot School of International Affairs at GW. This appointment speaks to an emerging awareness of the global impact of our science and specifically the disconnect between technical and non-technical communities. I see opportunities for organizations like the ACA to participate in outreach to the policy community, who (believe it or not) are hungry for education and technical enlightenment. The ACA membership is full of dynamic and articulate scientists and, as a consequence, I would like to see us take on a greater role and engage the policy community in interactions beyond our typical forums and 'comfort zones.' Returning to the local level, I hope to be able to chip away at the divide between the small-molecule and macromolecular communities within the ACA. While this is certainly not a lethal compartmentalization, anyone reading this is likely aware of the minimal overlap. Looking back at a number of ACA meetings, opportunities to have both camps in the same room at the same time often emerged around symposia based on education, best practices, and diverse keynote speakers. It is definitely not the VP's job to take over a meeting program, but I would certainly be supportive of events targeting both communities simultaneously. Moreover, our common interests in the development, support and use of national facilities can provide even more of a forum for working together across disciplines not only at meetings, but year-round. I am honored to have been elected to serve as the next Vice President of the ACA. This is an intellectually rich organization with a sound infrastructure. Consequently, opportunities for enhancement (as opposed to repair) are all the more intriguing.

Michael James
Canadian Representative

Distinguished University Professor, Department of Biochemistry, University of Alberta, Edmonton, Alberta.

Statement: I have been a member of the ACA, on and off, since my time as a graduate student working for my Master's degree at the University of Manitoba (1963). The first meeting that I attended was in Minneapolis in 1968. Over the years I have realized just how beneficial it is for us Canadians to have the opportunity to be members of the ACA, whether our interests are in mineralogy, chemistry, structural biology, diffraction physics, or instrument development. The ACA provides for all of these disciplines and brings together the best people to pass their knowledge and experience on to the younger generation of crystallographers. I still have a lot of energy to tackle new projects that are and will be of importance to Canadian crystallographers. Speaking of Canadian crystallographers I was surprised, and amazed, to learn that only 50% of us are members of the ACA. Why is that? One possible reason may be that our efforts in meeting attendance are focused on the specialties we have chosen in crystallography. By this I mean those of us who specialize in the structural biology of membrane proteins attend those meetings that are geared specifically for that sub-discipline. Or if we are mineralogists, we attend those geology meetings to discuss our discoveries of new minerals. While I can understand these reasons and even perhaps used them at times to rationalize my failure to pay annual dues, I don't think overall that these are good reasons. If one looks at the programs of the past few ACA meetings, I am sure that you will find topics into which your interests fit well. In addition, we all employ similar crystallographic techniques and to attend a meeting where these techniques are discussed is of paramount importance. Where else could you hear about the developments in serial femtosecond diffraction experiments? John Spence treated those of us who attended the 2012 Boston ACA meeting to the future of crystallography in his acceptance speech for the Buerger Award. The instrument manufacturers are all in attendance at these meetings and ready to discuss the next best thing for data collection since photographic film! (Just kidding.) Collectively we benefit a great deal by being members of the ACA, and I plan to strongly urge all of my Canadian colleagues to renew their ACA memberships.

Ilia Guzei
Communications Committee

Chemistry Department, University of Wisconsin-Madison, Madison, WI.

Statement: As IYCr 2014 is approaching, I believe this Committe provides us with a unique opportunity to reiterate to the general public and scientific community the significance of crystallography, the role it has played in scientific discoveries and everyday life, and the importance of teaching the graduate and especially undergraduate students symmetry and crystallography. My professional pursuits are a good match for this committee's activities. As a contributor to *Reflexions* and co-editor of *Acta Cryst. Section C*, I have experience with writing and evaluating scientific manuscripts, which goes along with the committee's coordination of ACA publications and preparation of reviews of crystallographic research. I enjoy organizing meetings and workshops and have been the ACA meeting Poster Chair three times; thus, helping with the annual ACA meetings and press conferences would be second nature to me. As an amateur photographer I possess skills in videotaping, an activity that is now being taken seriously at our annual meetings when recording historical and plenary lectures is necessary. As a US IUPAC Young Observer at the 2013 IUPAC Congress in Istanbul I was excited to represent the US as a crystallographer. There are many ideas about coordinating IUCr, ACA, and IUPAC activities, one of which – crystallographic education in undergraduate colleges – is particularly appealing. I will actively work with the other members of this Committee and with these three organizations to disseminate information about the role that crystallography plays in our lives and why it is important to continue funding fundamental and applied science.

Edward J Collins
Continuing Education

The University of North Carolina at Chapel Hill, Department of Microbiology and Immunology, Chapel Hill, NC.

Statement: It is critical to provide quality resources to both novice and experienced crystallographers. I have seen an alarming trend on NIH study sections demonstrating that protein crystallography, like small-molecule crystallography not too long ago, has been relegated to a necessary, but routine technique. We must continue to educate all of our people that they are valuable voices to the greater scientific community. Everyone values the information we provide, but they appear not to understand the real problems associated with our scientific discipline. I have a long-standing interest in crystallographic education. I am the course director for a macromolecular crystallography course at UNC. I have been involved in "education" centric sessions at ACA meetings for the past seven years. Andy Torelli, Peter Horton and I have put together a website that has images that may be used for data processing and phasing. These datasets have common pathologies that can be used to learn how to either avoid or work around these pathologies. What is particularly valuable is that the software developers were gracious enough to provide tutorials for how they thought data processing and refinement should work. This approach has received excellent feedback, but should be expanded to include small-angle and small-molecule data so that a larger community can be served. I plan to work closely with the Communications Committee to make resources such as this readily available to better serve our entire constituency.

Peter Müller
Data, Standards & Computing

Director X-Ray Diffraction Facility, MIT, Cambridge, MA.

Statement: Serving the crystallographic community through the ACA SIGs and committees is important to me. As a Co-Editor of *Acta Cryst.* and as a reviewer for many other journals, I have been involved in discussions about which data should be submitted to whom at what time and in which format. As a member of this committee it will be interesting to experience similar discussions from a different perspective. I was part of a group working on a white paper on data safety and archiving to ensure the availability of current diffraction data for future generations. Among other things, we discussed a CIF-like open format for raw diffraction data where the header of every image would explain exactly how the data should be interpreted. This would allow for the integration of the data even hundreds of years from now when our beautiful methods and programs may only be of historical interest. Having all this information properly included in the raw data files could make it possible to understand what "a frame" is even if diffractometers are largely unknown when the files are discovered. This is comparable to Adobe's digital negative (DNG) format for digital photo-cameras (which are not so different from modern area detectors). DNG is, "a publicly available archival format for the raw files generated by digital cameras. By addressing the lack of an open standard for the raw files created by individual camera models, DNG helps ensure that photographers will be able to access their files in the future." This Committee should push for effort towards preservation of crystallographic data.

PUZZLE CORNER

The solution to the fall issue's DISORDERED puzzle is shown, along with a new DISORDERED puzzle.

Periodic Table of Crystallographers

To commemorate IYCr14, Joe Reibenspies, with suggestions from many others, constructed the Periodic Table of Crystallographers on the facing page. An electronic version, which can be zoomed to see the individual pictures at higher resolution, can be seen at: ***xray.tamu.edu/ptable***. How many can you identify? Why is each associated with that particular element?

The solution will appear in the spring issue.

Crystallographers in pictures identified

In the fall issue, some names were missing from captions of photos taken at the Hawaii meeting. Readers have provided identities of some of these. The "??" person in the banquet picture at the bottom of page 37 is Ranjit Deka, Dept. of Microbiology, UT Southwestern Medical Center, Dallas. At bottom right on page 51 is Erica Ollman Saphire, Dept. of Immunology and Microbial Science, Scripps Research Inst. (Thanks to Dirk Zajonc)

Frank Fronzcek.

DISORDERED

Reorganize these words to find the natural sequence

TRUEDANE	DENATURE
GYNOHERD	HYDROGEN
DIMFLOSED	MISFOLDED
AVENTI	NATIVE
FLIDUSIDE	DISULFIDE

What he called his grant to study organization of random coil

Answer:

FOLDING MONEY

DISORDERED

Deconvolute these crystallographic words to find an ordered solution

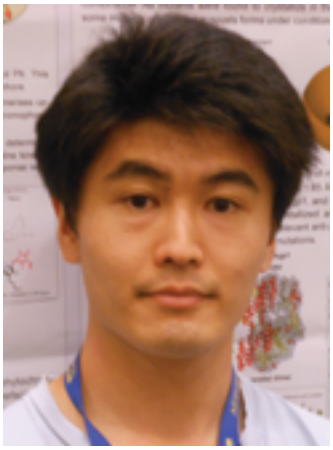
ILICITCRN	
TYROPAIL	
CUSTURRET	
DELAW	

When he texted "IYCr14", the meaning was

Answer:

Periodic Table of Crystallographers
2014 international year of crystallography
by Re I Be N S P I Es

The following notes were written by recipients of travel grants to attend the ACA meeting in Hawaii (2013). Recipients were asked to comment on their personal exeriences at the meeting: the venue, the events for young scientists, the overall program and their own presentation. They all were very grateful for the awards, and for many attendance would not have been possible without the support. These 'kids' are the future of our science - please keep this in mind and contribute generously to the ACA student travel fund.



Soshichiro Nagano

Hawaii was my first ACA meeting. I very much appreciated the diversity of the people who attended. By diversity, not just in terms of the topics, but also from the standpoint of the speakers. For example, in the *Reviewer Practices* session, talks were given by those who review the papers and that gave me a chance to see the situation from a different perspective than the one I have as an author.

The meeting also gave me a chance to speak to renowned crystallographers, as well as freely interact with the exhibitors. For me it was particularly encouraging to see the speakers at various levels in their careers. Not only could I obtain several new ideas for my own project from speakers close to my own age, but I witnessed substantial feedback from the more experienced researchers in the audience. Because I work on macromolecules I was also pleased that there were more biological delegates at ACA 2013 compared to a typical BCA meeting.

Some talks were really interesting, especially the ones covering the early history of crystallography that were very useful for a relatively young crystallographer like myself. Since such talks are not research based, therefore I don't expect the speakers would be worried about putting the talk online so why not archive them for viewing online? (Editors note: that is exactly what we are planning to do – see page 9)

I did notice that in some cases the video/audio systems were not optimal. I wish the projectors were a little larger. I understand the limitations that come with a conference held in a hotel, as opposed to BCA meetings where some talks are held in large lecture theaters of universities.

Hawaii was an exciting place, but I feel that the hotel was expensive. I guess people like me who pay their own way and/or rely on grants may be rare, but I wish more wallet-friendly locations could be chosen. That being said, the travel grant was very generous, but I wish the method of payment could be made more flexible. It was not easy to cash the check outside the US. Even by late August I had not managed to cash the check, and this impacted my finances so much that I really struggled for several weeks.

Overall, the meeting provided an excellent opportunity to exchange ideas and I would recommend attending to other young crystallographers.

Maike Bublitz

This meeting, my first at ACA, was an exceptional experience for me. I had attended other international meetings before so there were many familiar faces, which created a very good networking environment. The program was almost overwhelmingly diverse, giving me the opportunity to get a glimpse into many research fields beyond my own. I particularly appreciated the *Career Odyssey Panel* discussion. Many of the presentations (both lectures and posters) were closely related to my research on the crystallography of membrane proteins and the use of XFEL radiation. Being able to interact with the scientists working at the leading edge of my research field was of great value to me.

Hawaii is of course an amazing location, which made the experience even more special. Being lucky enough to win a free surfing lesson – sponsored by Rigaku – was another once-in-a-lifetime experience I will never forget. I hope I will be able to attend next year's conference in Albuquerque.

Colleen Lopez

I am a graduate student at Cal State University San Marcos in San Diego, California. My experience with the ACA conference was amazing. I most enjoyed the opportunity to give a lecture on my work presenting a one-hour experiential lesson on crystallization and diffraction to 5th graders in the San Marcos School District. The lesson was based on the California core science standards for 5th graders as stipulated by the California State Board of Education

I am incredibly passionate about my work and found the experience of sharing it with a room full of professionals with similar interests very rewarding. Many of the attendees offered ideas on how I could improve my project and find ways to share the concept with other individuals and school districts across the country. I spent time walking around during the poster sessions and thoroughly enjoyed talking to all the other aspiring students like myself. It was also very interesting to meet and listen to some of the most brilliant minds in the field. I was very fortunate to actually meet some of them and learn from their experiences.

The conference itself was incredible, but if I had to give one suggestion for further improvement I would suggest considering ways to increase the undergraduate student participation. Attending conferences like the ACA as an undergraduate student is a great educational experience. Such conferences allow students to practice their presentation skills and provide them a forum to meet experts in the

field, and in this way they will undoubtedly receive advice on both their education and potential future career paths.

While I am not currently a member of any professional scientific society, my positive experience in Hawaii has motivated me to seek such opportunities in the future. As my studies progress, I also see myself joining such societies to keep abreast of the many advancements in my field of interest.

Ghazala Sadiq

I was able to to network with industrialists and academics and by talking about my work I gained insight into a problem I am currently encountering with 'crystal twinning'. I particularly enjoyed the sessions on *Materials Discovery, Complementary Methods in Crystals and in Solution* and *Contemporary Crystal Engineering* as they involved the discovery of new functional materials.

I presented a poster entitled *Concerning the crystal chemistry and enantiomer separation of TAK* allowing me to discuss my work with my peers, generate new ideas and answer many questions that had not previously occurred to me. I had a number of discussions about the objective of my project and whether using additives to control the enantiomeric outcome was feasible. Pharmaceuticals are perhaps the most valuable materials known to mankind, and there are important intellectual property, regulatory and efficacy implications if one is able to discover new compositions of matter for active pharmaceutical ingredients (APIs). Generally I found my research to be well received, and there was interest in my results. I also had the opportunity to view other students' posters and discuss their research with them. I hope that I asked useful questions. I also found the exhibitors interesting, not only for the new technology that they presented, but also for highlighting the range of jobs available in science.

Maxime Cuypers

I have completed my first post doc and am currently looking for employment in biophysics with new perspectives. I enjoyed the overall mood of the entire meeting. The discussions were always pleasant and constructive. The diversity of topics covered often made it difficult to choose which session to attend. I did notice that the attendance of sessions of presentations of specific subjects of biophysics (i.e. neutron based presentations) that took place in large rooms was significantly lower than that of broader, more general interest presentations that were occurring in smaller rooms. Many of those switching sessions, depending on interests, had to stand in the back, which was uncomfortable. It would perhaps be good to take the "more general interest" presentations into consideration in order to avoid as much as possible this inconvenience in future meetings. I realize that organizing the sessions is a lot of work, however, rethinking the location of sessions would be an easy improvement. Also, the layout of the poster boards hindered access to the middle-alley posters (when the sessions were crowded). Some posters remained inaccessible.

I have been a member of the BCA (British Crystallographic Association), and this year I applied for the first time to the ACA. Choices have to be made each year depending on the conferences we plan to attend because, for a post-doctoral fellow in the present economical context, it is difficult to justify attendance to many different crystallography based conferences during the same year.

I would like to continue my ACA membership, since as a professional I have a need for up-to-date information and knowledge. I believe it is crucial to remain well informed about new developments and discoveries in research and that societies can play a great role in this regard.

I have been a member of the ACA since 2008 and previously attended the meetings in Toronto and Boston. As I am studying crystallography the ACA meetings are the ideal places for me to meet people and to learn new tricks, techniques and information on macromolecular crystallography. It was very important for me to attend the meeting this year as it is the final year of my PhD studies,

Agnesa Shala

and thanks to the travel grant and my supervisor I was able to. The highlight of the meeting for me is always the poster sessions, where whether you are the presenter or the spectator you can get overwhelmed with useful information. The beautiful setting of Hawaii helped make the meeting an even more amazing experience. I will continue being a member of the ACA community where the possibility of learning from your peers is never ending.

Hilary Stevenson

For me, one of the best parts of the ACA meeting was having the opportunity to present a talk in the *Femtosecond X-ray Pulses: Biological Applications* session. This gave me the opportunity both to speak about our new method and also to obtain interesting and engaging feedback from

the audience. Additionally, the presentation paved the way for several other interesting conversations with scientists I wouldn't have otherwise met.

A minor suggestion for the future would be to facilitate communication between graduate students before the conference. That way, students could coordinate events and activities. I make this suggestion because several students expressed regret that they didn't better plan to take advantage of what Honolulu had to offer.

I do plan on maintaining my membership in ACA. The connections and opportunities I have made through the ACA have been invaluable, and I hope to continue them.

Rachel Sullivan

As a first time attendee at an ACA meeting since becoming a member more than 8 months ago, I was pleasantly surprised at how many research areas were being covered.The posters and talks covered areas from materials for a sustainable future, metal-organic frameworks, dynamic and flexible structures in biomolecules, to structural enzymology and contemporary crystal engineering.

The contemporary crystal engineering session had several talks relevant to my PhD, including co-crystal design using the CSD by Peter Wood. This talk was particularly complementary to the new skills I had gained at the CSD workshop earlier in the meeting and it reinforced how useful the CSD software is to individuals who either design new systems, run crystal structure comparisons, or do fragment searches.

My 'favorite' talk was by Aurora Cruz-Cabeza, who worked with Joel Bernstein on conformational polymorphism. Polymorphism is of particular importance to my PhD as the small organic molecule on which I have been working on is a dimorphic enantiotropic system - not to mention the implications of polymorphism on the development of stable active pharmaceuticals in industry. Cruz-Cabeza's talk described the calculations that led to the development of a general set of rules that could be used to classify any molecule. This was particularly rewarding, as I was able to follow up my interest in her work and discuss it further by attending another conference in Oxford later on in August, where she was also presenting.

I thought the conference could have been improved if there were more talks on small molecules with less emphasis on proteins.

Emma DeWalt

I gave an oral presentation at the meeting that was titled:*Polarization-Resolved Nonlinear Optical Imaging for Protein Crystal Detection and Crystal Quality Assessment* in the *Complementary Methods in Crystals and in Solution* session. My talk focused on new developments in nonlinear optics for sensitively detecting small protein crystals, as well as methods to determine the quality of a crystal. I feel that my talk went well, and I received a question from the audience at the end.

Not only was Waikiki beautiful, but the conference rooms at the hotel were laid out intuitively and provided ample space for the talks. I also liked the diversity of topics presented. My only suggestion is to have clocks or timers available in all of the rooms, to ensure that there is time at the end of the presentations for questions and further discussion.

I am currently a member of ACS (American Chemical Society), SAS (Society for Applied Spectroscopy) and ACA. I plan on continuing my membership in ACA.

Karolina Majorek

I am a new ACA member and this was my first meeting. I really enjoyed the great diversity of the program, the informative talks, poster presentations, and the wonderful location. I also attended the CSD workshop, which will definitely help me make the most of the database. I think even more workshops should be organized in the future, as they provide a great opportunity to get first-hand knowledge about the tools available in crystallography. I appreciated the vendor exhibits, as they let me get up to date on the newest equipment on the market. I enjoyed the *Career Odyssey Panel* and the YSSIG Mixer. It was a great idea to give students the opportunity to hear from scientists following different career pathways: both in academia and industry. Young scientists like me, who are taking our first steps into the field, know that we should get to know more experienced scientists, but we are often shy or simply do not know whom to approach to get answers to our questions. I think more panels of this type should be organized, as they make it much easier to learn about our possibilities, and about the different ways to achieve our goals. It was a privilege to present a talk on my research among so many distinguished crystallographers, and I think more students should be given that opportunity. Being approached by other scientists, even days after my presentation, was extremely nice and rewarding, and it assured me that the work I'm doing is important. I look forward to attending ACA meetings in the future.

I really enjoyed meeting different people and talking to them about my research. I also appreciated the poster sessions and the one on one conversations. I currently belong to Sigma Xi, ACS, and ACA, and I plan to continue in all three.

My research consists of work done on Pt complexes that change structurally upon

Amie Norton

changes in environment. For example, the complexes I work with are vapochromic so that when exposed to vapor, they change color which in turn correlates to changes in structure. I use single crystal x-ray diffraction to determine the changes in structure. When presenting my poster on a Pt complex, I enjoyed getting to talk about the phase change that was going on in my system. I learned a lot about phase changes and about comparing polymorphs. One thing I learned was that mercury has a comparison function in order, to look at two polymorphs.

The feedback I received from the poster prize judges, my peers and other attendees was very positive. I gained a new appreciation for crystallography from listening to talks on the unique work being done in the field. I also enjoyed being able to share and trade ideas.

I am a postdoc at the University of Amsterdam, the Netherlands. I am interested in understanding the organic solid-state using a combination of database analysis tools, computational chemistry and experimentation. Iamcurrently studying topics such as conformational polymorphism and tautomerism in molecular crystals.

Aurora Cruz-Cabeza

I really enjoyed the GSAS-II workshop. It was a great way to learn new things and interact more closely with other meeting participants. I would recommend the workshops to future students and postdocs. They are all nicely organized and cover a wide range of topics.

I presented my work on conformational polymorphism as part of the *Etter Early Career Award Symposium*. and I received lots of nice and useful feedback.

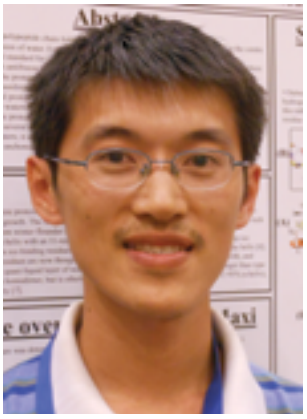
My favorite sessions of the meeting were *Contemporary Crystal Engineering* and *From Knowledge to Design: Data Mining in Materials Chemistry*. .I especially enjoyed the very nice mixture of industrial and academic contributors in the latter and the wide variety of talks in the former.

To end a nice meeting, I guessed the number of jellybeans in the ALS water bottle, which I was then able to take home with me!

The location was beautiful but also very expensive. I suggest arranging the meetings in more affordable locations in order to adapt to the current lack of funding.

I am a member of the ACA and plan to continue my membership.

I am a PhD student in Peter Davies' lab at Queen's



Tianjun Sun

University. This was my second ACA meeting, and I had a fantastic experience. There were many interesting sessions, and some were quite eye-opening for me. I learned about future directions for protein crystallography. Many people came to my poster and gave me a lot of good ideas, which I will try in the future. There were also very good social activities for younger attendees where I got the chance to know students from all over the world as well as experts in the field. Of course, the location was perfect – it was my first trip to Hawaii and I am looking forward to attending more ACA meetings in the future.

I am not currently a member of any professional scientific society, but I am interested in membership in ACA as I hope it can help me get to know more about the community of crystallographers.

Attending the meeting in Hawaii was an amazing experience for me - the beautiful scenery, cool structures and new techniques impressed me deeply. I was pleased to see so many top scientists giving talks. Some of the sessions I liked best were *Membrane Protein Scattering* and *Host Pathogen Interactions* because they were the closest symposia related to

Yong-Liang Jiang

my own research. In addition, I also learned new techniques for structure determination and validation, neutron scattering, and femtosecond x-ray pulses. As a first-year postdoc, I am not a member of any professional scientific society but I think being an ACA member would be good for my professional growth. I would like to see the ACA provide more opportunities for young scientists and hope that the ACA family will become better and better!

Sonia G. Thangavelu

I really liked the diversity of talks, ranging from small molecules to proteins. Since we predominately characterize small molecules and MOFs using x-ray crystallography, it was refreshing to hear talks outside of our respective field. Another event that I really enjoyed was the social mixer for young scientists. It was a

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great networking opportunity not only as a way to meet other graduate students but also to engage with established professors. I think it would improve future meetings to encourage the participation of more young scientists to come to the planning meetings. It is quite frustrating when students complain about certain issues (such as research funding/career options) and then do not attend the planning meeting to express their opinions. We need to better market the YSSIG at the meetings, perhaps by having more sessions focused on young researchers. I am a member of ACA (application currently in progress) and also a member of ACS.

Shuaiqi Guo

I am a graduate student studying the structure/function of antifreeze proteins in Peter Davies' lab at Queens University. I had a great time at the meeting. It was an eye opening experience and a chance for me to see cutting edge research from all over the world, and an excellent opportunity for me as well, to meet with experts and my peers in the field of crystallography. I was also very fortunate to be selected as a Pauling Poster Prize winner. This award added to my overall experience, and it will serve as a great incentive for me to work harder in the future.

I think the young scientist mixer event was great. It would be nice to have a few more events just like that if possible (e.g. a short trip to a local tourist attraction).

Shane Caldwell

This was my first ACA meeting and what a venue! I was glad to have the opportunity to take part in such a large assembly of multidisciplinary expertise from around the world. I appreciated the opportunity to rub shoulders with the greats of crystallography as well as to meet many of my peers, who work on such similar, and yet also diverse, research problems. Many talks and poster presentations were very compelling, especially all of the excellent research in structural microbiology and immunology. During my poster presentation I received great feedback, especially some excellent suggestions on how to better handle small-angle scattering data as well as suggestions about other experiments I can conduct with my system. What I liked best about the meeting was the friendly atmosphere, the amazing ACA staff, and the location. I would have like to see more coffee, and the AV/acoustics in the big room were pretty rough. I am a member of the ACA and plan to continue as a member and look forward to my next meeting already!

Christina Zimanyi

Giving a talk about my *exciting structures* was a great experience. I really enjoyed the award talks by Tom Koetzle and Alex McPherson and George Phillips' address at the banquet. As a relatively young crystallographer, it's great to have such an accessible way to learn the history of my field.

My favorite part of this meeting was the mix of talks, methods development, applications, and basic science. However, often these sessions overlapped, and that leads straight to my least favorite part of the meeting, which was the number of interesting sessions that overlap. I had to miss a few talks due to double booking. I definitely plan to continue my ACA membership, mainly to attend the annual meeting. This meeting was great for networking because attendees from both academia and industry were friendly and willing to talk about their work. I hope to return next year and be more involved in the YSSIG.

For me the two most enjoyable aspects of the meeting were being able to engage with the American community, and their the diverse areas covered by the various sessions. As an early-stage researcher it was incredibly useful to learn about work in the immediate area of my own project, topics

Andrew Cairns

outside this, and everything in-between! My work explores the structure-property relationship in materials, and in particular how disorder affects physical properties. I was able to see some very interesting talks throughout this meeting related to this—from PDF studies of nanostructured materials to new advances in high-pressure neutron diffraction.

I enjoyed very much the *Etter Early Career Award Symposium* and the YSSIG Mixer. One idea (imported from the BCA and ECM) might be to combine this sympoisum, the mixer, and a poster session into a separate event before the main conference, or early on in the proceedings, so as to encourage discussion and interaction between early stage researchers who might not know each other. I belong to the ACA, the ACS and the BCA and plan to continue in all three.

The ACA meeting was great partly because of the venue, but mostly for the scientific program. I had an opportunity to expand my knowledge and interact with various researchers as a first-time attendee. My interactions at the poster sessions were interesting. I got feedback on my own research that was very valuable to me.

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Ji Young Yoon

Also visiting the exhibitors, I had the opportunity to ask about their latest equipment and techniques. The event for young scientists gave me a good opportunity to network with other people working in different areas. Above all, the SAXS workshop was very useful to me. I was not familiar with that field, but I learned a great deal about it through the workshop. I look forward to attending many more meetings .

Oriana Fisher

This both my first ACA meeting and the first opportunity I've had to present my work at a conference. I was impressed by the number of talks and by the breadth of topics they covered. I liked being able to attend talks on topics closely related to my own research, while also having the opportunity to learn about topics that were not as familiar to me (including the SAXS workshop). In fact, it was sometimes difficult to choose which session to attend, as often there were multiple talks going on at the same time that seemed to be of interest. Presenting a poster was also a great opportunity to discuss my research with other people in the field and to get feedback from them. Of course, this year's location in Honolulu was a very welcome chance to leave New England for a little while, and I enjoyed getting to see some of Hawaii while I was there as well. Although this was my first year as a member of ACA, I plan to continue my membership.

Gyanendra Kumar

This was one of the best meetings I have ever attended. It was also nice that a lot of the abstracts submitted by young scientists were chosen for oral presentation. I personally loved the sessions that focused on advances in methods/ techniques in macromolecular crystallography and structure determination. I hope to see more of these kinds of sessions at future ACA meetings.

Halls in hotels are not built for lectures; the flat floor and low ceiling makes it difficult for the audience sitting behind the first two rows to see the slides. It may be a good idea to hold the meetings at convention centers or lecture hall complexes.

I am currently a member of the ACA, the ACS and AAAS and plan to continue to belong. I would like to see more workshops, and summer schools on theory and practice of macromolecular crystallography.

Paul Musille

This was my second ACA meeting, and I was honored to have the opportunity to present my work to an international group of scientists with broad research interests. As this was my first visit to Hawaii, it was also a great opportunity to explore a new place. Like my last experience at an ACA meeting, this meeting offered a huge range of topics that allowed me to both keep up with research close to my field and to gain knowledge about more distant fields. Additionally, the exhibit show was a great place to see all the newest technology and advances in techniques and equipment.

As a young scientist the ACA offers great opportunities to both socialize and network with other young scientists, senior researchers, and industry representatives. This remains one of my favorite parts of the meeting. Very few other venues offer field-specific social and networking opportunities that are so varied and catered towards young scientists. I hope to have many more opportunities to travel to and present my research at ACA meetings!

Robert Kirchdoerfer

I found the meeting to be an excellent forum to exchange ideas. The people who visited my poster were incredibly supportive in offering their own experience with difficult crystallization experiments, and I look forward to putting their ideas into action. The sessions discussing protein model quality will shape how I prepare and validate my own protein models and present my work in the future. I also enjoyed the many updates on synchrotron beam line instrumentation and look forward to implementing these new tools during our next beam time.

I would have liked to have seen more discussion on protein sample preparation and crystallization during the sessions, to discover new ideas for making and evaluating samples for crystallization.

I am currently a postdoctoral member of the ACA and look forward to continuing my membership. I strongly hope that the ACA will continue to support the development of young scientists and to educate them in the best practices in crystallography.

Hande Öztürk

I am very happy to have attended this year's conference, which allowed me to meet with many of the top scientists in the XRD and crystallography fields. During the coffee breaks I had a chance to talk to and question the authors of articles I have read, which was very helpful.

In addition to the workshops and the oral sessions, the poster sessions were extensive as well. I had the opportunity to have an idea of the projects that were being worked on by young scholars in my field and to see future trends in crystallographic research going on in different parts of the world. One suggestion I have concerns the poster sessions: In my opinion, for such an impressive number of attendees, we needed a bigger room for the poster presentations. Also for future meetings, it would be a good idea to categorize the posters according to their topics and place them accordingly so that visitors can take advantage of the limited time most efficiently.

Currently, I am not a member of any professional scientific society. I am starting to learn the focus of different communities in my field and ACA looks like a potential candidate for me. The main reason is the closeness of its focus to my research area. In terms of our needs as young scholars, I think regional meetings and scientific workshops always serve us well in order to network and increase our knowledge about different subfields. The proceedings from these meetings can give the organizers useful suggestions for upcoming conferences. Looking forward to attending the ACA meeting in 2014!

Vjekoslav Strukil

A few months ago, I was very pleased and excited to find out that I had been awarded an ACA travel grant intended to cover my expenses for my trip from Montreal, Canada to Hawaii. By actively taking part in the *Contemporary Crystal Engineering* session I was able to present parts of my postdoc research conducted in the Friscic group at McGill University and discuss the results among the assembled group of established scientists. It was a unique opportunity to learn more about the cutting-edge research in the broad field of chemical crystallography and also, more specifically, the advancements in sold-state chemistry and powder and small molecule diffraction. The scientific program was rather busy, but its diversity and audience-oriented sessions enabled participants to pick up topics of their interest. As I have only recently entered the field of x-ray crystallography, the knowledge I gained is definitely becoming an integrated part of my everyday research. The positive impressions I experienced during the meeting will encourage me to further exploit the possibilities of career development through ACA membership. Apart from extending my chemistry-related skills, meeting other people with whom one can share similar professional interests is always an exciting benefit of participation at an event such as this, and it greatly contributed to my personal development, especially in the breathtaking landscape and beautiful surrounding of the Hawaiian Islands.

Michael Thompson

In addition to being in a beautiful location, the meeting provided an excellent opportunity to broaden my understanding of the field of crystallography. I always enjoy going to conferences and hearing about developments and research from my own field (protein crystallography), but the ACA meeting was the first time I attended a meeting where there were experts in other crystallographic disciplines. I enjoyed listening to some presentations that were outside of my own field, giving me a deeper appreciation for the breadth of techniques and challenges that exist in the world of crystallography. Also, this was the first time I was given the opportunity to speak about my own research. Although I was nervous, I found that the meeting attendees were relatively unintimidating and friendly, and I left the session with many constructive and encouraging comments. I had a fantastic time at the meeting and, while I am still very new to the ACA, I look forward to exploring the many opportunities that go along with membership.

Jennifer Wierman

The meeting was a breakthrough for me. After giving my talk on the application of graphene in crystallography, I had numerous chances to sit down with experts within the field to dream and scheme about the future of microcrystallography and how graphene could alter the protein-crystal data collection set-up. The breaks became indispensable to free-flowing creativity, problem solving, and collaborative kickoffs. Projects with fellow graduate students, and beamline scientists, and even with industry materialized over coffee and umbrella-laden drinks. In short, I felt as if I were a part of the community, and helping to advance research on a larger scale. And to add to this euphoria, you can't get a much better setting than

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Hawaii. While the beaches may have held a level of distraction, gathering experts in the field with pineapple drinks in hand and a view of the ocean didn't slow progress.

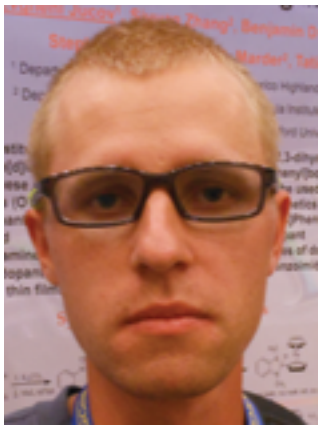
I wish I could have cloned myself and visited every interesting, yet overlapping, session. My only suggestion would be to make sure sessons in similar areas of interest don't overlap. There were several talks I missed due to a timing conflict. My goal is to encourage more of my peers to attend the meetings in the future. In this way, I can pirate their notes from those sessions! I belong to both the ACA and the Biophysical Society and plan to continue my membership.

Larissa Romanello

The things I liked most at the meeting were the financial support, the great themes of the lectures that were very interesting and varied, and the ease in establishing contacts with other researchers and students.

However, the financial assistance for the trip was paid by a check from a bank that does not exist in Hawaii so I had great difficulty in cashing the check at a currency exchange office, which charged a rate of nearly 10%. In my country the rate would be even higher. I think that it would be more helpful if we could receive assistance in a more direct way, such as the payment of the hotel.

I am not currently a member of the ACA because, as a student, my financial resources are limited, however, I intend to become a member soon.



Evgehni Jucov

Without the travel grant, I would not have been able to attend the meeting and visit one of the most beautiful and unique places on Earth – Hawaii. The meeting gave me an invaluable experience to present my research, to communicate with other scientists, and to meet with some of the most famous people in crystallography, such as Ilia Guzei, Allen Oliver, *et al*. The overall organization of the lectures and poster sessions was very effective for all the participants, and I'm looking forward to being able to attend the next Meeting in Albuquerque.

This was my second ACA meeting and, just as with the last, it was a great experience. I attended the workshop on GSAS-II and really benefitted from the work Brian Toby and Bob Von Dreele did putying it together. I was very pleased that I was selected for a an oral presentation. I met a number of colleagues in my field who were happy to make suggestions. As a member of ACA, ACS, and APS, among others, I often find meetings oversized and cumbersome. However, the ACA meeting being limited in size and in one hotel makes it easy to move from talk to talk without having to miss things you might be interested in. One thing that I would change is potentially providing a shuttle service if the student/postdoc hotels are separated from the main site. I was also disappointed that there was no *Would you Publish This?* session; I really enjoyed the discussions in that session last year. I am looking forward to next year and excited to see how the ACA is involved in the IYCr.

Kevin Gagnon

Attending the meeting was an amazing opportunity and a fantastic experience!

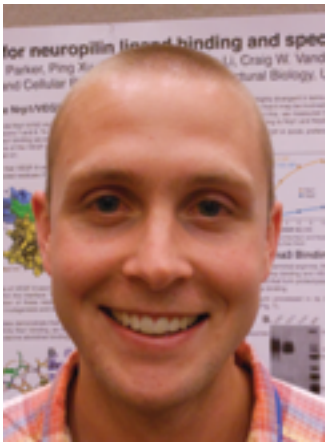
I really enjoyed the poster sessions, both presenting and visiting with other researchers. At the time of the meeting I felt like I was in a bit of a rut with my own work. Talking with fellow crystallographers and scientists gave me not only new perspectives on how to proceed but also a renewed fervor for my project. Additionally, the session on structure validation was not only insightful, but a great opportunity to hear from some of the leaders in the field in a more relaxed environment. As a young crystallographer it was incredible to hear them talk about how the latest problems in data analysis and validation are being solved. It is one thing to learn about the method in a classroom, and quite another to be in a room hearing how the methods of tomorrow are being hashed out. Truly amazing!

Kate Helmich

I don't have any suggestions on how to improve the meeting as a whole, but one thing that might make it more beneficial for young scientists might be to have more slots on the program, or even an entire session, devoted to student talks and to provide additional opportunities for students to present their work. The two student lecture award talks I attended were really great, and I would have really enjoyed the opportunity to hear from more of my peers in the field.

I am currently a member of the ACA and plan to continue this in future years.

For me, the most useful and enjoyable part of the meeting was the BioSAS Workshop. Through this workshop I was able to interact with many of the people who are leaders



Matthew Parker

in the biological small angle scattering field, providing me with critical resources and contacts for integrating SAS into my science. Additionally, it is very helpful that the resources used in the workshop, such as presentations and sample data sets, were made accessible to workshop attendees. I would like to see more formally organized opportunities for trainees to network among potential employers, including both academic and industrial organizations. I am currently a member of the ACA, the American Heart Association (AHA), the American Society for Biochemistry and Molecular Biology (ASBMB), and the ACS. I plan to maintain my membership with the ACA.

This meeting was a series of firsts for me: my first ACA meeting, my first time in Hawaii, and my first time being invited to present my own research at a conference. One of the things I enjoyed the most was how much I learned outside of x-ray crystallography, in addition to expanding my crystallographic knowledge. Despite it being a technique based conference, I found many researchers in the same field of biology as me (antibiotic resistance/tolerance), which allowed me to learn a lot about other

Dana Lord

bacterial systems related to my own project. Furthermore, I acquired some tips & tricks on difficult protein purifications as well as strategies for improving crystallization, all of which gave me new ideas for my thesis. I also thoroughly enjoyed the events for young scientist which helped me meet a lot of new people and feel more comfortable at the conference. I was the only student from my university who attended, and I previously had not known many people in the crystallography field. I definitely want to pursue structural biology for my post-doc, and the conference provided an invaluable platform for me to network. If I could suggest one change to improve the meeting it would be to avoid scheduling similar sessions during the same time block. For example, there were three sessions that attracted my interest on Sunday morning. However, many of the talks ran over and the times did not align with the other on-going sessions. Thus it was very difficult to visit multiple sessions during one time block. All in all, my experience with the ACA has been extremely positive and I plan on continuing my membership.

As I am in the middle of my graduate studies, the

Alan Wong

travel grant covered part of my flight and allowed me to present my latest research on the structural biology of a metalloprotease using x-ray crystallography. Attending the meeting also allowed me to learn more about techniques in the field of crystallography. I especially enjoyed the methods and development talks that showcased the use of crystallography and related techniques in new fields of research. I also enjoyed the poster sessions, where I met with individual scientists and discussed their research. The 2013 ACA meeting was a memorable experience, I will continue my membership with the ACA and look forward to attending future meetings.

Not only I did I learn plenty of new, interesting information, but I also got the chance to meet remarkable scientists. As a young scientist who has just started learning about the field of crystallography, I enjoyed every single talk and poster. The *Etter Early Career Award Symposium* was very interesting to me and especially the talk given by Aurora . Cruz-Cabeza that gave me a better understanding of what conformational polymorphism is. She also included some really good information about whether conformational change can be identified using

Maria Karakasheva

structural information alone. I also enjoyed the *Structural Enzymology* session. I was able to learn more about structures that are determined using x-ray crystallography and complementary methods. The *Career Odyssey* session was also helpful, especially for young scientists like me, because it involved participants who talked about the variety of crystallography-related careers and the opportunities currently available.

I liked the poster sessions a lot because people were able to communicate with each other and share their opinions about the topics that interested them. This time of the day was definitely the best time for interacting and learning.

I do plan to continue my membership in the ACA because I think this association is a great part of the field I am interested in

I am a postdoctoral scholar in the Andrej Sali group, University of California, San Francisco (UCSF). This was my second time attending the ACA meeting, following my first one in New Orleans back in 2011. As was the case back then, I really enjoyed interacting with lots of people from various fields. Everyone in the conference was quite open to share his or her ideas and scientific progress in detail. I got interesting feedback during my presentation which

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Seung Joong Kim

should be of great benefit in my future research. It was a great honor to have direct discussions with the big names in the field while presenting my poster. The poster sessions were well organized and covered many interesting topics; thus it was really fun to see all of them and talk in person to the authors. I thought that the SAXS workshop was a huge success and delivered both fundamental basics and practical applications of the SAXS experiments. Having this kind of workshop again would be very helpful to any people in the SAXS field. For last, everyone loves Hawaii and it was another unforgettable treat and lots of fun to be in Honolulu! I am very much looking forward to next year.

Thank you for considering my work worthy of an award! My favorite part of the meeting was being able to learn about new developments in synchrotron radiation technologies, and particularly those related to femtosecond x-ray nanocrystallography. This relatively new area of research is exciting and potentially a great tool for biochemists working on difficult targets. While I did appreciate hearing from junior investigators, I would also have liked to have heard more talks by senior scientists. I plan to continue my involvement with ACA in the medium to long-term future. Keeping in touch with evolving concepts in x-ray crystallography is extremely important for conducting cutting edge research. The ACA should continue to inform its members of major advances throughout the year using various communication media.

Jean-Philippe Julien

The meeting was a wonderful experience. The session topics, from proteins to inorganic molecules were diverse and allowed attendees to never feel excluded. As a computational researcher, hearing from great speakers like Tom Terwilliger and Paul Emsley, who actively work on software that many of us use on a daily basis, was enlightening. To my great surprise the SAXS sessions were pretty instructive for a non-specialist like me. I'm currently an ACA member and will probably continue it for next year. The location was also delightful, providing a relaxing environment after a day at the meeting. I strongly encourage the ACA to keep on the same track in terms of organization, topic choices and scientific quality. I would like thank the organizers, and the *Computational Tips & Tricks* session chairs Louise Dawe and Jason Mercer, for giving me the opportunity to give a talk..

Julien Jorda

What's on the Cover

The cover of the winter issue of ***RefleXions*** reflects the cover of the first issue of the new ACA/AIPP (AIP Publishing) journal *Structural Dynamics* featuring the first paper to be published.

Ultrafast structural and electronic dynamics of the metallic phase in a layered manganite: L. Piazza[1], C. Ma[2], H. X. Yang[2], A. Mann[1], Y. Zhou[3], J. Q. Li[2] and F. Carbone[1] Struct. Dyn. 1, 014501 (2014); ***http://dx.doi.org/10.1063/1.4835116***

[1]Laboratory for Ultrafast Microscopy and Electron Scattering, ICMP, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland, [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, [3]Department of Condensed Matter Physics, Brookhaven National Laboratory, Upton, New York 11973, USA

Abstract: The transition between different states in manganites can be driven by various external stimuli. Controlling these transitions with light opens the possibility to investigate the microscopic path through which they evolve. We performed femtosecond (fs) transmission electron microscopy on a bi-layered manganite to study its response to ultrafast photoexcitation. We show that a photoinduced temperature jump launches a pressure wave that provokes coherent oscillations of the lattice parameters, detected via ultrafast electron diffraction. Their impact on the electronic structure are monitored via ultrafast electron energy loss spectroscopy, revealing the dynamics of the different orbitals in response to specific structural distortions.

Cover legend: Electron diffraction pattern from an orbitally ordered bi-layered manganite, for different femtosecond laser pump powers. The different panels show the evolution of the orbital stripes (visible as satellites of the Bragg diffraction peaks). A 90 degree rotation of the stripes is evidenced in the bottom right pane.

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Cele Abad Zapatero, Maike Bublitz, Chris Cahill, Majed Chergui, Abe Clearfield, Ed Collins, Aurora Cruz-Cabezo, Maxime Cuypers, Bridget D'Amelio, Paul Davie, Emma DeWalt, Graciela Diaz de Delgado, Joe Ferrara, Kevin Gagnon, Majed Gergui, Ilia Guzei, Kate Helmich, Mike James, Yong-Liang Jiang, Julien Jordan, Evgehni Jucov, Jean-Philippe Julien, Maria Karakasheva, Seung Joong Kim, Robert Kirchdoerfer, Colleen Lopez, Dana Lord, Karolina Majorek, Chris McMahon, Peter Müller, Soshichiro Nagano, Amie Norton, Allen Oliver, Honde Ozurk, Matthew Parker, Chiara Pastore, Virginia Pett, Larissa Romanello, David Rose, Ghazala Sadiq, Amy Sarjeant, Agnesa Shala, Charlotte Stern, Cheryl Stevens, Hilary Stevenson, Vjekoslav Strukid, Rachel Sullivan, Tianjun Sun, Michael Thompson, Brian Toby, Bob VonDreele, Jennifer Wierman, Alan Wong

Cartoon on Page 22 from Nearing Zero by Hank Kim at ***www.lab-intio.com***

Nominations for 2015

ACA Awards: Nominations for the ***Warren, Buerger***, and ***Etter Early Career*** awards are due by May 1, 2014. Nominations for ***ACA Fellows*** are due February 28, 2014.

ACA Offices and Committees: In the fall of 2014 we will elect a new Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 15, 2014. Members of the nominating committee are George Phillips, Carrie Wilmot and Victor Young. Full details describing the criteria for all ACA awards and offices can be found on the website.

2014 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds. ***NOTE: It is now possible to renew online.***

ACA website: www.AmerCrystalAssn.org.

Send all nomination suggestions to: Marcia@hwi.buffalo.edu

FYI: The AIP Bulletin of Science Policy News

FYI summarizes science policy and budget developments in Washington affecting the physical science community. Summaries are issued two or more times every week. *FYI This Month* is distributed on a monthly basis, briefly summarizing major developments that were covered in more depth in *FYI*. Electronic subscriptions to *FYI* and *FYI This Month* are free; they are provided by AIP as a service to the science community. Subscribe at ***www.aip.org.***

Some of the latest *FYIs* include:

New Study on Student Performance in Math and Science: STEM education is seen as being directly associated with US competitiveness and is closely tied to employment trends. While many studies show student performances, the results of a recent study paint a picture of where US students place on an international scale.

National Science Board releases STEM Education Data and Trends: The National Science Board recently released two tools relevant to the biennial report, *Science and Engineering Indicators* (SEI). A website based on the SEI allows users to access data from the report related to student learning. The NSB also recently released another tool providing mobile access to the SEI report, the Science and Engineering Indicators Digest, and two companion reports.

House Science Subcommittee Hearing on New DOE Office of Science Bill: A draft bill now being considered would authorize spending levels for the DOE Office of Science. It is called the *Enabling Innovation for Science, Technology, and Energy in America Act* or the EINSTEIN America Act. The bill would provide program direction for basic energy sciences, advanced scientific computing research, high-energy physics, biological and environmental research, fusion energy science, and nuclear physics research.

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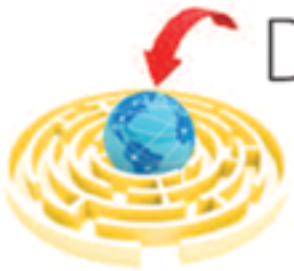

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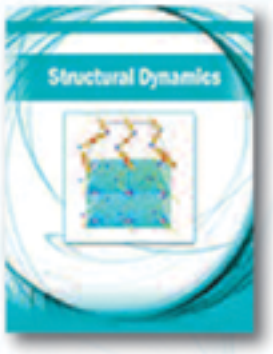

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Opportunities with New Sources – Chair: Soichi Wakatsuki

SAS and Fiber

Pathological Fibers: Prions, Amyloids & Friends – Chair: Joseph Orgel

YSSIG

Etter Early Career Award Symposium – Chair: Yulia Sevryugin

Career Odyssey Panel – Chair: Martin Donakowski

Blackboard Sessions: Data Processing with the Pros – Chairs: Andrew Torelli & Ed Collins

Small Molecule and Service

Computational Chemical & Biological Crystallography: Complementary Methods Bridging the Divide – Chair: Jason Mercer

Would You Publish This? – Chairs: Christine Beavers & Kevin Gagnon

Cool Structures – Chair: Shao-Liang Zheng

Industrial, YSSIG and Biomac

Industrial Research from Young Scientists – Chairs: Peter Wood & George Lountos

Immunology of Cancer – Chairs: Sherry La Porte & Steve Almo

Materials, Neutron and Powder

Discovering Emergent Phenomena and Magnetism with Neutron and X-Ray Powder Diffraction – Chairs: A. Liobet & B. Campbell

Producing & Transporting Energy: Thermoelectrics, Superconductors, Photovoltaics & Light Harvesting – Chair: M. McGuire

Instrumentation & Methods for Sructure Solution of Nanosized Materials – Chairs: Pavol Juhas & John Helliwell

Disorder & Inhomogeneity in Complex Materials Probed by PDF – Chair: Ram Seshadri

Earth / Environmental Sciences – Chairs: Claudia Rawn & Olaf Borkiewick

Innovative Ways of Finding Atoms from Powder Diffraction Data – Chairs: Graham King & Peter Stephens

GIG, Small Molecule and Service

General Interest – Chair: Graciela Diaz de Delgado

Engaging Undergraduate Students with X-Ray Crystallography: Curriculum Development, Undergraduate Research, Equipment Acquisition and Strategies for Faculty Success – Chairs: Kraig Wheeler & Roger Rowlett

Neutrons and Biomac

Neutrons in Biology: New Instruments and Structures – Chairs: Zoe Fisher & Andrey Kovalevsky

Neutrons in Biology: Structural Enzymology – Chairs: Zoe Fisher & Paul Langan

SAS, Biomac and Canadian Division

Solution Structure & Dynamics of Biomacromolecules (I) – Chair: Thomas Weiss

Solution Structure & Dynamics of Biomacromolecules (II) – Chairs: Gerald Audette & Thomas Weiss

Supramolecular Assemblies – Chair: Gerald Audette

New Algorithms in SAXS / WAXS – Chairs: Lee Makowski, Marc Allaire & Jan Llavsky

Small Molecule and Synchrotron

Wavelengths and Particles as Tools in Structural Analysis – Chairs: Vivian Stojanoff & B.C. Wang

SAS, Synchrotron and Canadian Division

Combined Techniques in One Beamline – Chairs: Pawel Growchulski & Allen Orville

Chemistry and Biology with Novel Scattering Techniques – Chairs: Nick Suter & Jacob Urguidi

Synchrotron

Automation: From Crystal to Solved Structure – Chairs: Aina Cohen & Stephen Ginell

ACA Albquerque - May 24 - 28, 2014

Who Needs to Register: Everyone must submit a registration form (including invited speakers) with the appropriate fee. Registered participants will receive conference materials and a name badge securing admission to the Opening Reception, the Exhibit Show and Scientific Sessions, at the ACA Registration Desk within the convention center.

Schedule: The 2014 Meeting will have a 4-day, 5 concurrent session pattern such that there will still be as many talks as during a 5 day meeting. The meeting will start with a workshop on Saturday, May 24, and scientific sessions on Sunday, May 25, and will end on Wednesday, May 28, after the Awards Banquet.

YSSIG Social Events: **Due to the new shorter meeting format the *Mentor/Mentee dinner* and the *YSSIG Mixer* will be combined into a single 'not to miss' event- stay tuned for further details that will be posted on the meeting website.**

Obtaining a VISA: Advanced planning by foreign travelers is critical. We recommend all foreign travelers consider the following when making plans to travel to the US:

Identify whether a VISA is needed.

VISA applications should be made 90 days in advance of the travel date. For further information contact: the US Department of State (travel.state.gov/visa/visa_1750.html).

Staying Green: The full set of abstracts will be availabe through the ACA website. Program information will also be available through your smartphones and tablets. We are not planning on having a meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Info: FREE WI-FI will be complimentary in the sleeping rooms, so bring your laptops and stay connected to home and office. The room rates at the Hyatt are competetive with other properties in the vicinity. We are able to offer these rates by committing to fill a certain number of rooms. By staying in the conference hotel you will help us meet our room block commitment, which also brings with it the free meeting space that helps keep registration fees affordable.

All of our contracts include a number of lower-cost rooms available to students. Room sharing can make them even more reasonable - use the ***Room Sharing*** feature under accommodations on the meeting web site.

As further incentive to stay in the conference hotel, a number of lucky attendees will be selected at random to receive one night's accommodation free!

Financial support: Young scientists will be eligible to apply for travel support through the ACA and the IUCr. Applications 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 factors such as ethnic origin, religion, citizenship, language, political stance, gender, or age, in accordance with the statutes of the International Union.

Registration Fees

Category	Early (before March 31)	Late (after March 31)
Regular Member	**$500**	**$700**
Retired Member	**$195**	**$295**
Post doc Member	**$250**	**$350**
Student Member	**$195**	**$295**
Nonmember*	**$700**	**$950**
Post doc Nonmember*	**$350**	**$450**
Student Nonmember*	**$285**	**$385**
Guest**	**$ 65**	**$ 65**
Workshop: PHENIX	**$50**	**$100**
Social events		
Opening Mixer	**included in reg. fee**	
Banquet	**$70 ($35 students)**	
YSSIG Event	**TBD**	

* The nonmember registration fee includes a complimentary one-year ACA membership.
Those registering as nonmember post docs or nonmember students must include documentation of this status with the registration form.
**Guest registration includes Opening Reception and Exhibit Show.
Register on-line or download forms to register by fax or mail.

www.amercrystalassn.org/content/pages/2014-homepage
Questions: aca@hwi.buffalo.edu

ACA Small Molecule Course 2014

The 10-day course will be offered from July 7 to July 16, 2014, at the University of Notre Dame in South Bend, Indiana, US. This intensive course will emphasize both theoretical and practical aspects of chemical crystallography. Diffraction theory, symmetry operations, structure solution and refinement, powder diffraction techniques, and high energy sources are some of the topics that will be discussed.

No prior knowledge of crystallography is expected from attendees. However, a good understanding of undergraduate level chemistry, physics and mathematics is desirable. Attendees are advised to read either: *Crystal Structure Analysis: A Primer, 3rd Ed.* by Jenny P. Glusker and Kenneth N. Trueblood (Oxford Univ. Press, 2010) or *Crystal Structure Determination, 2nd Ed.* by Werner Massa (Springer, 2004) as preparation for the course. While the course is geared towards graduate level attendees, applications from strong undergraduate students will be considered.

The course is limited to a total of 25 attendees. In previous years there has been a broad demographic of students from both the US and abroad with affiliations in academia, government and industry. Anyone interested in the course is encouraged to apply. The faculty comprises experienced crystallographers with varied research backgrounds from academia, national laboratories and industry.

Instruction is divided into three sections: theory lectures are given during the morning sessions; workshops and data collections will occur in the afternoon and evening sessions. Participants will receive hands-on experience preparing crystalline samples for single-crystal and powder diffraction experiments; setting up and collecting diffraction data; processing data; and solving and refining structures. Several single-crystal and powder instruments will be available for the duration of the course, and attendees are encouraged to bring their own samples for data analysis. Commonly used software packages and crystallographic databases will be made available on university computers. Attendees are not required to bring their own computers.

A limited number of partial scholarships are available for student-level attendees, based on scientific ability and the expected benefits from participating in the course. Some meals will be provided, and there are many dining options both on-campus and within easy walking distance off-campus.

South Bend is located 80 miles east of Chicago, IL and 100 miles north of Indianapolis, IN. The campus is linked by public transportation to O'Hare and Midway International Airports and Union Station (Amtrak).

For further information regarding tuition, accommodation and transportation, please see our website at ***www.acasummercourse.net*** or e-mail us at ***info@acasummercourse.net***.

Applications will be considered on a rolling basis, with a deadline of April 1, 2014.

We encourage international participants who require visas for travel to the US to begin the application process early.

Allen Oliver, Amy Sarjeant & Charlotte Stern

Annual Statement of Ownership, Management, and Circulation

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17. I certify that all information furnished on this form is true and complete.
(signed) Marcia Colquhoun for American Crystallographic Association, Inc.

FEBRUARY 2014

19-21 **NIBB 2014**. Neutrons in Biology and Biotechnology, Grenoble, France. *www.ill.eu/html/news-events/events/nibb-2014-neutrons-in-biology-and-biotechnology/*

21-23 **Bruker/MIT Symposium: Modern Approaches to Structure Solution.** Cambridge, MA. *web.mit.edu/x-ray/bmit14.html.*

APRIl 2014

7-10 **BCA Annual Spring Meeting**, U Loughborough. *crystallography.org.uk/spring-meeting-2014/.*

23-26 **44th Mid-Atlantic Macromolecular Crystallography Meeting & 11th Annual SER-CAT Symposium**, University of Maryland, IBBR Shady Grove Campus. *www.mid-atlantic.org.*

MAY 2014

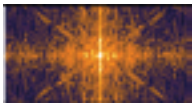
18-21 **Molecular Machines: lessons from integrating structure, biophysics and chemistry.** EMBO EMBL Symposium, Heidelberg, Germany. *www.embo-embl-symposia.org/symposia/2014/EES14-03/index.html*

20-24 **ACA 2014 Annual Meeting, Albuquerque, NM, Albuquerque Convention Center & Hyatt Regency Hotel.** ***Program Chairs: Christine Beavers & Petrus Zwart. Local Chairs: Zoe Fisher & Kate Page.*** *www.AmerCrystalAssn.org*

30-8 **International School of Crystallography. 47th course_Structural Basis of Phyarmacology: Deeper Understanding of Drug Discovery Through Crystallography,** Erice, Sicily. *www.crystalerice.org.*

JULY 2014

9-11 **Emerging Photon Technologies for Chemical Dynamics,** Sheffield, UK. *http://www.rsc.org/conferencesandevents/rscconferences/fd/fd171/index.asp*



AUGUST 2014

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

JULY 2015

25-29 **ACA 2015 Annual Meeting,** Philadelphia, PA, Sheraton Philadelphia Downtown**.** ***Program Chairs: Kraig Wheeler & Louise Dawe.*** *www.AmerCrystalAssn.org*

AUGUST 2015

23-28 **ECM 29,** Rovinj, Croatia**.** ***Program Chair: Nenad Ban.*** *ecm29.ecanews.org*

POSITION AVAILABLE

Position Title: Senior Research Associate - Time Resolved Crystallography

The University of Chicago Center for Advanced Radiation Sources (CARS) is seeking a Senior Research Associate (SRA) to become part of the BioCARS national user research facility at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL). The successful applicant for this full-time scientific position will be responsible for providing user support, originating research projects and leading R&D efforts to expand capabilities of synchrotron beamlines in the area of time-resolved crystallography.

The position requires a Ph.D. in the Biological or Physical Sciences, coupled with a minimum of seven years of experience in solving biological problems via innovative experimental and computational approaches. In addition to providing support for scientific users from the biological and physical sciences communities conducting research at Sector 14 of the APS, the SRA will also be expected to engage in collaborative original research with BioCARS users and staff. In addition to identifying, acquiring and integrating new instruments into the facility, this SRA will also be responsible for development and maintenance of all current instrumentation. Additionally, this individual will oversee a Biosafety level 3 facility. Strong computer skills are also required; specifically experience in EPICS, python and C Programming language as well as knowledge of Linux based operating systems. This position also serves as the primary point of contact for all issues related to the facility including coordinating with technicians and staff regarding vacuum, mechanical or electronic systems.

The SRA is expected to possess excellent organizational, verbal and written communication skills. These skills are critical to planning work flow and supporting user groups, as well as to disseminating the work of BioCARS in peer-reviewed and other publications, presenting findings at national meetings and planning and conducting workshops to train junior level personnel in time-resolved crystallography techniques. In addition, the SRA will have the opportunity to serve in the role of Principle Investigator, writing proposals to secure funding from federal and non-federal agencies to support such research and development.

The ability to work well as a team member and independently is required, as is the capacity to work in an environment with strict safety regulations. The successful applicant must be able to satisfy the requirements for access to ANL.

Interested candidates must apply through the University's Academic Jobs website at https://academiccareers.uchicago.edu/applicants/Central?quickFind=53172

A CV, including a list of publications, and a statement describing past and current research accomplishments must be uploaded to be considered as an applicant. Review of complete applications will begin February 1, 2014 and will continue until the position is filled.

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