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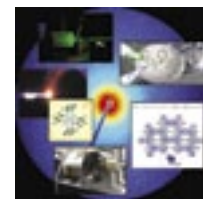
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Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)

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They say that time seems to speed up as one grows older. That certainly appears true to me as I write my final *President's Column*. Reflecting back on the range of my experiences during 2010, I find much to be pleased about. There was our successful ACA meeting in Chicago as well as my being able to participate

in interesting meetings at AIP, the USNCCr for Crystallography, the Council of Scientific Society Presidents, and the First North African Crystallographic Conference. The ACA is the voice of our community of scientists, responsible for promoting the power of diffraction and scattering in structural studies and their importance in a wide range of fields. My interactions over the past year have provided valuable opportunities to represent the ACA and to solidify our place in the scientific community. We are trying to enhance the visibility of the ACA by getting our organization to appear as a prominent hit when 'crystallography' is Googled. We have gotten the ACA listed on Wikipedia and are also exploring appropriate social networking sites.

Another benefit of attending these meetings is to learn about valuable resources available to us. The USNCCr is a part of the National Academies, which is represented by staff members on the Board of International Scientific Organizations (BISO). The International Visitors' Office (IVO), within BISO, provides services for monitoring international visa situations. This office can facilitate and expedite individual US visa cases for visiting scientists, postdoctoral fellows, and graduate students – at no charge. They generally cannot be of assistance after a visa application has been denied. If a US visa applicant has not received a response in twenty-one days, the applicant should fill out an IVO questionnaire so BISO can follow up on his or her case. The questionnaire can be found at: sites.nationalacademies.org/pgal/biso/visas/PGA_048017.

An important action that Council took at our fall meeting was to vote to change the format of ACA annual meetings. We plan to change from a five-day meeting with four parallel sessions each morning and afternoon to a four-day meeting with five parallel sessions each half day. We will continue to start the meeting on Sunday to take advantage of any special weekend airfare rates and end the meeting on Wednesday afternoon. The new format retains a total of forty sessions, but SIGs that traditionally held a session each half day (for a total of ten sessions in five days) will have to consider if they want to continue with ten sessions or offer a session each half day, which would result in eight sessions under the new format. It was noted that there was already some overlap of session topics at ACA meetings as well as at the IUCr Congress and the European Crystallographic Association annual meeting. Several factors led to Council's decision. Time savings

as well as financial savings for our members are major factors, since attendees would have one less day away and one fewer night of expenses. The majority of meeting attendees stay for three or four days. Comparisons to other crystallographic and society meetings demonstrated that most of these are three to four days with similar registration fees to that of the ACA. We are checking to see if the hotel contract for our 2012 Boston meeting can be modified from a five-day meeting to four days. If so, we may implement the new format in 2012. Failing that, we will try the new format in 2013. Sites being considered for future meeting are Las Vegas, Oklahoma City, a return to Hawaii, Los Angeles and/or the Washington, DC area. We will keep you posted as planning develops.

When I stood for election as Vice President, one thing I wanted to work on was to ensure that ACA remains relevant and vital for all our members, especially young scientists. Working toward that goal, I am pleased to report that at its fall meeting, Council voted to include a YSSIG representative as an *ex officio*, non-voting member. Jamaine Davis will take on that role in 2011, providing direct input to Council from the YSSIG, which will allow us to better serve that important community.

Another way we hope to better serve our twelve SIGs and to maintain balance in our meetings is by increasing the variety of vendors who exhibit at our annual meetings. Based on feedback from the survey we did in Chicago, we are working to attract new vendors and to lure back companies that had come to our meetings but have not been exhibitors in recent years. Increasing vendor participation will allow us to learn of and potentially test new products and, not insignificantly, increase the revenue stream from our annual meetings.

You can help the ACA to remain a vibrant organization by renewing your membership and by doing it electronically. It is fast, simple, secure, and it is a greener option. It also saves the ACA your membership dollars by cutting down on the cost of mailings. So, if you haven't already renewed your membership, please take time to do that right now. We can't succeed without our members.

This year has been a wonderful experience for me. It has been a pleasure to work with the professional staff at ACA Headquarters in Buffalo. Marcia and Crystal (and Patti and Jen in the past) made my job infinitely easier this year. I have been honored to serve as the President of the ACA in 2010 and have enjoyed working with so many of you that are involved in the broad disciplines represented in the ACA.

There are many things to work toward in the coming years – expanding our membership, developing new SIGs to better serve the interests of our members, increasing outreach and education efforts, especially to teachers and young scientists, and helping those young scientists prepare for the multidisciplinary approach to research that is now the norm for success. Now that I have passed the gavel to Tom Koetzle, I look forward to 2011 when I can serve as Past President and watch him lead us into the next decade. Lastly, I want to thank you for your support and for your continued participation in the ACA.

Judy Kelly

Highlights of the October 2010 ACA Council Meeting.

*Back row: Marv Hackert, Jim Britten, Bill Duax, Tom Koetzle, Bob Von Dreele.
Front row: S.N. Rao, Marcia Colquhoun, Judy Kelly, Bernie Santarsiero, Carrie Wilmot.*

Reports: President *Judy Kelly* announced that the 2011 *Transactions* Symposium would be cosponsored by the Small Molecule, Synchrotron, and General SIGs, and would celebrate the 2011 International Year of Chemistry with the content inspired by the work of *Philip Coppens*; *Time Resolved Studies and Photochemistry (AM) and Charge Density (PM)*.

Treasurer *Bernie Santarsiero* reported that the 2010 Chicago meeting with a final overall cost of approximately \$435,000, did come in slightly in the black. Meeting costs have escalated dramatically (since 2003 there has been a 50% increase in the cost per attendee) even when we have negotiated and cut expenses wherever possible.

Executive Officer *Bill Duax* and Director of Administrative Services *Marcia Colquhoun* reported that there were 1,840 paid-up ACA members in 2010. This year elections were conducted electronically. Postcards were sent out with login information. *Crystal Towns* has been promoted to the position vacated by *Jen Shephard*.

This was the last ACA Council meeting for *Bob Von Dreele* (Past President) and *Jim Britten* (Canadian Representative). The next Council meeting will be May 27, 2011 in New Orleans.

Annual Meetings: Council unanimously decided to reduce the ACA annual meeting from 5 days to 4 days starting in 2013 (see President's column). Balancing the budget of the 2011 New Orleans ACA meeting in the Spring was discussed; even considering the Council approved registration increases (\$50 for a regular registration and proportionately for other categories) it was clear that other cost-saving measures would need to be taken.

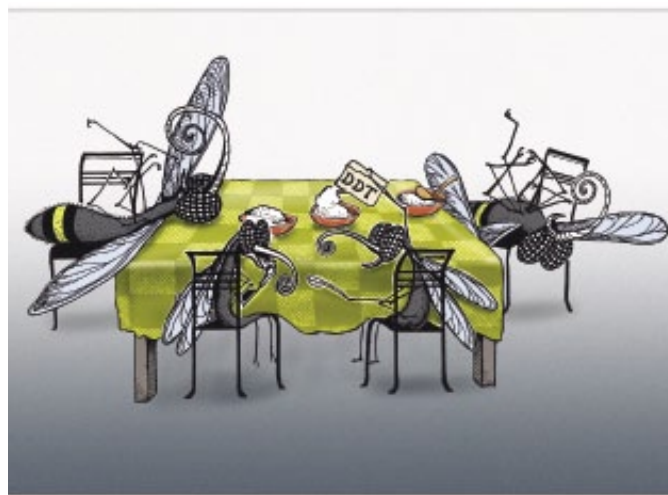
Workshops: These are one day (occasionally two day) one-off meetings held just prior to the annual meeting. They have to be revenue neutral. The deadline for submitting a proposal is September 1st of the year preceding the meeting (August 15th for IUCr years like 2011). Two proposals for 2011 Workshops were received and will be held in New Orleans (see page 40).

Summer Courses (formally Summer Schools): These are annually recurring, generally ~one week long, and very hands-on. They are financially subsidized by the ACA and the USNCCr,

and approved for four years of support at a time. Currently there are no summer courses in macromolecular crystallography and the Small Molecule Summer School will be in the final year of its current cycle (see page 44). Canada is now running an annual chemical crystallography workshop, which in 2011 will be held in Montreal. The SIGs have identified possible summer courses and organizers; one small molecule, four macromolecular, and possibly one powder. The proposal deadline is January 15th of the year prior to the starting year (i.e. Jan 15, 2011 for a summer course running years 2012 – 2015).

The Continuing Education Committee (CEC) had been hard at work redrafting documents so that the expectations and requirements for running a workshop or summer course will be more specific. The ACA will also request a Letter of Intent (LOI) so that the initial approach to the ACA does not involve a significant time investment by potential organizers.

Carrie Wilmott



"Of course, that's the problem with the older generation — they're so intolerant."

From the Editor's Desk

Erratum: - Fall 2010 issue of *RefleXions* - page 43: *Adam Lietzan* wrote to tell us: "I am honored to have an image from my work acknowledged in *RefleXions*. However as a point of clarification, the summary for the image mentions that I'm a part of the Kumar lab. I am actually a member of the Martin St. Maurice lab at Marquette University. Kumar was a previous graduate student in the lab."

RefleXions staff: *Bomina Yu* did a great job on collecting and assembling information for the awards pages in this issue (6-7). If you hear of an award to an ACA member please send the information to *Bomina (bomina@gmail.com)* so she can include it in an upcoming issue. Self-notifications are allowed - please let us know. All the book reviews were done by *Joe Ferrara* - lucky for us that Joe is such an avid reader. *Virginia Pett* worked with *David Sayre* to add his living history to the ACA archives and *Sidney Abrahams* penned the inaugural **Puzzle Corner**.

The images on pages 37 and 42 are part the **Puzzle Corner**. If you see yourself or anyone you know send the name and location of the photo to acareflexions@gmail.com so we can archive the photos with full attribution.

Voting is not a Spectator Sport: In 2008 voter turnout in my Congressional district was at 80% and the margin of victory was over 12 percentage points. In 2010, the same two candidates were running, turnout was ~50% and the margin of victory was less than 1% with an 847 vote margin returning the incumbent to Congress (phew!). In this year's ACA election participation was a disappointing 15% and the margin of victory in one race was 1 vote. I would wager that there is not one ACA member that does not have a preference for one candidate over another whether it be for an ACA office or for a local or national office (irregardless of whether you live in the US or elsewhere). Standing by and letting someone else decide our future should not be an option - we must all VOTE at every opportunity that presents itself.

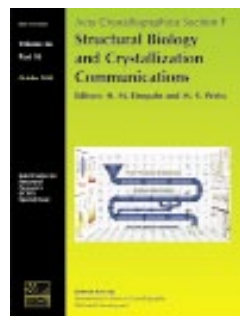
Cartoon: The cartoon on page 3 in this issue was created by *Nick Kim*, U. Waikato, New Zealand. www.nearingzero.net

Judy Flippen-Anderson

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Acta Crystallographica Section F Showcases Structural Genomics Publications



The application of high-throughput methods to structural biology has generated an abundance of new macromolecular structures. In order to help ease the resultant publication backlog, *Acta Crystallographica Section F* now offers a special publication strategy to showcase these structures and the experiments upon which they are based. The first example was published in December 2009 and contained eight papers from the RIKEN-UK structural genomics consortium in a special section of the journal.

More recently (October 2010), the journal published a special issue that focuses exclusively on 35 structures, grouped into context, from the Protein Structure Initiative Joint Center for Structural Genomics. The issue, which is open access, is available from journals.iucr.org/f/issues/2010/10/00/issconts.html. This milestone publication has been enthusiastically welcomed by the community, and new requests and proposals for further special issues and special sections are under consideration.

For more information, please contact the Editors, Howard Einspahr (hmeinspahr@yahoo.com) or Manfred Weiss (mweiss@helmholtz-berlin.de).

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Brunger wins inaugural DeLano Award



The American Society for Biochemistry and Molecular Biology (ASBMB) has created the *DeLano Award for Computational Biosciences* in memory of Warren Delano, whose tragic passing a year ago came as a shock to many. Known for creating powerful visualization tools for three-dimensional structures and making the source code freely accessible, DeLano was legendary in computer programming for the biosciences.

Notably, his molecular graphics program PyMOL allowed the average biologist to visualize and manipulate biomolecular structures for the first time ever. The award, established by DeLano's family, friends and colleagues, will be presented annually to an investigator who develops the most readily accessible and innovative computational tool or application that helps advance the field of molecular life sciences. The inaugural award will be presented to ACA member *Axel T. Brunger* of Stanford University.

Brunger, Prof. of Molecular and Cellular Physiology and HHMI investigator was also advisor to the undergraduate DeLano. He is being recognized for the many contributions he has made to structural biology. His program X-PLOR enabled scientists to refine three-dimensional crystal structures, which previously took months, in just days. X-PLOR was then incorporated into the software suite called CNS (Crystallography & NMR System), which includes most of the steps for macromolecular structure determination. More than a decade later the paper describing CNS is still cited in over 1000 articles a year. Brunger's concepts and strategies helped provide the foundation of much of modern structural biology. Brunger will present his award lecture at the 2011 ASBMB annual meeting in Washington, D.C.

Majkrzak and Axe named 2010 NSSA Fellows

Among the fourteen scientists named 2010 Fellows by the Neutron Scattering Society of America (NSSA) were ACA member *Charles F. Majkrzak* (see *RefleXions*, summer 2010, p. 28) and *John Axe* from the Brookhaven National Laboratory (BNL). The program recognizes NSSA members who have made significant contributions to the neutron scattering community in North America in one or more of the following areas: advances in knowledge through original research and publication; innovative contributions in the application of neutron scattering; contributions to the promotion or development of neutron scattering techniques; and service and participation in the activities of the NSSA or neutron community. Axe was recognized for "seminal studies of commensurate and incommensurate structural phase transitions, and service to the US and international neutron community." Both Majkrzak (1996) and Axe (1973 with Gen Shirane) are recipients of the ACA Warren Award.

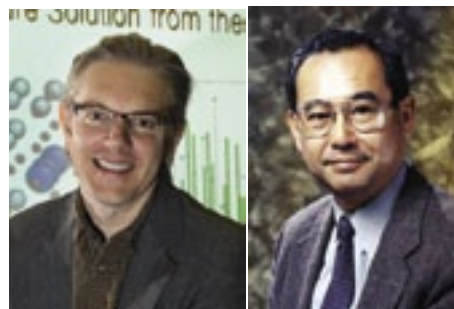
Kerfeld honored for Exemplary Contributions to Education



ACA member *Cheryl A. Kerfeld*, Assoc. Prof. in the Dept. of Plant and Microbial Biology at UC Berkeley, where she studies proteins involved in photoprotection of photosynthetic organisms. She is also a structural biologist and head of the Dept. of Energy Joint Genome Institute's Education and Structural Genomics Programs. The JGI's education

program was conceived to develop educational programs and tools centered on large-scale DNA sequencing and its bioinformatic analysis. These freely available programs and tools are invaluable resources for a range of institutions where faculty may not be familiar with bioinformatics and genome-scale research. The ASBMB is honoring Kerfeld with the *Award for Exemplary Contributions to Education* for encouraging effective teaching and learning of biochemistry and molecular biology through her own teaching, leadership in education, writing, educational research, mentoring and public enlightenment. Her award lecture "Sequence and Consequence" will be given at the 2011 ASBMB meeting in Washington, D.C.

Billinge and Egami win 2010 J. D. Hanawalt Award



The ICDD has awarded ACA members *Simon Billinge and Takeshi Egami* the *J. D. Hanawalt Award for excellence in the field of x-ray powder*

diffraction. Egami is currently Director of the Joint-Institute for Neutron Sciences at the Univ. of Tennessee. His research interests include neutron scattering, high-temperature superconductivity, electronic oxides, and the structure and dynamics of liquids and glasses. Billinge, who was a student of Egami's, is now Prof. of Materials Science and Applied Physics and Math at Columbia and Senior Scientist at BNL. Billinge's group studies the nanoscale structure-property relationships in functional nanomaterials using novel x-ray and neutron scattering techniques coupled with advanced computing. The pair was honored for their work in developing and extending the technique of Atomic Pair Distribution Function analysis of non-Bragg structures as exemplified in their book, "Underneath the Bragg Peaks". Their method allows scientists to study complex materials on the nanoscale.

Egami and Billinge presented their award lectures at the 59th Annual Denver X-ray Conference. Egami's presentation focused

on “*Recent Advances in the Pair Distribution Function Technique*” and Billinge spoke on “*Structure at the Nanoscale: Atomic Pair Distribution Function Analysis of Nanostructured Materials*”.

J.D. Hanwalt pioneered the development of a powder diffraction database in the 1930s that is still in use today. Takeshi Egami is also a former winner of the ACA Warren Award (2003).

Robin Rogers to receive Award in Separations Science and Technology



Administered by the ACS and sponsored by Waters Corp., the Award recognizes the development of novel applications with major impact and/or practical implementation in the field of separation science and technology. The scope of the award is as broad as possible, covering all fields where separation science and technology is practiced. The 2010 award went to ACA member ***Robin D. Rogers***.

At the University of Alabama, Rogers is the Robert Ramsay Chair of Chemistry and a distinguished research professor, as well as Director of the Center for Green Manufacturing. He is also Editor for the journal *Crystal Growth & Design*. His research interests focus on utilizing ionic liquids and green chemistry for sustainable technology through innovation. His laboratory has developed novel strategies for the separation and purification of value added products from biomass, for which he holds a number of patents. Rogers will be honored at the Awards Ceremony at the 241st ACS National Meeting, where he will also deliver his award lecture in the Division of Industrial and Engineering Chemistry Separations Science and Technology Symposium.

The 2011 Gregori Aminoff Prize in crystallography goes to Lia Addadi and Stephen Weiner



This Prize rewards contributions in crystallography, including areas concerned with the dynamics of the formation and determination of crystal structures. The Royal Swedish

Academy of Sciences will award the 2011 Prize to ***Lia Addadi*** and ***Stephen Weiner***. Addadi is a Dorothy and Patrick E. Gorman Prof. and Chair of Biological Ultrastructure at the Weizmann Inst. where she studies the interactions between crystals and proteins, antibodies, or whole cells. Weiner, also at the Weizmann is the Walter and Trude Borchardt Professorial Chair in Structural Biology. His research focuses on biomineralization and archaeology. Together they are being recognized “*for their crystallographic studies of biomineralization processes, which have led to an understanding of mechanisms of mineral*

formation.”. Addadi and Weiner have successively identified the biologically controlled texture of biominerals that occurs along specific crystallographic planes on protein crystals, which in all aspects control their formation, orientation, size, shape and assembly, and give rise to the complex shapes of many beautiful marine organisms. The award is presented at the annual meeting of the Royal Swedish Academy of Science.

Hecus awarded the Fast Forward Award and the “Rusnanoprize”



Developed as a spin-off from the Institute of Biophysics and Nanosystems Research at the Austrian Academy of Sciences in Graz in 1992, Hecus X-Ray Systems specializes in the development and marketing of x-ray analysis systems for research and industry. This year they were recipients of the ***Fast Forward Award*** given by the Styrian government recognizing the most innovative ideas of the year. Hecus’s innovative technology in x-ray optics combined with micro

calorimetry (S3-MICROcaliX) was among the six projects honored. Within a few weeks, Hecus was honored again with the ***Rusnanoprize*** from Russia. The international Rusnanoprize was established in 2009 by the Russian Corp. of Nanotechnologies to inspire and recognize innovations in the field of nanotechnology and nanoindustry. The annual prize is awarded to researchers for their discoveries and innovations as well as to companies for practically implementing them. Hecus is being recognized for their implementation of innovative technologies in nanodiagnostics.

Pamela Björkman to receive MUN honorary degree of Science



The Memorial University College (Newfoundland, Canada) awarded ACA member ***Pamela Björkman*** an honorary degree of science at their fall convocation. Björkman was recognized for her work in medicine. She is the Max Delbrück Prof. of Biology at the California Inst. of Tech. and an HHMI Investigator. Her novel structure of a human leukocyte antigen (HLA) protein, HLA-A2, revealed how T

lymphocytes could see antigen and HLA protein at the same time and suggested the underlying pathology of autoimmune diseases: T cells mistakenly recognize a self molecule for a foreign antigen that should be destroyed. At Caltech, her research continues to focus on the structural mechanisms of recognition in the immune system. One of her current projects is to try to make antibody-like reagents against HIV. Her work has also been recognized with the Gairdner Award in 1994, election to the US National Academy in Science in 2001 and the L’Oreal-UNESCO Women in Science Award in 2006.

Memories of Jim Stewart (1931-2010)



Our colleague, Jim Stewart, was a renaissance man. He was a devoted, energetic, and patient educator who had an uncanny ability to detail, systemize, catalog, and recall which allowed him to immediately quote from history, literature, and recent newspaper/magazine articles. New topics under discussion or questionable points prompted his immediate quest for answers which were quickly returned. Jim touched many of us with his wit and thoughtful comments. An avid

environmentalist, he practiced its principles long before that term gained its present popularity. His Great Depression upbringing together with a deep understanding of thermodynamics were evident in the homes he designed and built, in his choice of automobiles, and many other aspects of his life.

We met in 1956 at the U. of Washington as graduate students under Ed Lingafelter. Jim's long involvement in crystallographic computing began there on an IBM 650 computer. Jim's subsequent consulting at Sandia National Labs on programming, mutual visits over the years, and personal interactions of our families provided the intertwined thread for our long friendship.

His quest for a solar-heated, energy efficient house began with the "Hyattsville" one, adjacent to the University of Maryland (UMD), continued after his retirement with sequentially; the "McConnellsburg Cabin", "Torrie" (a 4 story house taking advantage of the picturesque Pennsylvania ridges), and finally the one level in-town house, "Ayr But An Ben", which also had a walk-in basement. Slightly different, but potentially improving energy efficiencies were used in all of these *via* insulation options including solar window input and leaning sarcophagus-type hot water heating, foam insulated roof/wall panel construction, total exhaust air heat exchange systems, ground source heat pumps for hot water and house heating and use of insulated concrete panels for basement sections. Over those nearly 50 years, meticulously kept records were maintained for various energy consumption units (purchased as # of kWh, cu ft of gas, and gals of propane @ \$\$ on dates @ mean temperature, but also each converted to GJ & totaled; a strict one on CGS units) allowing a comparison of improvements he designed into them (achieving a remarkable 3.5 times improvement in total E/floor area from "Hyattsville" to "Ayr But An Ben"). And of course, he was interested in comparing these results with my various homes because of the very different climate here in Albuquerque.

Because Bernice and Jim were avid readers, each of the houses contained enough books to fill more than 3 walls, 9' high. He introduced me to the Great Courses series of DVD lectures and would not hesitate to review the detailed thermodynamics of heat pumps to me, possibly because he was disappointed that I did not use ground source heating in my latest house.

He was keen on hybrid and future total electric cars; their drive trains and/or related motors. Again he kept detailed spreadsheets on his cars. For example, the spreadsheet on the 2005 Prius JTDKB20U653041174 had columns for gal bought, cost, MPG, T in F, true MPG, dash total gal, true cum MPG, dash gal, dash total gal, dash cum MPG, % error, % fill error and \$/gal!

We had long discussions on fair taxation and "consumption" taxes, present tax sources and their distribution; on national debt, deficit budgets, the monetary system, and gold; on free will, the origin and evolution of Christian faith, religious fundamentalism, in Islam as well as the West, and their interface with other religions. And when he judged me lacking, a week or so later the UPS would deliver a book for me to read.

I miss the weekly, sometimes more, phone conversations which supplemented the many e-mails exchanging various articles and data. I am sure that all of you who knew him will also greatly miss him.

Bruno Morosin

I first heard the name of James McDonald Stewart when I was a graduate student at Louisiana State in the early seventies. When I first joined the group my advisor Steve Watkins told me that Jim was one of his great 'heroes' in the field of crystallography. In those days, the software system that we used for data collection, reduction and structure solution was Jim's XRAY69. The XRAY package was extremely effective and educational. Whenever our group had unresolved problems we would either call or write Jim about them. He always explained the software and the crystallographic principles involved in detail. We benefited a great deal from Jim, not only because of his pioneering software system, but also because of his willingness to teach computational crystallography any time and any place.

After joining the National Bureau of Standards (NBS, now NIST) in 1983, I had the opportunity to meet Jim a number of times at the local crystallographic colloquium in Washington DC, where he was very active and gave frequent lectures. From 1986 to 1988, I worked as a NIST guest scientist, and also as a research chemist at the chemistry department of UMD under Jim's guidance. We received a three-year grant from ICDD to prepare x-ray powder standard patterns of electronic materials for the ICDD Powder Diffraction File (PDF). Jim was involved in an advisory capacity on the software for powder data collection and data reduction. I enjoyed our friendship very much. He was a great mentor, a wonderful, gentle, and humble scientist.

In the mid eighties, one of Jim's graduate students, Yuming Zhang, also worked at NIST on a project concerning the crystallite size/strain of materials. This project was co-directed by Camden Hubbard, and Bruno Morosin. The computer software suites 'XRAYL and CRYsiz', and the certification of an instrumental profile standard (LaB₆) were developed as a result of this project. Jim often came to NIST to hold discussions and to supervise Zhang. I also benefited by learning about various aspects of both the software and the principles of residual strain analysis. Zhang told me on many occasions that Jim was the nicest and most dedicated professor he had ever known.

Although Jim retired formally from UMD, his eagerness to teach never ceased and he stayed active by teaching at Juniata College for many years after his retirement. Jim continued to instill in the minds of young students an appreciation for the importance and elegance of chemical and crystallographic principles.

Jim was a great teacher and a giant in the field of crystallography. He opened the door of computational crystallography by creating the computer suite 'XRAY'. His vision and his software have transformed the field of crystallography forever. Many software systems being used nowadays are based on his concepts and the strategies applied in 'XRAY'. Jim's patience, unique way of teaching, rapport with students, and in-depth knowledge of both crystallography and computer science earned him tremendous respect from his students. I have the utmost respect for Jim; and like my graduate advisor, I will also always consider him as a great hero and teacher in the field of crystallography. His receipt of the ACA Fankuchen award in 2001 was a well-deserved acknowledgement of his great contributions. Most importantly, his influence will live on in the continued development and application of the computational areas he helped create.

Winnie Wong-Ng

My memories of Jim Stewart span 45 years; all are wonderful. We first met in the mid sixties when I was an NRC post-doc in Ottawa. Jim was a computing guru at UMD where he coordinated the development of the *XRAY System of Crystallographic Programs for any Computer*; a radical approach then as most software was written for a target machine. This was an era when computers were mainframes supported by large budgets and staff. Crystallographers faced serious portability problems with time and money being wasted on adapting programs to the different hardware types, operating systems and Fortran versions!

Jim was always a relatively shy person, except when it came to discussing computing. He then literally glowed with enthusiasm and could talk authoritatively about all aspects of the field. Jim attracted many converts to his XRAY philosophy of restricting machine-specific aspects of languages; in particular, to use only US-Standard ('pidgin') Fortran. Software contributors to XRAY, and later those to XTAL, usually became his close friends and remained so for life. I collaborated with Jim from 1968 and visited his lab and home a number of times. These were memorable and productive occasions. Jim had two main priorities in life; his family, followed closely by his computing interests. During these visits we would often work at night when access to UMD computers was faster and cheaper. Jim always dealt with family matters first, and then we'd go to do battle with the latest coding problem.

Jim was a born teacher and had the best people skills of anyone I knew. He was famous for his 'community' coding sessions when he brought programmers together to write code in real-time! This required special people skills, and Jim did it regularly. In more recent times, I believe Jim could easily have been a billionaire developer with *Microsoft* - which, coincidentally, has its HQ close to where he was born. Most programmers I know work best solo. But not Jim, he relished the interaction of ideas and egos and made it productive. It was also fun because Jim was just as apt to jump up and recite a poem of Robbie Burns or sing

a little ditty - his way of keeping the ideas and code flowing.

Jim loved anything technological, and especially autos and energy-efficient houses. The mention of autos or solar houses would always provide a welcome diversion from the intensity of coding. A fair slice of our time together in Washington, Ottawa and Perth, was spent discussing these. When I eventually installed a full photovoltaic system at home - a trivial addition compared to his efforts - he was delighted.

It was hard to resist Jim's enthusiasm for computing; it embraced relative strangers. A computing center director at UWA who gave crystallographers continual grief over access and charges, suddenly became quite generous after a meeting with Jim. He held similar sway over the UMD computing center where he was an Honorary Fellow. He routinely ran his jobs from the main control screen in the central machine room. Such access was unheard of in the days when computer managers were high priests and users were considered, well, unclean! Everyone who knew Jim has stories to tell of his persuasive powers - he had a way with people; the UN could have done with his skills.

Outside of the family, Jim wasn't much interested in social gatherings. His favourite beverage was Pepsi, and for him coffee was a definite walk on the wild side! Raised as a strict Protestant, his upbringing cultivated a lifelong interest in efficiency, reuse and avoidance of waste. He recycled drink cans before it became fashionable; he kept a fuel/mileage log on his autos and knew their efficiency to two decimal places. This frugality, conservativeness (in the truest sense of the word) coupled with a real generosity of spirit, were lifestyle benchmarks for younger colleagues - though, alas, few of us could live up to them. Jim had no apparent interest in sport. Yet he was a avid walker and would walk to work in Washington's tropical heat or polar cold rather than drive and in so doing leave younger and fitter people in his wake.

Jim's collegial approach to software development involved experts in the field directly. When the distribution of XRAY tapes became too complicated, Jim and Bob Munn coalesced RatFor and Macros into an approach that could be targeted at specific machines. A new package, XTAL, based on RatMac, was released in 1984. This remained well-supported, with 30 contributing authors, up until the late nineties when version 3.6 was placed in SourceForge as shareware. The XTAL development model depended on healthy computing budgets and widespread programming skills; alas, both have greatly diminished.

Jim's contributions to crystallographic software and teaching over 50 years were recognized with the ACA Fankuchen Award in 2001. Friends and colleagues who were fortunate enough to be in LA on that occasion were as proud and emotional as he was!

I close with a quote from XTAL. This is one of the 65 messages issued if an input error occurred - important therapy in an era when the next possible turnaround may be 24 hours away.

Fireworks ended - and spectators gone away...

And how vast and dark! - the Haiku poet, Masaoka Shiki.

No more turnarounds in this session, old friend - we'll miss you a lot.

Syd Hall



David Sayre was awarded the Eighth Ewald Prize of the IUCr in Osaka 2008 “for the unique breadth of his contributions to crystallography, which range from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by x-ray diffraction and microscopy, and for never losing touch with the physical reality of the processes involved.” He is seen here accepting the Prize from Iris Torriani, Vice-President of the IUCr. As part of the ACA History Project, he summarizes his scientific contributions below. David’s full statement will be deposited at the Center for the History of Physics (AIP). This is the second in a series of narratives by individual crystallographers. If you would like to contribute your story, contact Virginia Pett, pett@wooster.edu.

Thank you for inviting me to contribute to the ACA archive on the history of crystallography. In your invitation you sent a *Notes for Authors* containing specific questions expressive of what you hope to receive from your contributors. I will try to answer those questions.

Q. What are the main contributions that you have made?

There are two. Much the more important is the concept of x-ray diffraction microscopy, dating from 1980. I was then at IBM Research. Also, much earlier (in 1952), there was the squaring method of direct phasing. I was at that time a graduate student under Dorothy Hodgkin at Oxford. And there was a third thing. At IBM, which I joined in 1955, I became almost immediately a member of the original Fortran group. That may not have been crystallography, but it certainly benefited crystallography.

Returning to the x-ray diffraction microscopy (XDM), it occurred years later, at a time when I was concerned about the future of large-biomolecule x-ray crystallography. Was the crystallinity of the specimen really necessary? Much would be gained if it could be dispensed with. The Fresnel zone plate was known to be a possible basis for an x-ray microscope, and in the 1970s two very relevant new technologies were in the air for that: the synchrotron x-ray source, and (in the computer industry) nearly nanometer-scale fabrication technology.

In 1973 I took a sabbatical year at Dorothy Hodgkin’s laboratory, and gave a talk on those matters. Janos Kirz, professor of physics at Stony Brook, was also on sabbatical with Dorothy that year, and the upshot was that we became lifelong friends and colleagues. He was close to Brookhaven National Laboratory, which would indeed, in 1979, receive the funding to build the National Synchrotron Light Source, which started delivering photons in 1985. I, on the other hand, had access to IBM’s fabrication technology. Janos was one of the first to be ready for the photons, with his Fresnel zone-plate scanning transmission x-ray microscope (STXM). I, in the meantime, had been invited to speak at the 1979 Workshop on Imaging Processes and Coherence at Les Houches in France, and in my talk I asked why x-ray crystallographers, if given stronger x-ray

sources and better detectors, could not do diffraction imaging of non-crystalline (as well as crystalline) specimens. Accordingly, in 1985, when NSLS came on line, graduate student Wen Bing Yun was also ready and, using a single diatom as a specimen, got confirmatory (continuous and speckled) diffraction patterns. That left mainly the question of phasing, and I stated the concept of phasing by oversampling fairly clearly first in 1991, and more clearly in 1998. Thus, finally all the components of 2D imaging were brought together, first using an artificial specimen in 1999 and subsequently using a freeze-dried yeast cell in 2005.

Starting in 1999 the literature on diffraction microscopy has grown enormously in both size and scope — too much of it to be handled here. Fortunately David Shapiro, writing for us in the January 2008 Special Issue of *Acta Cryst. A*, has given a very helpful guide to that literature.

Returning now to x-ray crystallography, in my doctoral thesis at Oxford and in 1952, I gave an early direct phasing method, the Squaring-Equation method. It is now mainly of historical interest only. But it revealed very early the importance of atomicity as a key determinant of phasing, and does it in a very simple and attractive way. It has thus been followed by better methods which are, however, considerably more difficult to understand, and for that reason it is still mildly retained for teaching purposes. It came to me all in a flash one day early in 1950, when I was a graduate student in Dorothy Hodgkin’s group in Oxford, and I will take a few lines to tell that story. Earlier, in wartime 1943-45, I had worked in electronics and circuit design in airborne radar at MIT’s Radiation Laboratory, and had been much impressed by Hendrik Bode’s theorem: that if an electrical network is lumped-constant, and its amplitude characteristic is known, its phase characteristic is also known. Then, in 1947, I learned of x-ray crystallography and was captured by it. I, of course, also learned of its phase problem, and tried from time to time, but in vain, to find a basis for making a direct translation of the lumpedness of an electrical network into the atomicity of a crystallographic specimen. However, the thought was now ingrained in me, and one afternoon early in 1950, I was in the library looking at Fourier integral theorems, and came to the well-known one between multiplication and convolution and, for some reason which is still unknown to me, I simplified it to *self*-multiplication (squaring) and *self*-convolution, and imagined it to myself with equal atoms, and there it was — all in a flash — the phases had to be such as to make the theorem hold. Unfortunately the equal-atom part of my simplification departs too much from chemical reality to make the method widely usable, and in 1953 Karle and Hauptman, using a totally different approach, corrected that fault, and allowed direct method research to move on further, to the next stage of its modern development.



Q. What people or experiences influenced you to become interested in science in general and crystallography in particular? Were there mentors or colleagues who were important to your development as a scientist and crystallographer?

My father was a very good organic chemist, and it was a foregone conclusion that I would follow him in some type of scientific career. Apart from that, I don't think I have had mentors, though I can name 3 or 4 people with whom I had conversations that significantly altered my thinking. Lindo Patterson and Henry Lipson suggested, as a good topic for my 1949 M.S. thesis, "The Fourier Transform in X-ray Crystal Structure Analysis", which completely underlies the principal work which I have done in the latter half of my life, and Alan Turing was the person who added to that by directing my attention to Shannon's ideas about sampling density. Also, in my early work life, it was Bode's theorem that put me onto the squaring method of direct phasing. Otherwise, however, I seem to be guided mainly by my own thoughts.

Q. Were you active in the ACA?

I have not been consistently active but was active enough that I was president of the ACA in 1983. My main effort was to encourage crystallographers to be not only good at their crystallography, but equally to be good at the science that was making use of their crystallography. I think that that has caught on, and has been extremely valuable to all.

Also, at Jerry Karle's request, I organized for the 1981 Ottawa Congress, an extremely satisfying International Summer School on Crystallographic Computing, modeled on Michael Woolfson's wonderful schools, and attended by 185 participants from 31 countries.

Q. A little more information about XDM, please.

It is also known as "x-ray crystallography without need for a crystal", which I first proposed in 1979. The essence of XDM is diffraction not from a crystalline specimen but from a non-crystalline one. The strength of the Bragg spots is lost, so one needs a strong x-ray source and good x-ray detectors. The diffraction pattern is continuous and contains all the information at and between what would have been the Bragg spots if the specimen had been crystalline, and that larger amount of information greatly assists in reconstructing the specimen image. So x-ray structure analysis acquires an almost limitless number of new usable specimens, at least among specimens which can tolerate the higher imaging exposures. The quality of the imaging is best with the crystal form, but the arrival of so many newly usable specimens creates a whole new world of imaging possibilities. As for available literature on the subject, there was, previous to the year 1999, only our own small 3-4 person group in Stony Brook working on these ideas, so a rather small literature existed. Our 1999 paper in *Nature* changed all that, however, and there has been, starting in the year 2000, an almost overwhelming wealth of literature. For a best entry into it, see the Shapiro paper in the January 2008 Special Issue of *Acta Cryst.*

Q. What aroused your interest in XDM?

The difficulties, and (especially in biology) the unnaturalness caused at present by the rule of crystals only.

Q. What were the major obstacles to your work?

Waiting for new and better sources and detectors.

Q. What were the sources of funding?

My salary was paid by IBM. In 1973 I became a close colleague

of Janos Kirz, a physicist at Stony Brook and Brookhaven, and now at Berkeley, on x-ray imaging. For the last 35 years it has been he, or his colleague Chris Jacobsen, working with the appropriate funding sources, who supplied the needed students, photons, and apparatus for the work. It absolutely could not have been done without them.

Q. Were there collaborators?

Yes., physicist Veit Elser and graduate student Pierre Thibault at Cornell. They did outstanding work in producing the bulk of the reconstruction software for us.

Q. How did things actually work out?

Beautifully, bringing us to the successful 2-dimensional imaging of a yeast cell in 2005. Actually in that work we had produced a tilt series of 2D images, allowing us in 2008 to prepare a five degree tilt pair of images of that cell, giving us in effect a working version of a low-beam-exposure stereo-3D method of biological cell viewing. At the 2008 Osaka IUCr congress this image was shown in my Ewald Prize lecture and also in David Shapiro's talk.

Q. What was the initial reception given to this work?

Until 1999 wait and see, from both the crystallographers and the diffraction physicists. From 2000 on, a very high production of papers from the diffraction physicists, but a continuing wait and see from the crystallographers. See next paragraph.

Q. What are the long-term ramifications of your work?

A big and unwanted ramification would be if the two populations (crystallographer and diffraction physicist) decide to split over the crystallinity issue. But the preceding paragraph tells us that that unwanted possibility exists. And it would be bad for both parties, and for the sciences that we serve. Let us — ACA and IUCr — NOT let that happen.

Q. Please comment upon changes in the profession as a whole today.

I think that the young people, who now come from all over the world, and from both genders, are marvelous. If only everything could be like that.

Q. Do you have any additional comments?

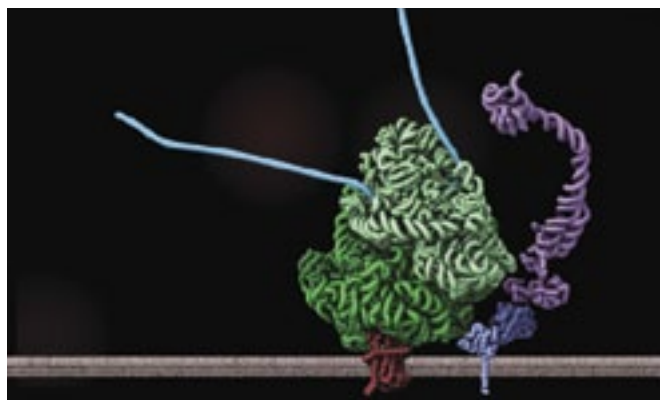
I cannot leave this write-up without emphasizing the contributions of Janos Kirz, physicist at Stony Brook and Berkeley. We met in 1973, when both of us were spending a sabbatical year at Oxford in Dorothy Hodgkin's group, and have been very close colleagues from that time on. None of the early work on XDM could have occurred without his wisdom and deep scientific abilities, for it was he and his colleague Chris Jacobsen who year after year saw to it that the students, photons, equipment, knowledge and insights needed for it were there. Deep thanks, Janos.

David Sayre



Science as Art - Art as Science

Imagine the surprise when the earliest molecular models were presented to the public by Hoffmann in his 1866 Faraday Lecture, or the anticipation when Fischer used bread clumps and toothpicks to model the stereochemical properties of carbohydrates in the 1890s. A few of us were around in 1968 when a color monitor was first used to display 3-D images of molecules. The challenges then were daunting – it was not until 1975 that it became possible to fit a protein structure to density with molecular graphics. Early programs like ORTEP, DISPLAY, BILDER, FRODO evolved and matured, but were seldom used outside the lab. Later, visualization software, such as GRAMPS, and 16mm movies taken from the graphics terminal in the 1970s made it into the lecture room and laid the groundwork for videos now easily made from programs like KiNG or VMD (molvis.sdsc.edu/visres/sculpture/subjects.jsp). David Goodsell (mgl.scripps.edu/people/goodsell) took molecular visualization into the art gallery and Edgar Meyer started carving wooden sculptures of molecules (molecular-sculpture.com/); Byron Rubin (www.umass.edu/microbiol/rasmoll/history.htm#bender) and Julian Voss-Andrae (www.julianvossandreae.com/) made secondary skeleton sculptures in metal.



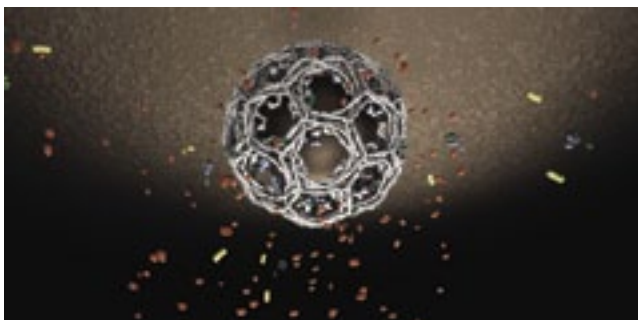
Still animation ER membrane translocation (Janet Iwasa).



Rapid prototyping (3dmoleculardesigns.com, Scripps) made it possible to create precisely scaled models (image at left, Edgar Meyer). To commemorate the sesquicentennial of the polio vaccine in 2005, the Smithsonian commissioned scaled bronze sculptures of the polio virus capsid structure and the capsid+receptor complex (Hogle's lab, HMS). Mixing fantasy with art and

science, images of molecules have been juxtaposed with flowers or in sculpture gardens (molecular-sculpture.com/Campus-sculptures/Imagine.html). Can we place life-sized bronze sculptures of biomolecules in public spaces, like a model of penicillin in a hospital terrace or a blockbuster drug in the offices

of a pharmaceutical company? These sculptures of monumental molecules will have lasting value, telling future generations about the 'golden age' of crystallography and the heroic efforts to elucidate the individual molecules of life.



Endocytosis - one stage of an animation depicting the assembly and disassembly of a clathrin cage (Janet Iwasa).

The recent increased use of physical, hand-held static models has been well complemented by the growing use of dynamic visualization tools. In the past decade, an increasing number of scientists have turned to 3-D animation software to create Pixar-quality movies of dynamic molecular events. These molecular animators, including recent MacArthur Foundation awardee Drew Berry (www.macfound.org/site/c.1kLXJ8MQKrH/b.6241243/k.30C1/Drew_Berry.htm), Janet Iwasa (<http://iwasa.hms.harvard.edu>), and Graham Johnson (fivth.com) use animation software from Hollywood, such as Autodesk Maya, Maxon Cinema 4D and Blender, to bring static molecular structures to life within their natural biological context. Efforts are currently underway to give these animation programs some of the capabilities of molecular viewer software (www.molecularmovies.com/toolkit/, mgltools.scripps.edu/epmv) and to provide tutorials specifically targeting researchers (www.molecularmovies.com/learning/).

Imagine going to the cinema to see the latest 3-D blockbuster, a film pulsing with dramatic tensions between molecules competing for scarce resources, or with heroic (photogenic) scientists using cutting-edge technology to combat dreadful diseases – yes, fellow crystallographers, that too is part of our heritage, so why not go public with it, in 3-D!

With the centennial of the discovery of x-ray diffraction and the International Year of Crystallography just around the corner, here is our chance to make a visual and lasting impact on public consciousness and sensitivity.

Janet Iwasa & Edgar Meyer

Useful links: biovisions.mcb.harvard.edu/ - www.proteopedia.org/wiki/index.php/Main_Page

Delightful eyesfull: www.youtube.com/watch?v=mbcWGU8fpxA&feature=related%20? - www.nytimes.com/imagepages/2010/11/16/science/16anim5.html - www.nytimes.com/imagepages/2010/11/16/science/16anim6.html - www.nytimes.com/2010/11/16/science/16animate.html?scp=1&sq=science%20animation&st=cse - www.nytimes.com/2010/11/16/science/16animate.html?hwp

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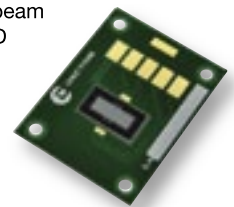
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Crystallography – World of Wonders

An educational outreach workshop was held as part of the 2010 ACA meeting in Chicago. This workshop was geared towards school teachers, and carried Illinois continuing education certification. Sponsorship by the ACA, the USNCCr and a supplement from the NSF allowed the teachers to attend the workshop at no charge. Unfortunately, due to inclement weather that caused severe flooding, many of the 29 registered attendees could not make it to the workshop.

The workshop combined presentations from a number of instructors with hands-on exercises that could be taken back to the classroom. As an intriguing start to the day, **Bruce Knoll** (Bruker) demonstrated that with modern instrumentation, users need very little training to mount a crystal and start collection of



a dataset. By lunchtime, the diffractometer had finished collecting data on aspirin, and the automated software had gone through all steps of structure solution without requiring user input. While the data were being collected, **Claudia Rawn** (Oak Ridge National Lab/UT

Knoxville) took the teachers on a *Materials Discovery Tour*, introducing them to basic concepts of bonding, structure, and structure-property relationships. Her powerpoint presentation was balanced with a number of hands-on exercises, including stacking of closed-packed layers of spheres, identifying several metal, ceramic and polymer spheres based on known properties like density, and polymer chain entanglement. A highlight of her session was the construction of basic crystal structures (face-



centered cubic material and rocksalt) from legos, which was so popular that all other presenters and even the AV staff participated! These activities were followed up by **Cora Lind**'s (University of Toledo) introduction to diffraction basics, which exposed the teachers to waves and slit experiments and drew analogies to

diffraction experiments. With the aid of diffraction grating slides and lasers, the concepts of repeat distance and atom identity determining spot location and spot intensity were demonstrated. After lunch, **Katherine Kantardjieff** (CSU Pomona) introduced remotely enabled instrumentation and how it can be used to expose a wider audience to crystallographic experiments. This was followed by a highly entertaining presentation by **Jim Kaduk** (IIT), who showed that powder diffraction can provide interesting information about everyday materials like peanut butter, oreos and many other frequently encountered compounds. The last two sessions by **Colin Groom** (CCDC) and **David Goodsell** (Scripps Research Institute, representing the RCSB PDB) gave the workshop participants a chance to learn about crystallographic databases, and to try them out hands-on.

A few of the teachers could stay for **Venki Ramakrishnan**'s



opening lecture to the ACA meeting, and were thrilled to have a chance to meet him and get his autograph.

The workshop feedback from the participants was very positive, encouraging us to run similar workshops in the future. Teacher attitudes changed from apprehension in the morning to excitement after the first few hands-on exercises, and by the end of the day, several participants were making plans for how to use what they learned in their own classrooms! Several of them also took additional hands-on kits to share with their colleagues.

Cora Lind

Photos: Workshop speakers Bruce Knoll (middle of left column) and Claudia Rawn (bottom of left column). Venki Ramakrishnan and Cora Lind with two of the Chicago high school teachers (right column).

**19th Annual BHT Regional Meeting, McMaster,
Hamilton, Ontario, November 5, 2010**

While retaining the BHT acronym in deference to the founding locations (Buffalo, Hamilton, Toronto), the group has expanded to include active participants from Kingston (Queen's), London (Western), Guelph, Waterloo and Rochester, as well. Attendance at the meeting was close to 100, supported by our loyal partners: Art Robbins, Bruker, Formulatrix, MiTeGen, Hampton Research, Molecular Dimensions, Qiagen and Rigaku. As usual, overall organization was overseen by *Lynne Howell* and local arrangements by *Murray Junop* and *Alba Guarne*.

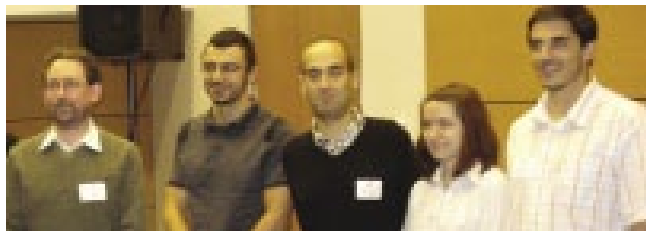
This year's special guest was *Paul Adams* (Lawrence Berkeley lab). Paul's name has been familiar to most of us in macromolecular crystallography for many years (Xplor, CNS, etc), and this year he gave a workshop on the latest developments in automated structure solution with Phenix. The high level of interest was demonstrated by the spirited discussion that followed on topics ranging from salvaging marginal data (not recommended) to automated molecular replacement using the entire PDB (not quite ready for prime time).

The afternoon session consisted of research talks by trainees *Lindsay Matthews* (Guarne lab), *Chris Goulah* (Malkowski), *Noboru Ishiyama* (Ikura), *Da Duan* (Allingham), and *Chris Garnham* (Davies). After the coffee break, the newest faculty member from Toronto, *Trevor Moraes*, introduced himself and his research program, and was followed by a talk from his trainee, *Charles Calmettes*. The session was rounded out by exciting results from *Joel Weadge* (Howell), *Peter Stogios* (Savchenko) and *Kosta Popovic* (Privé lab). Planning for the 20th anniversary meeting was placed in the capable hands of *Matt Kimber*, and the day ended with a lively wine-and-cheese reception, sponsored by Rigaku and Qiagen.

David Rose



Left to Right: Charles Calmettes, Joel Weadge, Da Duan, Noboru Ishiyama, Christopher Goulah



Left to Right: Paul Adams, Kosta Popovic, Peter Stogios, Lindsay Matthews, Christopher Garnham

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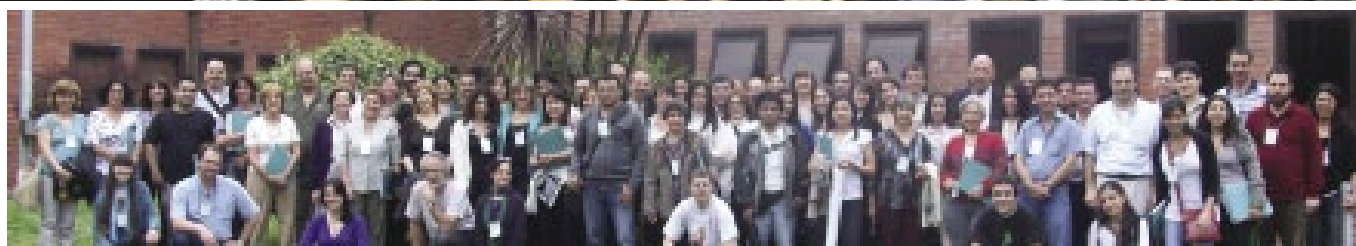
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6th Meeting of the Argentinian Crystallography Assoc. (AACr), Buenos Aires, Argentina, October 2010


The meeting was attended by approximately 100 participants from different areas of the country, giving it a true national relevance. It included poster sessions (more than 75 presentations, many of which were introductory work from promising young crystallographers) and many invited talks covering a broad variety of topics (polymorphism in pharmaceuticals, structural aspects of polymers, biopolymers and proteins, metals, alloys and texture, new minerals, geology, etc). Invited speakers included crystallographers from Brazil (*Adailton Bortoluzzi, Javier Ellena, Aldo Craievich, Iris Torriani and Alejandro Ayala*) and Argentina (*Raúl Bolmaro, Fernando Colombo, Susana Conconi, Graciela Punte, Elena Brusau, Ricardo Baggio, Alejandra Diez, María Vera, Adriana Serquis, Silvia Alconchel and Paula Abdala*).

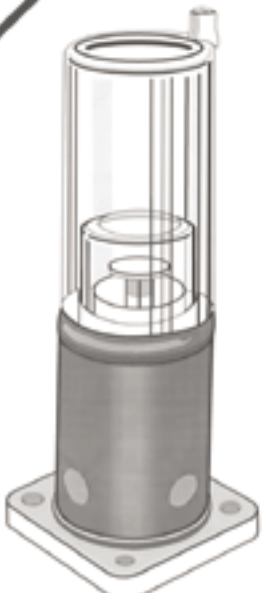
As a satellite activity the 2nd School of Crystallography was held from November 18 to 22. The school focused on the solution and refinement of crystal structures by single crystal methods, and was taught by *Oscar Piro* and *Ricardo Baggio*. There were 42 undergraduate and graduate students from almost all the main regions of Argentina (Buenos Aires, Río Negro, Neuquén, Mendoza, Bahía Blanca, La Plata, Rosario, Santa Fe, Córdoba, San Luis and Posadas) as well as a students from Brazil, Peru and Colombia, giving the school a true Latin-American flavor.

The ordinary AACr Annual Assembly was also held during the meeting and the current officers of the association were confirmed for a one year term to come. In addition, it was confirmed that the 7th meeting will be held in Bariloche from November 2 - 4, 2011, and the 8th, to be held in 2012, will be in Santa Fe. Following what seems now to be a well established tradition for AACr meetings, it was decided that a 3rd school, focused on powder diffraction by x-ray and neutron techniques using Rietveld methods, will be held in Bariloche, from November 7 – 18, 2011, and a 4th school, most likely focused on crystallography and vibrational spectroscopy will be held in Santa Fe following the 2012 AACr meeting.

Daniel R. Vega

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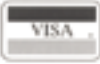


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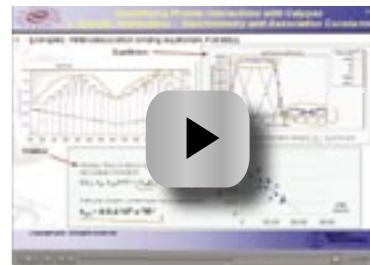
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Methods of high-pressure single-crystal x-ray diffraction: A satellite workshop of the 26th European Crystallographic Meeting, Darmstadt (Germany), September 3-4, 2010



Single-crystal diffraction provides the most accurate structural data on the compression of crystalline solids. The methods for high-pressure diffraction developed over the last 3 decades are mature and easy to use in both the laboratory and at synchrotron sources, but are not well known throughout the crystallographic community. In 2008 a group of high-pressure crystallographers from Europe and the US met in Padova (Italy) to discuss how to promote high-pressure single-crystal methods. On the occasion of a second meeting a year later in Copenhagen (Denmark) we agreed to meet on a regular basis and decided to offer a workshop open to everybody in association with the 26th ECA meeting.


The workshop, hosted on the campus of TU Darmstadt and organized by *R. Miletich*, *A. Grzechnik* and *H. Ehrenberg*, attracted 50 participants from all over the world for 2 days of lectures and demonstrations. *Ross Angel* gave a general overview of the entire workflow for a high-pressure experiment, and the additional challenges to be overcome compared to ambient-pressure measurements. *R. Miletich*, *C. Hejny* and *B. Periotto* presented on diamond-cells, how to load them, and then perform the data collections on the diffractometer. *M. Alvaro* reviewed software for data integration before the workshop split in to separate sections in which *R. Angel*, *D. Gatta*, *T. Balic-Zunic* and *A. Grzechnik* showed how to integrate high-pressure data with several commercial and freeware software packages. The second day was devoted to the separate subjects of equations of state (*T. Boffa-Ballaran*) and intensity data reduction and refinement (*K. Friese*, *R. Angel*), followed by structure validation and structure analysis (*T. Balic-Zunic*, *K. Friese*). The majority of the second afternoon was devoted to discussing detailed data issues with the participants, along with a demonstration by the research group of *R. Miletich* on preparing and loading diamond-anvil cells. The workshop was concluded with a short presentation by *H. Ahsbahs* on a new generation of diamond-cell design, and a review of synchrotron beamlines available for single-crystal diffraction.

Participants included researchers from many fields at all levels of experience with high-pressure single-crystal x-ray diffraction ranging from beginners to experts. More than one third of the participants were PhD students. The contribution to the workshop from all participants was immense; comments on the presentations (available at www.crystal.vt.edu/crystal/


[hpworkshop.html](#)) and subsequent discussions enlivened the workshop. With its completion, we hope that all of the participants (including ourselves, the speakers!) are now more confident that they can perform single-crystal high-pressure x-ray diffraction measurements and can complete the data reduction and analysis to obtain the highest-quality results. It has been proposed that the workshop will be taught again at the 2012 European Crystallography Meeting in Bergen.

We would like to acknowledge the generous support of Agilent Technologies (formerly Oxford Diffraction), Stoe & Cie GmbH, Incoatec GmbH and Scimed GmbH that allowed us to offer travel grants to some student participants, and to cover catering costs.


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Puzzle Corner

A recent invitation to contribute to a new electronic archive, presently under construction as an ACA History Portal of crystallography, led to the realization that such written material might well be enhanced if accompanied by photographs of earlier crystallographic gatherings such as the 1st IUCr Congress of Crystallography at Harvard in 1948 (1), for which serendipitously the names of all 157 of the 310 participants present had been recorded by Robert C. Evans, General Secretary of the IUCr, thereby greatly increasing its value and interest. The chance that a crystallographer in a group photo may not be recognized, however, often scales with group size and time elapsed since taken. The possibility that many other older group photographs might be received by the History Portal that include unidentified crystallographers proved reminiscent of the Puzzle Corner in BCA's *Crystallography News* (2,3), which often challenges its readers to identify earlier crystallographers. Sometimes BCA members are also asked to identify the circumstances under which such photographs were taken, while other puzzles offer very different kinds of challenge. The ongoing popularity of this feature suggests the possibility that emulating our transatlantic cousins might help overcome the identification challenge while offering our members a little diversion.

The ACA's version of Puzzle Corner is anticipated to resemble that of our Book Review section, both of which are planned as regular features but with each of variable issue length. Members' reactions to this new feature will be warmly welcomed, as will be photographs received of historic crystallographic interest even when all in it are known.

(1) www.iucr.org/__data/assets/image/0014/24143/hires_iucr_i.jpg (when you look at this photo you will notice that the front row a number of folks for whom awards have been named - Fankuchen, Warren, Buerger, Patterson, Ewald & Hodgkin).

(2) www.crystallography.org.uk

(3) *Carl Schwalbe*, Editor of *Crystallography News*, is warmly thanked for his advice and support.

The first photo with unidentified participants is below. Send photos, puzzles or general suggestions to sca@mind.ne or acareflexions@gmail.com

Sidney Abrahams



Moscow (?) - from left to right: V. I. Simonov, J.M.Cowley(?), ? , M. Marezio, Aafje Vos, F. Herbstein, N. Kato and S. C. Abrahams

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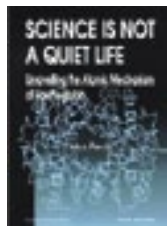
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Science Is Not a Quiet Life: Unravelling the Atomic Mechanism of Haemoglobin: Edited by Max Perutz, ISBN:978-9810227746



I have to thank Angela Criswell for bringing this book to my attention. We thought it would complement Michael Rossmann's recent webinar *From Haemoglobin to West Nile Virus*. I was so enthralled by the book that I gave Angela's copy to a student just starting her career in the study of hemoglobin only to find that it is actually quite hard to find. Anyway,

I did find a replacement copy and the book is worth reading, especially if your library or supervisor has a copy.

The book is divided into 12 chapters. The first provides a non-crystallographer's introduction to crystallography titled *Diffraction Without Tears: A Pictorial Introduction to X-ray Analysis of Crystal Structures* that first appeared in his 1992 book *Protein Structure: New Approaches to Disease*. This chapter does what it says, both in schematic pictures and state-of-the-art graphics. State-of-the-art graphics from the 40s to the 80s, that is. Those of you with 3D monitors will appreciate how difficult it was when Fourier transforms were calculated by hand.

Each subsequent chapter consists of a short introduction by Perutz followed by a series of papers associated with the period of study. The papers within in each chapter are in chronological order, but across chapters they are not. Reading the papers in strict chronological order might give a better historical perspective.

In chapter 2, *Early Studies*, we see the inception of protein crystallography in the 30s with J. D. Bernal. This chapter has a paper titled *The Composition and Swelling Properties of Haemoglobin Crystals*—this is the beginning of the use of humidity control to systematically change the properties of protein crystals. The next chapter, *Solution of the Phase Problem* discusses the heroic efforts Perutz and his collaborators, including Lawrence Bragg and Michael Rossmann, used to determine the structure at 5.5Å. The development of isomorphous replacement, first using different salt concentrations, then heavy atom derivatives, unfolds before us in the papers presented.

Chapter 4, *From the First Molecular Structure Model to the Allosteric Mechanism* covers the evolution of the structural model, from 5.5Å to 2.8Å, with the elucidation of the allosteric effect. *Structure of Myoglobin: A Three-Dimensional Fourier Synthesis at 2Å Resolution* by Kendrew *et al.* is provided for historical perspective. Chapter 5, *The Haemoglobin Battles* describes how Perutz used synchrotron data collected in 1980 at LURE to increase the resolution to 1.74Å, and used other methods to show how the binding of oxygen changed the structure and induced the allosteric effect. Perutz then turns his efforts to understanding the *Molecular Pathology of Human Haemoglobin* starting with hemoglobin in sickle-cell anemia, and then other less common conditions.

Chapter 7 covers *Haemoglobin as a Drug Receptor* while chapter 8 presents the case for evolution via *Species Adaptation in Haemoglobin*. Chapters 9 and 11 cover the topics *Early Shots at the Folding and Unfolding Problems* and *Haemoglobin as an*

Oxygen Sensor That Regulates Expression of Nitrogenase Genes, concluding the work on hemoglobin.

I skipped chapter 10 above because here Perutz goes in a different direction with *Present Work: Polar Zippers and Neurodegenerative Disease* where glutamine repeats are the polar zippers. The final chapter, *Glaciers*, is quite interesting. This has nothing to do with cryo-crystallography, and tells us about Perutz' effort during World War II to test the hypothesis that large icebergs could be converted into unsinkable aircraft carriers. This required field work in the Alps to gather data to test creep in glaciers and provided much enjoyment since Perutz enjoyed skiing - a skill needed to reach the glaciers he was studying.

Cooking for Geeks by Jeff Potter, O'Reilly Media, ISBN-13: 978-0596805883



I heard an interview with Mr. Potter on NPR's Science Friday a few weeks ago and immediately bought a copy of this book. The author is a software developer who likes to cook. The "Geeks" in the title are software developers, but let's face it, most of us crystallographers are geeks too and a lot of us like to cook. My last argument for reviewing the book is that cooking is really just applied chemistry.

The book pays due homage to *Mastering the Art of French Cooking* by Julia Child and *On Food and Cooking* by Harold McGee. The author treats cooking like running a program. Potter starts with a discussion on initializing your kitchen and calibrating your tools. Much attention is paid to heat and time and the interchangeability (to a degree) of the two. His favorite tool is an infrared thermometer for temperature calibration but he also describes the use of sugar to calibrate ovens to 365°F.

There are some useful discussions about the tasty products of chemical reactions that occur during the cooking process: Maillard reactions, caramelization and protein denaturation. Although the description of the last reaction was a little weak and the description of using alcohol to make aroma molecules lighter is obviously wrong, I found the rest enlightening. For example, I really like the idea of replacing the glass window in my oven with Pyroceram® to make a proper 850°F pizza oven. All I have to do is convince my wife nothing will happen to the house.

The other 'hack' I am interested in trying is *sous vide* (under vacuum) cooking. In this method the food item is placed in a sealed plastic bag brought to an exact temperature, 140° F for example, in a water bath and allowed to reach thermal equilibrium. The results are supposed to produce delicious and tender meat and fish. I am sure there are enough low temp controllers and pumps around here that I can cobble something together in a few hours. Speaking of fish, did you know that if you brine salmon for 20 minutes in 5-10% saline solution and rinse, the albumin will set and won't leach out during grilling? This works for mahi-mahi too.

Another interesting trick is to create a recipe by averaging a number of existing recipes. However, I am sure it is the outliers that make for the interesting results. Throughout the book you will find sidebars with interviews from experts and recipes that demonstrate the topics being covered.

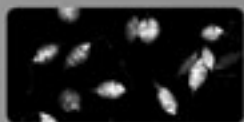
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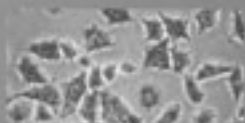
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***William and Lawrence Bragg, Father and Son: the Most Extraordinary Collaboration in Science* by John Jenkin, Oxford University Press, 2008, ISBN: 978-0-19-923520-9**



I remember seeing *William and Lawrence Bragg* just after its publication in 2007 but had forgotten about it until I recently found a copy on Amazon. I learned a lot from this book about the origins of x-ray crystallography, history that predates the last biography I read about a crystallographer: *J. D. Bernal: The Sage of Science* by Andrew Brown.

While William Bragg was a brilliant scientist in his own right—for example, he applied the Fourier transform to diffraction data in later years—it was his son Lawrence who explained Max von Laue’s experimental results, deriving in 1912 what we today call Bragg’s Law. Even more amazing to me is the fact that he did this during his first year as a fellow at Cambridge. Lawrence is the youngest scientist to have won a Nobel Prize, awarded when he was just twenty-five years old.

The first half of the book chronicles William’s life until he returned to England after twenty-three years at the University of Adelaide. Jenkin goes on to describe the overlapping lives of William and his sons Lawrence and Robert, who was killed at Gallipoli during World War I. Unlike the first half, this part of the book is not laid out in chronological order, so you have to pay attention to the dates.

The most exciting part of the book is the final third. Students of crystallography could learn just about everything they need from this section. Jenkin, a retired physicist from La Trobe University in Melbourne, shows how Lawrence formulated the theory of diffraction and began to solve structures by inspection. During WWI, Lawrence contributed to the war effort by developing sounding methods for locating German artillery.

As director of the Cavendish Lab at Cambridge, Lawrence cultivated crystallography in the UK. Among his proudest moments were the 1962 Nobel prizes for the structures of hemoglobin and myoglobin, and for the structure of DNA, both awarded to members of labs he headed.

***Don’t Be Such a Scientist: Talking Substance in an Age of Style* by Randy Olson, Island Press, 2009, ISBN: 978-1-59726-563-8**

***Am I Making Myself Clear? A Scientist’s Guide to Talking to the Public* by Cornelia Dean, Harvard University Press, 2009, ISBN: 978-0-674-03635-2**



I saw these books reviewed in *Science* and was intrigued. I have read both and have learned, or perhaps relearned, how to communicate better. While it is important to be able communicate amongst ourselves as scientists, what these books enforce is that it is

also important, perhaps more important, to be able to communicate to the non-scientists with which we share the planet.

Randy Olson was a marine biologist who became a screen writer and director in his late thirties. The title comes from the result of his first acting lesson in which the teacher screamed at him “Don’t be such a scientist!” for being too analytical in class. Some of Olson’s film credits include *Flock of Dodos: The Evolution-Intelligent Design Circus* and *Sizzle: a Global Warming Comedy*. His book outlines the differences between the way scientists think and communicate among themselves and with the general public. He explains how to express ideas to the general public with clarity and respect with the following four rules: don't be so cerebral, don't be so literal minded, don't be such a poor storyteller and don't be so unlikeable. The underlying method he describes is the arouse-and-fulfill strategy.

He uses the movies *An Inconvenient Truth* and *Too Hot Not To Handle*, both produced by Laurie David, as examples of how to communicate to the general public. *Too Hot Not To Handle* uses the conventional format for a science documentary; lots of facts and interviews with prominent scientists. *An Inconvenient Truth* has many fewer facts, some personal stories and a few errors that do not change the general trends that show the earth is warming. Olson is not recommending that errors be allowed but stresses that what is important to the general audience is the trend not the fine details. We all know the result: *An Inconvenient Truth* was a phenomenon; *Too Hot Not To Handle*, well at least I can watch it on Google video.

Cornelia Dean is a writer for the *New York Times*’ Science Times. Her book comes from the perspective of a journalist who has learned to cover science. There is a lot of overlap in the concepts between this book and *Don’t Be Such a Scientist*, but there are enough differences that you should read them both. Dean’s book is a detailed how-to guide on the subject of communicating science to non-scientists. She covers the topics of knowing your audience, journalism and journalists and discusses science, scientists as sources of information, using public relations effectively, working with modern media including radio and TV, hardcopy and online documents, and the web. Dean also provides good hints for writing op-ed pieces, being a witness and dealing with lawyers. In the last section of the book, she explores the obligation we have to help make policy and work with the general public.

I had one complaint about *Am I Making Myself Clear?* The type is quite small and was hard to for me to read. It turns out that is by design. Dean suggests small type forces the reader to pay attention longer. I found it annoying. On a positive note, I did find one tidbit interesting: she says that English is a Germanic language and we should use words of German origin, rather than Latin or Greek, in constructing sentences for general reading. For someone who spent four years learning Latin and only one learning German, this was a revelation.

Olson’s book also convinced me to rent *Flock of Dodos*. This movie has a number of elements for which Olson is criticized by scientists: too much humor, not enough facts and short sound bites. I watched it and walked away very worried. Remember that dodos did not adapt to a rapidly changing environment; watch the movie, think carefully about who the “dodos” in the movie really are, then read the two books above, if you haven’t already.

Present at the Flood: How Structural Molecular Biology Came About by Richard Earl Dickerson, Sinauer Associates, 2005, ISBN: 978-0878931682



Present at the Flood (PATF) is a retrospective that provides a detailed overview of the personalities and work that is at the origin of structural biology. Each chapter has an introduction and then a series of papers that elucidate a particular step in the process. For brevity, some of the papers are abridged. However, a number of those papers also appeared in their entirety in *Science is not a*

Quiet Life by Max Perutz, also reviewed here. Each chapter is well referenced and has a set of study questions at the end (with answers at the end of the book).

Dickerson begins with an introduction to the problems of protein and DNA structure that is elucidated in later chapters. In Chapter 2, he covers the work of Astbury and Wood and introduces fiber diffraction. Then he reviews the models for chains of amino acids that evolved through the work of D.W. Bragg, who mistakenly generated the cyclol model, then the work of Pauling and others.

In chapter 4 we see how the model for the α helix is developed by Pauling. Interestingly, Pauling used a rolled up tube of paper to visualize this model. Perutz had missed an important datum because all the fiber diffraction patterns, collected to date, were on perfectly oriented samples. The 1.5 Å reflection needed to confirm such a model was outside the diffraction conditions. Once Perutz tilted a fiber sample he saw the reflection and confirmed Pauling's model. This left the Cavendish lab on edge, so when the structures for hemoglobin, myoglobin and DNA were ready there was no delay in publication. The phrase, *I wish I had made you angry earlier*, summarizes the conversation between Bragg and Perutz on the observation of that reflection.

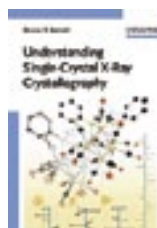
In chapter 5, he recapitulates Perutz' concept of crystallography without mathematics, providing a good introduction to many concepts for novices with a direct path to understanding the diffraction pattern for a helix with points of electrons along the path. Next he reviews the dead ends associated with the determination of the model and the final, correct structure. Of course, discussion of the history of the structure of DNA would not be complete without mentioning the tragedy of Rosalind Franklin. He suggests that one should read the first 8 books in the bibliography and come to their own conclusion, a valid suggestion.

Chapter 6 reviews Perutz' breakthrough in discovering multiple isomorphous replacement, which allowed Kendrew to solve the structure of myoglobin and Perutz the structure of hemoglobin. Dickerson takes the reader through the solution of the phase problem and the slow increase in the understanding of these structures. It is very clear that 2D projections were not enough and full 3D models were needed. I want to point out that the first paper reprinted is actually a parody on crystallography, the solution of the structure of the fictitious protein globlobin. I thoroughly enjoyed it.

In chapter 7, we see the transition from the low resolution structure of myoglobin, 6 Å, to the high resolution 2 Å structure

through modern computational methods. We learn also that the placement of the heme in the original myoglobin structure was wrong but corrected at 2 Å. The 5.5 Å hemoglobin structure is discussed, and the cyclol model is revisited and buried forever. Chapter 8 reviews the state of affairs after the initial structures were solved and the exponential growth of the PDB. The epilogue, Chapter 9, finishes the story with a *whatever happened to* the main characters in the book.

Understanding Single Crystal X-ray Crystallography by Dennis W. Bennett, Wiley-VCH, 2010, ISBN: 978-3-527-32677-8



I came across this book while browsing the "stacks" at Amazon. I remembered Bennett from the traveling salesman algorithm he published in the late 1980s for 4-circle diffractometers, and I met him while he was on sabbatical in Wisconsin. With the wisdom gained by the 25 years that have elapsed since I last took a crystallography class, I can honestly say I wish I had this book when I was in school.

The power of the book is that he begins each topic from first principles and derives the detailed concepts with full mathematical rigor. If I were to teach a course in small molecule crystallography, this is the book I would use. I disagree with his use of $\Delta f'$ and $\Delta f''$ instead of f' and f'' to represent the real and imaginary contributions to the scattering factor, but I am nitpicking. There are some typos in the book, and I would like to see the community do for *Understanding Single Crystal X-ray Crystallography* what it has done for Rupp's *Biomolecular Crystallography*.

The book is divided into sections on crystal lattices and symmetry, diffraction theory and experiment, structure solution, and structure refinement, and features 9 appendices. Each chapter includes a set of problems for the student to solve. He develops the concept of the crystal lattice through vector and matrix mathematics. Then uses these tools to develop point groups and space groups. Much attention is paid to interpreting the space group tables found in the *Int. Tables for Crystallography*.

In chapter 3, he develops the theory of x-ray diffraction from first principles, ending with the equations for calculating structure factors and electron density. Chapter 4 covers the experimental aspects of data collection, including classical film and serial diffractometer methods and modern area detector methods. Chapter 5 is devoted to the discussion of random and systematic experimental errors, with an excellent description of statistics.

The next chapters are devoted to structure solution, with Chapter 6 discussing Patterson, heavy atom (isomorphous replacement and anomalous scattering) and Fourier methods. Chapter 7 discusses direct and probability methods for structure solution.

The final chapter reviews all aspects of structure refinement, including linear and non-linear least squares, weighting, constraints and restraints. The basics of macromolecular structure refinement are provided, but not in enough detail for a macromolecular course but it would be a very good supplement to Rupp's excellent book.

Joseph Ferrara

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Professor of Biochemistry and of Computer Sciences, University of Wisconsin-Madison.

Statement: Like others before me, I am both honored and flattered to have been elected to help lead the ACA. I have attended ACA meetings (not all) since my graduate school days, and have always found them to be quite stimulating, as I consider myself to be both a crystallographer and a structural biologist. Some of my colleagues don't understand the difference but, by my book, the former is interested in the science of crystallography for its own sake, and the latter is motivated by biological questions. Because of my broader interests in diffraction, I think I can appreciate the whole range of activities that the ACA supports, and will endeavor to promote them all.

I also have a keen interest in teaching crystallography, and education is the basis for future development of our field. I have written a broadly used piece of software called XrayView that illustrates the Ewald construction graphically, and have contributed a Pymol software plug-in for printing physical models of the packing of protein crystals in various space groups. I teach a full semester course on protein crystallography, including homework exercises to grow crystals, collect data, solve, and refine a protein structure.

As for particular goals I think the ACA should work on in the immediate future, I will listen to others, as I have never been on the ACA council, but plan to catch up on areas that need work and pitch in enthusiastically. One area that I KNOW needs work is validation of coordinates that come from the crystallographic community, both small molecules and macromolecules. The recent exposure of fraudulent or seriously mistaken structures of both types creates disproportional damage to our field. There are ways we can work with journal editors and the data repositories to reduce the chances of these events from recurring, and at the same time enhance the value of these growing informatics resources.

Crystallography, like all fields, evolves over time. I am proud to be a part of the maturation of the technology and its widespread usage and dissemination. Those who worry that crystallography is dying because some experiments can now be done by non-specialists should not grieve for the olden days, but push ahead to new frontiers. There are many puzzles waiting to be solved, new x-ray sources on the horizon, and new methods ripe for development. Let our diverse backgrounds and interests push us to new heights!

David Rose, Canadian Representative

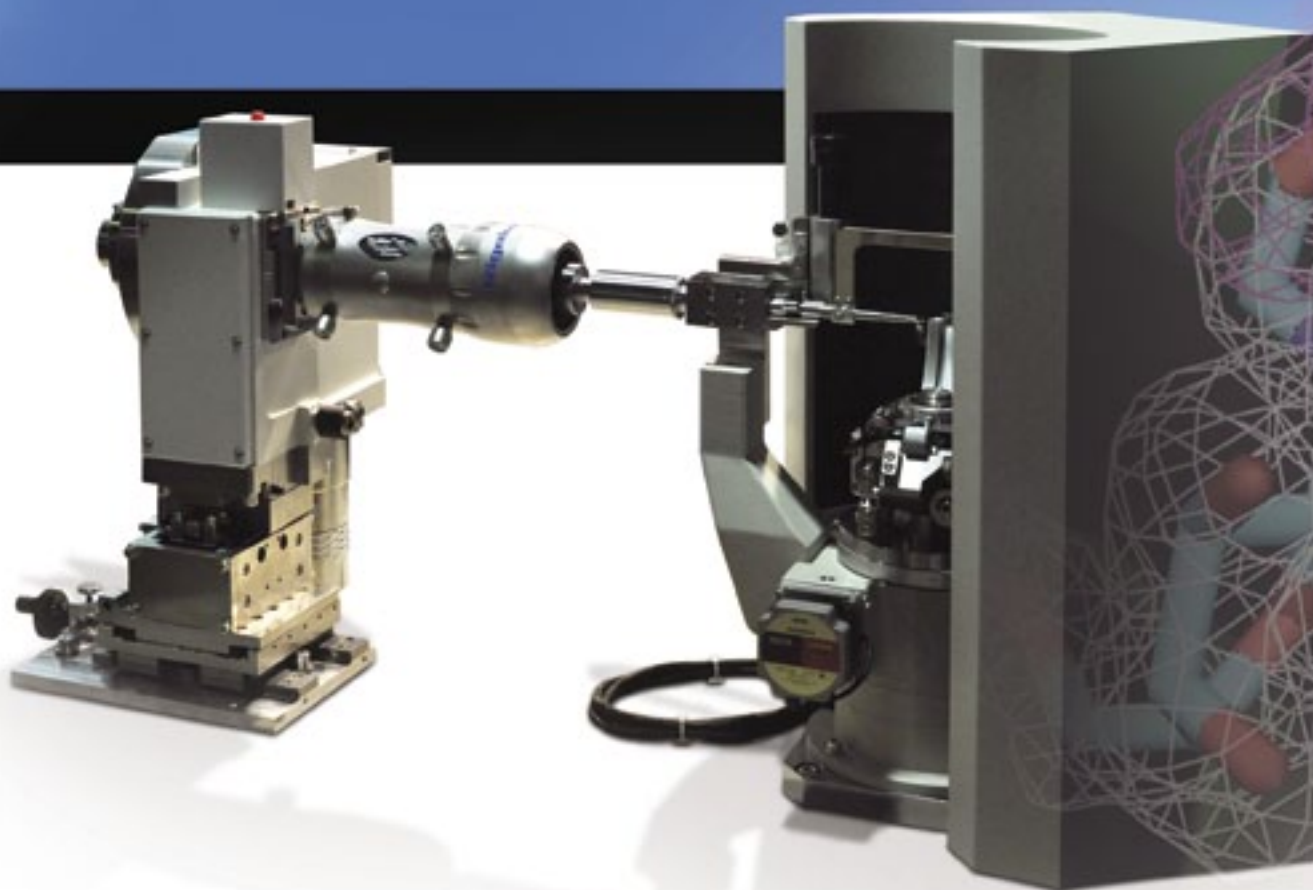
Professor and Chair, Department of Biology, University of Waterloo.

Statement: As the official organization supporting research in all aspects of crystallography in the Americas, the ACA has been my professional home for over 25 years. At ACA meetings, I have met colleagues ranging from undergraduate students to Nobel laureates. I have learned more about technical advances in our discipline and recent research results from ACA meetings than from any other single source.

My formal service to the ACA (beyond being a member) began almost 10 years ago. I was

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inspired to take part in order to promote the organization to colleagues at all levels, but particularly at the trainee level. ACA meetings are unusually welcoming to young scientists, helping them to make the connections that will be so important in establishing their careers. However, the meetings are only as good as the participants; a goal of mine is to encourage and facilitate attendance by my senior colleagues.

As Canada has no regular national meeting for crystallographers, the ACA has traditionally filled this void. Canadians are represented in disproportional numbers among past ACA Presidents, and among meeting attendees. The ACA has recognized this by establishing a special seat on Council for a representative from Canada. I was fortunate to have occupied that seat from 2002-2005, during which time I worked to increase Canadian visibility, for example by promoting a special Canadian Pauling Poster Prize. I had the pleasure of working with Louis Delbaere to improve communication across our community, and to increase interactions between the ACA and the Canadian National Committee of the IUCr. More recently, as Chair of the Canadian Division of ACA, I have tried to facilitate Canadian representation among session speakers, by negotiating with SIGs for Canadian co-Chairs of selected sessions. I have also worked with the Canadian Light Source to increase their visibility at Canadian Division and ACA meetings. In 2009, I served as Local Chair of the ACA meeting in Toronto, an experience I will always remember fondly. In addition to overseeing a fabulous group of volunteers supporting the ACA staff at the meeting, we took steps to revitalize the tradition of events for accompanying persons. The ACA family is truly that: a family.

It will be an honor and great pleasure to continue my participation in the ACA as Canadian Representative on Council. Jim Britten has raised the Canadian presence on Council to new heights and leaves huge shoes to fill. However, I hope that my experience in several capacities and my commitment to the ACA as a focus and advocate for national and international crystallographic research, will equip me to serve the community well in this position.

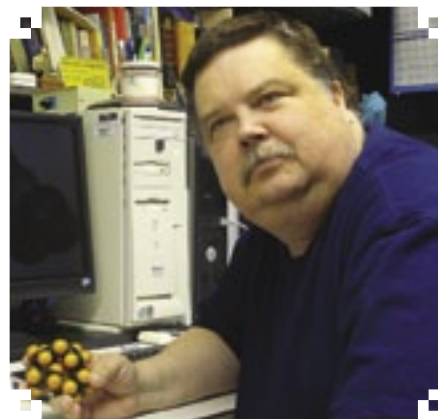
Stephan L. Ginell, Communications



Biophysicist/Crystallographer, Biosciences, Argonne National Laboratory, Argonne, IL 60439.

Statement: Communications is our life! Be it publishing scientific results, presenting at meetings, teaching, or casual discussions with colleagues. There is, however, the role of communications with the general public that is often overlooked. Communicating our scientific results and agendas (why we do structures) to the general public is critical in gaining approval for larger funding initiatives, such as synchrotron and neutron radiation facilities and structural and functional genomics as well as for the general success of our society. In order for the general public and our legislative leaders to strongly support science they need the information on why. A strong and focused PR presentation to support the research of ACA members is essential. Additional areas that I would like to see supported more are the communications between the different disciplines of crystallography and communications between the crystallographic community and other areas of science. I will strive to make communications amongst the members of our scientific community and with the general public a high priority.

Joseph H. Reibenspies, Data Committee



Senior Research Instrument Specialist, Texas A & M University, College Station, Texas 77843.

Statement: I am honored to have been elected to the Data, Standards and Computing Committee. As an old programming hack I have written and debugged thousands of lines of crystallographic code over last twenty-five years. I understand the importance of crystallographic software to our community and how that software interacts with the average scientist.

As a laboratory manager and director I know the importance of standards to the operation of a crystallographic facility. I have personally written dozens of Standard Operating Procedures (SOP) and Standard Administrative Procedures (SAP) for my laboratory to fulfill the requirements of the Good Laboratory Practices as well as numerous training manuals, laboratory notes and technical manuscripts. I have also written and edited a powder diffraction book and co-authored hundreds of scientific papers. Documentation is a critical link in the crystallographic chain of information and is the one that is most often overlooked.

As a professional crystallographer I have solved literally thousands of structures, collected thousands of data sets and sorted many hundreds of gigabytes of crystallographic information. With so much information to process it is important that the community set standards and make recommendations on how to process and disseminate this information to other scientists and among ourselves.

It is in this light that we must maintain and support the various databases that

we rely on to gather and disseminate this information. These databases must be available in a format that all scientists can readily access. This is also true for the crystallographic software that is available now and will be in the future. As a programmer I realize that coding the program is the easy part, explaining it to others is the real task.

The aging of our present programs is another serious concern we as a community will face in the next ten years. Many of the programs that we rely on were written by individual scientists or groups for their own personal use. These programs were distributed to others and have now become the standard for our community. The programs do not have a commercial base and as such are generally free and open to the public. The question that we face is what will become of these programs when their authors have retired and their groups disbanded.

To these ends I support various initiatives:

1) *Software stewardship*: Popular software that is now freely available must be supported and the stewardship of the software must be established for long term stability.

2) *Expanded access of crystallographic databases*: Access to the crystallographic databases should be at the institutional level. All scientists and engineers would benefit from structural information if that information is readily available on a web based system. This initiative would involve well documented web based search engines and institutional licenses.

3) *Standardization of data formats*: Software and instrument vendors should be given incentives to produce or export their data in a standard format.

4) *Broader appeal for the crystallographic sciences*: In particular the proper use of crystallographic software. I believe that this can be accomplished at the local level, if established crystallographic laboratories would share their knowledge and experience with their neighbors. The established laboratories would need incentives and compensation to undertake this task as it would be a drain on their resources; however the rewards would be a larger well informed community and a

source for future graduate students and trained employees.

5) *“White papers” from selected symposia (ACA conferences) on subjects related to Data, Standards and Computing*. The “white papers” would be written by the symposia chairs from material presented at ACA sponsored symposia and reviewed by the committee and the ACA. Selected “white papers” would then be made available on-line for use and reference by various funding, academic and industrial institutions. For example a researcher could support their funding proposal by referencing a “white paper” that was the end result of an ACA symposium or a department could employ the ACA “white paper” as a mechanism to advance a crystallographic agenda. In any case the “white papers” would be welcome documentation of ACA promoted initiatives and a source of information for researchers and administrators.

I will also work with the Data, Standards and Computing Committee and the ACA to advance these and other initiatives that would best fit the Committee’s and ACA’s mission. In this race for science we have been handed a golden baton, it is up to us to hold it, improve our position in the race and eventually pass it on to the next runner or we may drop it. The choice is ours.

Jeanette A. Krause, Continuing Education



Director & Sr. Research Associate, Richard C. Elder X-ray Crystallography Facility, Dept. of Chemistry, University of Cincinnati, Cincinnati, OH 45221.

Statement: It is an honor to be elected to serve on the Continuing Education committee. I first served on this committee from 1997-1999 and, as mentioned in my statement so many years ago, and which is still true today - the world of crystallography is alive, well, and continually evolving. Thus, we are constantly in a process of continuing our crystallographic education whether it is on our first day or after many years in the field. There is much to be learned from our colleagues regardless of specific crystallographic sub-discipline. I will strive to continue the legacy of high-quality workshops and tutorials that has become the norm of the ACA.

Contributors to this Issue:

Sidney Abrahams, Ross Angel, Aaron Bart, Jennifer Cash, Yuan Cheng, Margit Fabian, Christopher Farrow, Joe Ferrara, Rita Giordano, Varin Gosein, Sudipto Guha, Syd Hall, Hua He, Chris Hill, Janet Iwasa, Ryan Jackson, Kyra Jones, Judy Kelly, Serah Kimani, Kevin Kirouac, Emmanuelle Laffly, Meytal Landau, Cora Lind, Angeline Lyon, Kyle McLaughlin, Edgar Meyer, Tara Michels-Clark, Bruno Morosin, Kyle Morris, Victor Naumov, Yi Peng, Virginia Pett, George Philips, Li Qiu, David Rose, Karthik Sathiyamoorthy, David Sayre, Stacy Smith, Daniel Vega, Weina Wang, Nobukiko Watanabe, Carrie Wilmot, Winnie Wong-Ng, Wen Yang, bomina Yu, Linda Yu

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The following notes were written by recipients of 2010 ACA and IUCr travel grants. They were asked to comment on their personal experiences at the ACA meeting: what they thought of the venue, the events for young scientists, the overall program and their own presentation, were they first timers and whether or not they are ACA members. They were unanimous in giving thanks for the award and many indicated that they would not have been able to attend without the additional support provided by the student travel fund. These 'kids' are our future – please keep this in mind when you are asked to contribute to the travel fund.



Yuan Cheng

ACA 2010 was definitely a fantastic experience for me. The Global Phasing workshop was a perfect start for the week. It was so joyful and efficient to learn about those cool programs directly from the software developers. I really expect to attend more ACA workshops in the future.

The quality and scope of the science presented at the meeting was highly impressive. I was very glad to be able to learn about the latest progress in many different fields of x-ray crystallography in such a short period. My favorite sessions include *Longer Wavelength Phasing*, *Pushing the Envelope on SAXS* and *Structural Enzymology: Mechanistic*.

My overall experience in Chicago was really unforgettable and I look forward to attending the meeting in New Orleans.

This was my 4th consecutive ACA meeting and I felt that it was especially momentous. As the Chair of the Young Scientist Special Interest Group (YSSIG) I was very pleased to see so many young scientists attend the YSSIG annual meeting. There were several new faces and ideas that I feel will enhance the effectiveness of the activities and events of next year's meeting in New Orleans. It will be exciting to see all the things that we have planned come



Ryan Jackson

crystallographers settled in their careers. Relationships were made that will help me as I advance through the stages of my career. The sessions were excellent! I enjoyed the talks of the Nobel laureates and found all of the talks I attended to be very well prepared and of exceeding quality. This year I was able to chair the Etter Award Symposium, which was a great experience. I was very impressed with the quality of research other young crystallographers are doing. I was able to present my research at the poster session and was very pleased with the opportunity. I stood at my poster for the entire session and felt that my data and presentation were well received. Overall I loved the meeting this year. I felt it was very well organized and gave me ample opportunity to meet people and learn more about the field of crystallography.

This was my second ACA meeting in a row and I thoroughly enjoyed every second of it. Chicago is such a vibrant city of great architectural beauty and it was an apt location for a meeting that discusses crystals that could be considered miniature architectural wonders as well as their structures and associated recent



Karthik Sathiyamoorthy

technological developments and findings. The Nobel laureates lectures were highly inspiring and it established to me clearly again that persistence and hard work are the keys to

success. It is something that every young scientist like myself needs to always keep in mind. The sessions were overlapping and I often found myself wanting to be in two places at once but I managed to attend most of the talks relevant to my field and interests. The session on the precession camera and others with historical references were fascinating. The meeting was truly international and my poster was well received. I had many students and faculty approach my poster, ask questions and give good feedback. I eagerly look forward to my next ACA meeting at New Orleans and sincerely thank ACA for the travel grant that truly dissolved the dilemma of whether I would be able to come to this meeting.

My ACA experience this year at



Weina Wang

Chicago was very valuable to me in several respects. When I first arrived at the meeting, I was welcomed at the front desk with a package of meeting materials including 4 different ribbons: travel award winner, first time attendee, student, and mentee, which defined my roles throughout the meeting. This meeting was the first large crystallography meeting I have been to. Talks that focused specifically on different aspects of macromolecular crystallography were of great interest to me. There were also lots of opportunities to talk face-to-face with fellow students and senior scientists who were otherwise known only from reading their papers. It was also the first time I presented a talk at an international conference and I received a lot of nice comments and feedback that was valuable to me as a senior graduate student. In addition, I really enjoyed the *Professional Odysseys* session hosted by the Young Scientist SIG where many insightful comments were shared by the three panelists. This year's ACA meeting was an exceptional experience for me and I look forward to attending next year in New Orleans.



Nobuhiko Watanabe

Chicago was my first ACA meeting. I had an excellent time attending lectures and interacting with other scientists. The informative scientific sessions covered a broad spectrum of the current crystallographic research. Among all of the lectures I attended, the keynote lectures by the Nobel laureates were very inspiring to me. The workshop prior to the conference was very educational. Though it was just one day, the amount of information presented and skills it taught were priceless. During my poster session, I had the opportunity to present and discuss my recent results with professors and students. I would also like to thank my supervisor for taking me to the Mentor/Mentee dinner. In this casual setting, I had a great time talking with other mentors and their students about scientific and non-scientific topics. Overall, Chicago was an exciting city and I had a great time staying there.



Kyra Jones

ACA 2010 in Chicago provided an opportunity to enjoy and explore a wonderful, vibrant city on my first trip to the US. I even tried a Chicago-style pizza and was delighted to watch a few explosions being filmed for the upcoming *Transformers* movie from my hotel room. During the conference, I attended the events run by the Young Scientists such as the mentoring dinner and the mixer. I enjoyed meeting other students and networking with both up-and-coming as well as experienced scientists. I found the presentations to be very educational and enjoyed attending both the talks and

poster sessions. We are in the process of starting a new lab and being able to speak to the exhibitors was very useful. It was nice to be immersed in an environment in which other students and scientists understood the methodology I am using in my research and to learn about other areas of crystallography. I was nervous, as this was the first presentation I ever gave at a scientific conference, but I felt the talk went very well. I really enjoyed sharing my research results and the questions I received were inspiring and demonstrated interest in my research. I am now a proud ACA member and I am looking forward to attending future conferences.

I was pleased to see that the ACA meeting attracted a wide variety of crystallographers, chemists, biologists and physicists from a broad international community. I was



Margit Fabian

able to attend talks by experts, visit the poster session and the exhibitors and network with other young scientists. I felt especially fortunate to hear the plenary lectures by the 2009 Nobel laureates in chemistry. All three presentations gave me new information and I am very grateful for the opportunity to participate at the conference and listen to these revolutionary talks.

The colorful and throbbing city of Chicago was a worthy choice for ACA 2010. It was my first conference in this area and I learned much in field of biomaterials and new methods for structure analysis. I enjoyed all the presentations, particularly the session on *What can your Beamline offer you*. The meeting was a great event for me and I looking forward to being at the next one.

As a graduate student, I enjoyed the conference very much, especially the invigorating talks and the beautiful scenery of Chicago. There were many talks that could actually make me rethink my



Hua He

own research and spark fresh ideas. It was also very nice to meet other graduate students, sharing the sweet and the bitter as we progress toward earning a PhD. This was my first time to give an oral presentation at any kind of conference and I was very grateful for the opportunity to gain valuable feedback from professors who are big names in the area. These are the experiences that someone would have never had if he/she was just confined in the lab. I also had a chance to look around the city of Chicago. I can't believe that they have such a beautiful lake view right from the city. I really wish I could come back again



Rita Giordano

This was my first time at an ACA meeting and my first time in US. I was able to learn more and more about crystallography and I appreciated the session on *Radiation Damage* for the interesting and useful discussion regarding the subject of my thesis. I found the meeting really absorbing for the wide range of different topics covered, from small molecules to macromolecular crystallography, I gained a new perspective on other research areas.

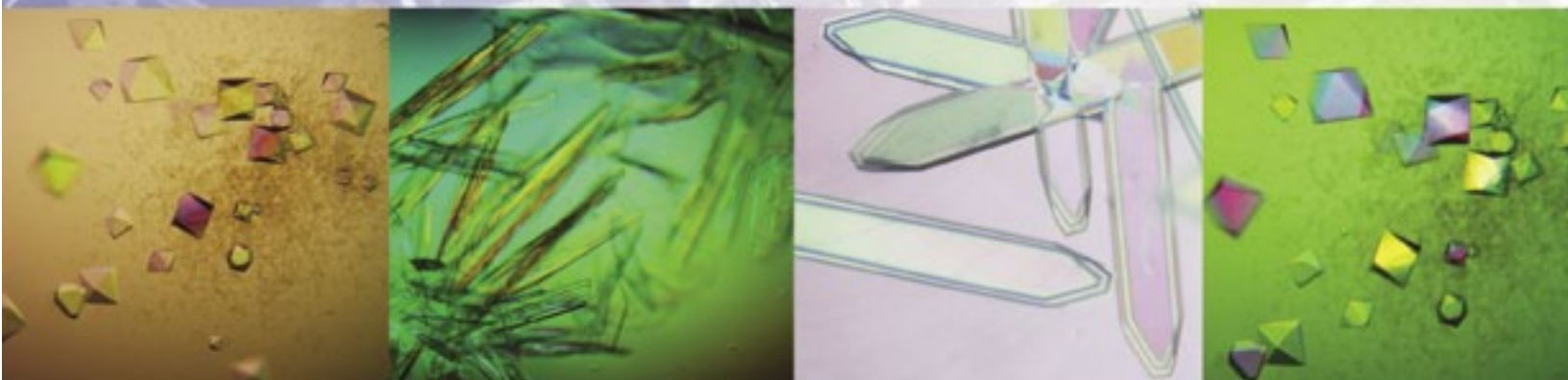
I liked the Young Scientists mixer; that was a very good way to get to know other students and young scientists. During the dinner I had very interesting conversations and expanded my network of contacts in the crystallographic community.

The poster session was very well organized, I had the opportunity to speak with many of the experts in my field, and get important advice and suggestions regarding my work. During the other poster sessions I was able to exchange different ideas with other participants.



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Wen Yang

For me the 2010 meeting was successful in both organization and scientific content. With so many scientific sessions it was easy to select lectures that interested me.

The exhibit show gave us all a chance to see new products and learn of recent developments that make crystallization, data collection and structure determination easy and essentially automatic. All of the posters and stories were interesting, especially when we could have a chat with the authors about their findings. I gave a poster presentation and it was a good chance for me to share my work with many famous scientists and younger ones. I also got some very useful suggestions and thoughts while standing by my poster. In addition, the events for young scientists were a good platform to exchange ideas and research techniques. The two things that most impressed me were the lectures from the 2009 Nobel laureates and the *Exciting Structures* session which gave us information on what's hot in structural biology today. I was also very surprised and excited to meet some structural software founders and my former friends and collaborators, exactly amazing. I hope to attend the 2011 meeting in New Orleans.

My talk in Chicago, *Phase progression of alumina nanoparticle catalyst supports as a function of synthetic temperature* was presented in the *Local Structure* session. Though a bit intimidating, it was a privilege



Stacy Smith

to present my research to a crowd filled with experts in the field of local structure and small molecule crystallography. I was able to meet and talk with many of these experts. I was also truly honored

to be named an Etter Student Lecturer by the Neutron Scattering SIG. My presentation was early in the conference, so for the rest of the week I could relax and enjoy the flow of information. Each session contained interesting and informative talks; I learned about incommensurate structures, symmetry mode analysis, non-ambient experiments, weird and functional materials, energy-related materials, phase transition mechanisms, and powder diffraction in general. I attended the three plenary lectures given by the 2009 Chemistry Nobel Prize winners where I learned a great deal about both ribosomes and macromolecular crystallography. Many of the posters I attended also dealt with biological macromolecular analyses and helped educate me on this previously unfamiliar topic. I enjoyed meeting many of my peers at the Young Scientists mixer and equally enjoyed the banquet where I finally connected faces with names for many of the ACA leaders and staff.

Chicago was my first ACA conference, and it reintroduced me to the wide world of crystallography. The diverse topics presented widened my vision to some of the many exciting challenges in crystallography. At the same time, it was a joy to see new research in my field of interest, applications of the atomic pair distribution function. The session on *Local Structure* was outstanding.

The poster session was one of the best I have ever attended. My poster was on a rather specific topic, the application of the atomic pair distribution function to nanoparticles and small molecules. Nonetheless, since the ACA attracts a diverse crowd I met some new people during my poster session and was able to stir up interest in my work. One interaction with another young researcher re-kindled my interest in a dormant project; I've lost a bit of sleep on it since then.

I had a very good experience at the meeting



Christopher L. Farrow

and I look forward to attending again in the future. I left with more ideas than I have time for, and that's the way I like it. I saw some old friends, some of whom came from across the globe. Thanks to the organizers for putting together such a great conference (in a great city!) and giving young scientists an opportunity to get engaged with the wider community.

I would like to thank Charles W. Carter for allowing me to present my work in the *Biological Impacts of Structural Biology* session. This was a great opportunity for me to get exposure and feedback for my current research. Overall, this year's meeting was



Kevin Kirouac

excellent. I saw many enlightening lectures and poster presentations and had the opportunity to speak with a broad range of scientists with diverse backgrounds and interests. I also

met many fellow PhD students and post doctoral fellows who shared their experiences and future goals and who will likely become future collaborators. The fantastic lectures on ribosome structure and mechanism by three Nobel laureates were a true pleasure and a highlight of the meeting. In addition, Chicago was a beautiful city and was a great venue for the conference.

This was my second ACA meeting and it was a wonderful experience. I was much more familiar with the organization of the meeting, and was therefore able to get the most out of the plethora of research presented by the many talks and posters. It was nice to meet face to face the people whose research has inspired the works of so many others.



Linda Yu

This meeting was especially exciting for me, since I was there not only to

present my own research, but also to support my fellow labmates in their presentations. In the same poster session where I presented my work on pyruvate carboxylase, an important enzyme that has been implicated in obesity and type 2 diabetes, Christine Huang presented her poster on propionyl-CoA carboxylase, a member of the same family of biotin-dependent carboxylases. Another labmate, Kehui Xiang, blew us all away with a recount of his journey to the structure of Symplekin, and how he finally triumphed over the especially frustrating task of removing a free phosphate in the active site that was inhibiting complex formation. Last, but not least, my PI, Liang Tong, presented an in-depth talk focusing on the recently solved structure of propionyl-CoA carboxylase, a huge protein totaling 750kD, and its implications on our lab's future research into other enzymes that are involved in fatty acid metabolism.

I had the pleasure of meeting professors, post-docs, and students from all over the world whose research differs considerably from my own. I was also fortunate enough to meet people whose research goals are very similar to mine, specifically Martin St. Maurice of Marquette. I found that discussing project successes and failures both with those who initially had no idea what I was talking about, as well as with those who are intimately immersed in the same research, was tremendously rewarding. I left the meeting anxious and excited to return to lab so that I could begin exploring answers to the many questions inspired by my new acquaintances. Each year I am more and more impressed by the ACA, and I am genuinely looking forward to next year's meeting.

This was my second time at an ACA meeting. The first was in Knoxville, 2008. This time I particularly enjoyed the talks by the 2009 Nobel Prize winners and many sessions especially *Structural Insights into the Cause & Treatment of Cardiovascular Disease and Macromolecular Complexes & Assemblies*. The oral sessions were really informative and introduced me to modern research methods.

Moreover, as a structure-based drug design new learner, the poster sessions provided me a great opportunity to learn

what others have done in same the field. I had great conversations with them. They not only answered all my questions, they also gave me lots of suggestions, which will be very helpful to my research. I was amazed to talk to other researchers in different fields from different universities and companies, and learned various



Li Qiu

techniques from their more than 300 posters. All of this useful information will help me determine which projects can be promising, and what career path I will follow.

I really enjoyed this wonderful meeting in the beautiful city of Chicago. I am definitely looking forward to the next one.

The ACA meeting in Chicago was very exciting and well organized. The presentations by three Nobel Prize winners were very inspiring and thought provoking. The Sheraton was a perfect venue for this conference given its centralized location and its proximity to downtown Chicago. In addition, the rooms for the sessions accommodated the attendees comfortably, however, the ambient temperature was quite cold in the hotel. The events for young scientists, including the mixer, were a great way to interact with other crystallographers and informally talk about one's research, and to generate new ideas. The program covered a wide variety of



Varin Gosein

topics, but seemed to lack enzymology. Also, most of the talks seemed to focus on techniques rather than using structural biology as a tool to answer fundamental biological questions like the talks in the Etter Award symposium. The program did however expose me to new

fields that I would have otherwise passed over. Given that this was my second meeting, my presentation went very well and I received a lot of input from others, including professors and post docs with lots of experience. I am an ACA member and overall this meeting was very informative and intellectually stimulating.



Tara Michels-Clark

As a first year graduate student my experience in Chicago was unique. It gave me an opportunity to meet many new people who share similar research pursuits. My educational background is in mathematics, so as someone new to crystallography I felt this conference was a wonderful chance to learn about the crystallographic community and the research that is current in the field. Chicago was a great city and the Sheraton was central to many great restaurants.

The conference activities like the young scientist mixer were a fun outlet to meet other young scientists and make not only professional connections but also new friends. The poster session showcased a lot of great work. I was able to talk with several who had resolved some very complicated protein structures. This was quite impressive and gave me a chance to see some of the more varied applications of crystallography. The meeting program had a wide range of topics making it easy to glean a lot of new information and ideas. I particularly enjoyed the local structure talks, especially those utilizing computational methods like density functional theory. This is most similar to my area of research modeling disordered crystal structures using evolutionary algorithms. My presentation at the Etter Award Symposium was well received and I was able to talk with several people who gave me additional ideas to pursue in my research. I plan to attend future ACA

meetings and will certainly suggest this meeting to other graduate students at the University of Tennessee.



Aaron Bart

This was my first ACA meeting and what an experience! There were so many great events and lectures during the week it was hard to prioritize which ones I would attend. I made it a point to expand my knowledge of

the field by going to lectures that were far from my own research, this was aided by the diverse range of topics the meeting had to offer. I very much enjoyed the various social events that were catered towards the young scientists; it was nice to have a relaxed setting to speak with mentors. I was also able to present a poster of my research and it was quite refreshing to have a very well informed audience in crystallography and structural biology, which provided some very interesting discussion. I had a wonderful time and learned quite a bit. It feels great to be an ACA member and I look forward to the meeting next year.

Many would agree that the ACA 2010 meeting was a success; I'm glad to have been part of it! I was particularly impressed by the wide coverage of different aspects of x-ray crystallography on the program; there was always something interesting to look forward to in every session. As a student, I found the talks that were focused

on emerging technologies and methods development very useful. It was a huge honor to be in the midst of the 2009 Nobel laureates and to hear their thrilling stories on the amazing ribosome. I was impressed by the quality of



Serah Kimani

poster presentations in the meeting and it was great to engage with the presenters and to learn of the fascinating research that is happening out there. As a poster presenter and a first time attendee, I'm glad to have had an opportunity to present my work on a platform with a lot of experienced crystallographers; I received very constructive comments that will help my work in the future. It was great honor to have been awarded the RCSB Protein Data Bank poster prize.

The mentor/mentee dinner was a disappointment. The venue was small and congested and did not provide the much-needed space for interactions. The Young scientists' mixer on the other hand provided a great environment for mixing and mingling. The venue was great; there was plenty of space inside and outside and the service was of high standard.

Overall, it was a great meeting and I would love to participate again. I am grateful for the travel award that enabled me to get to Chicago from South Africa.

This was my first ACA meeting and I was very excited to attend as well to have the opportunity to give a talk, especially as the BioMac SIG Etter Student Lecturer. After speaking in the *Exciting Structures* session, I was able to discuss my work with other crystallographers and received a lot of good feedback. I really enjoyed the opening plenary lecture by V. Ramakrishnan. I also enjoyed going to talks in the different sessions, in particular the Etter Award Symposium where students gave all the talks and the wide range of research covered was very interesting. I also learned more about fiber diffraction, an area I knew very little about before attending, by sitting in on two of the fiber diffraction sessions. As a graduate student looking to further



Kyle McLaughlin

my career in crystallography, I found attending the YSSIG meeting as well as the mentor/mentee dinner very rewarding. Overall, the ACA was a great experience, as I was able to

discuss research in an informal setting with other students and crystallographers. Thank you again for this opportunity and I am look forward to attending ACA meetings in the future!

ACA Chicago marked the first time I gave an oral presentation at a conference, and I wasn't sure what to expect. I was pleased to find out that all the details were taken care of, the environment was very welcoming and supportive, and people



Angeline Lyon

were interested in what I had to share.

The conference was very well organized, with a diverse range of sessions that allowed me to learn more not only about macromolecular crystallography,

but also about new techniques in data collection and structure determination. The overall environment was also warm and friendly, and I had the chance to meet many people in related areas, as well as having the pleasant surprise of meeting colleagues from graduate school.

Overall, the Chicago ACA conference was a great experience, and I enjoyed it very much. I'm very happy to be a member of such a great organization, and I look forward to attending future ACA meetings!

Chicago is a great city to visit in the summer and the Sheraton was right in the middle of downtown with close-by attractions and restaurants. The downside was the accommodation fees that were very high. The hotel charged extra for wifi, using the health club, and breakfast; all of which



Meytal Landau

are usually included in the room fees. Since food was not provided at the conference, overall expenses were very high.

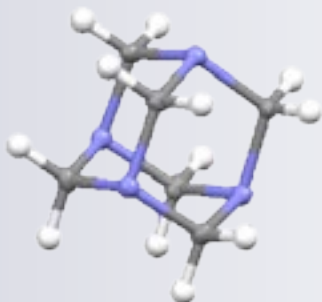
Cryocool Gas Stream Cooler

Revolutionizing the Speed and Resolution of Data Collection for Crystallographers!



Cryogen Free Model

Hexamine at 10 K (LHe Cryocooler). The X-ray C-N bond length is the same as from neutron data.



Cryo Industries of America, Inc. (CIA) has been manufacturing gas cooling systems for over 25 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, 4.5 K to 600 K.

This innovative design features 'Never-Ice' technology to produce the most efficient and economical stream cooler on the market.

Ice-Free Sample at 8 K using LHe Cryocooler



Warning: Once you have acquired a taste for LHe-temperature crystallography, even 90 K data collection tends to become a bit distasteful. (Warning provided by Cryocooler user)

There was a nice pub night for the Young Scientists, giving the opportunity to getting to know colleagues in a relaxed and informal environment. The program was broad enough to cover most of my interests. I learned about new fields and the current focus in my area. The down side was that some of the interesting sessions (for me) were held at the same time. Also, it was hard to follow so many talks over more than 5 days.

This was my first ACA meeting and I am very glad that I got the opportunity to give a talk; I enjoyed it. I got good feedback about the presentation and about my research which made me very happy. The questions I received were good and for me they reflected people's interest and understanding of the presentation. I also had helpful discussions following the talk.

I am an ACA member and I enjoyed the meeting and feel that I gained much from interactions with colleagues and from some of the talks. I also enjoyed walking in the streets of Chicago. I will come back next year if I have something new to present and to discuss.

I am a graduate student from the Universidad Peruana Cayetano Heredia in Peru, and Chicago was the first time I attended an ACA meeting. I profited



Chris Pacheco

considerably, both personally and scientifically, not only by attending several lectures but also by giving a poster presentation which helped me remarkably because I received advice to improve my work and motivation to go forward. My participation in this event provided me an invaluable experience indeed.

I also think that discussions on different topics during the meeting were pretty good giving many attendees the opportunity to learn and combine information from many areas. Furthermore, I think that events for young scientists were important in motivating them to getting more involved

in the scientific community.

I am an ACA member and definitely would like to come back next year and hope that more young scientists have the opportunity to attend such well developed meetings as this.

I thought Chicago was a very good location for an ACA meeting. It was within walking distance of several restaurants and



Jennifer Cash

entertainment. I also thought the hotel itself was very nice. As far as the events for young scientists, I didn't like the setup for the mentor/mentee dinner. I had expected it to be a more open format where we could walk around and talk to different people, but we were very restricted to the space where we initially sat down. Also, it took almost two hours for us to receive our food, making for a very late dinner. I was very interested in the talks pertaining to macromolecular crystallography. However, the topics seemed to be very redundant with many of them focusing on RNA/DNA/protein complexes.

I would like to have seen more talks that focused on macromolecular crystallographic techniques or maybe more broad topics that included signaling proteins. Even though I also listened to talks that were outside of my current interests, I found many of them difficult to follow as they seemed to be very specific in their subject matter. Some of the talks I enjoyed most were actually given by graduate students.

ACA 2010 was a meeting of many firsts



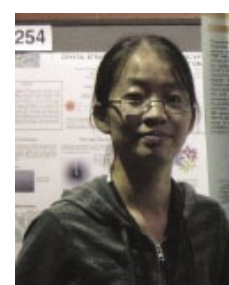
Kyle Morris

for me. It was my first visit to America, my first ACA meeting and my first chance to be able to speak at such a large meeting. I have been left very impressed. As a final year PhD

student I was delighted to win the travel award enabling me to come to the meeting and felt privileged to be selected to give a talk. I felt the hotel accommodated the meeting well with a variety of different sized lecture halls. I gave my talk in one of the smaller venues opening the *Prions, Amyloids and Friends* session to a full audience, who were receptive and asked probing questions. I was pleased that these prompted helpful discussions with people inside and outside of my field in the following days. Other talks in my and other sessions were very interesting, and although I am biased, the quality of the other student talks was something to be admired. Following from this, the young scientist mixer event was great to get to know other students like myself and to compare experiences but the busy social calendar (special thanks to Buddy Guy's *Legends & Rayonix*) and poster sessions also made it easy to meet a good variety of scientists at different stages of their careers.

I am now an ACA member and hope to see another meeting in the near future!

As a young investigator of protein crystallography, I thoroughly enjoyed the wonderful sessions, particularly *Membrane & Associated Proteins Software Integration & Databases, Data Collection Strategies, Exciting Structures, and Macromolecules, Complexes & Assemblies*. I was excited by those great talks and also learned more about crystallographic development. Most impressive were the excellent lectures given by the 2009 Nobel laureates in Chemistry that inspired us to keep exploring our great world by crystallography. I also liked the interesting talk by Ray Triebel. Furthermore, the poster sessions were well organized to give us a great chance to



Yi Peng

discuss results and exchange ideas. As this was my third ACA meeting, I was so glad to reunite with many old friends as well as to make new friends. Finally, I am pleased to have experienced this wonderful meeting in Chicago. I look forward to future ACA meetings.

This was my first time at an ACA conference and even though I am not a core crystallographer it was a great learning experience. The location was excellent, being in the heart of Chicago, and also because I am from Champaign-Urbana which is only a two and a half hour drive away.

The YSSIG mixer on Sunday was a great way to increase interaction



Sudipto Guha

among the younger members of the community and it is something I've not seen in other conferences so far. I met a lot of other young scientists from various fields and from all over the world and it was great fun to talk about our respective areas of research. The three keynote talks by the Nobel laureates were a high point of the conference for me.

My poster was well received and I was kept busy throughout the entire poster session and had a number of stimulating discussions with the people around. I would also like to commend the organizers for the exhibitor program that was very informative and also showcased the latest technological innovations in the field.

The ACA meeting was a great way for me to learn about all the different types of crystallographic research. This was my first meeting, and it was a surprise for me to learn that even though crystallography itself is already a pretty narrow field

within biology and physics, there are numerous diverse subfields within it, many of which I had never heard about. It is somewhat intimidating, but also inspiring to know how broad, deep, and specialized modern science is.



Victor Naumov

I gave a presentation on my own research and was pleased at how well it was received. It also felt satisfying to walk around the exhibition floor, look at all the robots, emitters, detectors, and other gadgetry, and talk with their creators. Seeing all this advanced technology keeps reminding me about the ever-accelerating progress of science and about the great privilege allotted to me to be starting my career at such an exciting point in history. It also reminds me of all the effort it takes to succeed in this competitive environment and inspires me to work even harder.

As a young scientist in the Garcin Lab at the U of Maryland Baltimore County, it was a very exciting to present my research about the biochemical and structural characterization of soluble guanylate cyclase. Beyond this personal experience, I also had the great opportunity to attend

the lectures of the 2009 Nobel laureates.

I have been enthralled by the research accomplished over 30 years by these pioneers in the structural characterization of the ribosome machinery, leading to a better understanding of its workings. In 1980, after over 25,000 attempts, Yonath and co-workers obtained the first ribosome crystals, a prerequisite for crystallographic analysis. In 2000, Steitz, Moore, and coworkers solved the first structure of the large subunit, and Yonath and Ramakrishnan obtained the first structures of the small subunit. The first steps of a very challenging project were accomplished, allowing a better understanding of the mechanism and regulation of translation and the design of new antibiotics. For a young scientist aspiring to make a difference in research, these accomplishments are both mind-blowing and inspiring.

Emmanuelle Laffly



The ACA gratefully acknowledges contributors to the various award fund

2011 Award Winners

M. J. BUERGER



Gerald B Ansell
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Abraham Clearfield
Philip Coppens
Karl F Fischer
Richard Gilardi
Theodor Hahn
Andrew Howard
Heinz Jagodzinski
Carroll Johnson
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Tom C Terwilliger
Thomas R. Webb
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Etter Early Career
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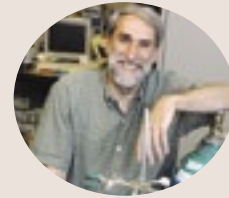
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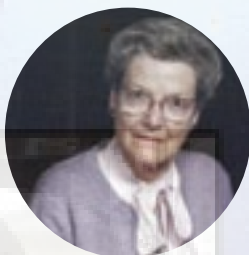
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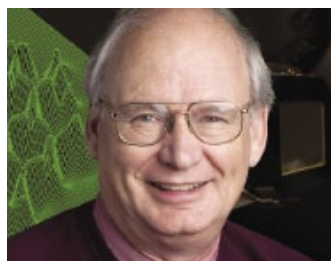
Bernard Santarsiero

Silver Honor Roll
 (donations of
 500-1000)

*Deceased



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 cklein@xula.edu



Local Chair
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Program Chair
Chris Cahill
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Poster Chair
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 Univ. of Wisconsin
 iguzei@chem.wisc.edu



May 28 - June 2, 2011
Sheraton French Quarter
 New Orleans, Louisiana

Deadlines:

Abstracts: January 31, 2011
Travel Grant Applications: January 31, 2011
Advance Registration: March 31, 2011
Hotel Reservations: April 14, 2011
Abstracts accepted online only
40% of all talks will be from contributed abstracts
Submit abstracts - register - full call for papers
www.AmerCrystalAssn.org
meeting2011.amerystalassn.org

Workshops

Symmetry-mode Analysis
Organizer: Branton Campbell

Introduction to PHENIX for Beginning to Advanced Crystallographers
Organizer: Paul Adams

Award Symposia

Patterson Award in honor of Keith Moffat

Margaret C. Etter Early Career Award in honor of Yuriy Mozharizskiy
Organizer: Jamaine Davis

Transactions Symposium

Time Resolved Photochemistry and Electron Density
In Honor of Philip Coppens on his 80th Birthday
Organizers: Peter Lee, Yu-Shang Chen and Jason Benedict

Evolution of Powder Diffraction Software
in Honor of Lachlan Cranswick
Organizer: Peter Stephens

Plenary Lecture

Ned Seeman - Winner of the 2010 Kavli Prize in Nanoscience

Banquet Speaker

Elizabeth Wood Award Honoree: Daniel Nocera

Microsymposia

Biological Macromolecules

Use of Databases in Structural Biology - Chair: Wladek Minor

Protein Structure Initiative: Tools for the Home Lab - Chair: Ward Smith

Structural Enzymology: Mechanistic - Chair: Zachary Wood

Membrane Protein Crystallization - Chair: Carla Slebodnick

Biological Macromolecules & the Canadian Division

Macromolecular Assemblies - Chair: Chris Hill

Structural Enzymology: Biology - Chair: Michael Murphy

Biological Macromolecules & Synchrotron

Microcrystals and Back to Merging Datasets - Chairs: Dominika Borak & Alex Soares

Structural Enzymology: Spectroscopy and Complementary Methods - Chair: Allen Orville

Biological Macromolecules & Young Scientists

Data Processing With the Pros - Chairs: Ed Collins & Andy Torelli

Phasing and Refinement for Dummies: No Book Required - Chairs: Ed Collins & Andy Torelli

General Interest & Service

Educational Inspiration: Crystallographic Teaching Techniques - Chair: Amy Sarjeant

Industrial

Challenges and Opportunities in Structure Based Drug Discovery - Chair: Nickolay Chirgadze

Panel Discussion: Industrial Access to National User Facilities

Materials & Powder

Resonant Scattering of Materials - Chair: Angus Wilkinson

Materials & Powder & Neutrons

Materials for a Sustainable Future - Chairs: Ashfia Huq & Claudia Rawn

The Devil is in the Details: Local Structure and Diffuse Scattering - Chair: Karena Chapman

Diffraction Studies of Magnetic Materials - Chairs: Yan Gao & Bryan Chakoumakis

Earth Materials - Chairs: John Parise & Ian Swainson

Crystallography and the Search for New Materials - Chair: Svilen Bobev

Materials & Powder & Neutrons & Small Molecule

In Situ Diffraction Studies - Chairs: Craig Bridges & Christine Beavers

Materials & Powder & Neutrons & the Canadian Division

Evolution of Powder Diffraction Software: in Honor of Lachlan Cranswick - Chair: Peter Stephens

Materials & Powder & Neutrons & Industrial

Diffraction Studies of Industrial Materials - Chair: Clarina De La Cruz

Small Angle Scattering

Surfaces and Interfaces - Chairs: Zhang Jiang & Masafumi Fukuto

Small Angle Scattering from Colloids - Chairs: Gegory Beuacage & P. Russo

Information in SAXS/WAXS Data - Chairs: Hiro Tsuruta & Lee Makowski

Small Angle Scattering & Synchrotron

Combined Tech. for Determining the Structure of Complexes & RNAs in Sol'n - Chairs: Yun-Xing Wang & John Tainer

Service

Undergraduate Research Symposium - Chair: Katharine Kantardjieff

Would you Publish This ? - Chair: Carla Slebodnick

Small Molecule

Modern Aspects of Crystal Engineering - Chairs: Travis Holman & Len MacGillavry

Cool Structures - Chair: Allen Oliver

Small Molecule & Service & General Interest

Small Molecule Machines - Chair: Christopher Incarvito

Scholarly & Pragmatic Aspects of Crystallographic Publication Practices - Chairs: Larry Falvello & Ilia Guzei

Synchrotron

Fast Science - Chairs: Tim Graber & Marco Cammarata

Maximizing the Scientific Results of Your Synchrotron Visit - Chair: Steve Ginell

Synchrotron & Small Angle Scattering

What Can Your Beamline Offer You - Chair: Ashfia Huq

Biological Macromolecules, Industrial, Synchrotron & Small Angle Scattering

New Bio-Science From Emerging Opportunities & Sources - Chairs: Bob Sweet & Dean Myles

ACA New Orleans - May 28 - June 2, 2011

Staying Green: The full set of abstracts will be distributed only on CDs with a hardcopy Program Schedule. We will have the 5 X& note pad portfolios but will not have a new meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Update: In an effort to reduce housing costs we have renegotiated the contract with the Sheraton to include **FREE WI-FI** in the sleeping rooms, so bring your laptops and stay connected to home and office for free. The room rates at the Sheraton are competitive 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. This helps keep registration fees in line and allows us to offer the 'extras' outlined above.

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 two nights accommodations free!

Financial support for young scientists will be available through the ACA and the IUCr. Applications for this support should be made by the abstract deadline on the meeting web site.

The Organizing Committee will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Union.

Registration fees

Fee	Registration fees	
	Advance (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**	\$ 50	\$ 50

WK.01 Symmetry Mode Anal.

Student	\$150	\$180
Others	\$185	\$215

WK.02 PHENIX

Student	\$120	\$155
Others	\$155	\$185

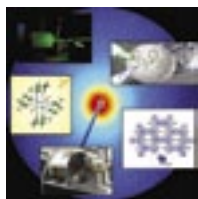
Mentoring Dinner Sponsored by the YSSIG

Mentor	\$50
Mentee	\$25
Banquet	\$70 (\$35 students)
YSSIG Mixer	Free for students and post-docs \$25 for all others

* 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, Exhibit Show and Get Together on Sunday morning. Register on-line or download forms to register by fax or mail:

www.amerystalassn.org/content/pages/2011-homepage
 Questions: aca@hwi.buffalo.edu



What's on the cover

The cover highlights a few of Philip Coppens' contributions to many areas of chemical crystallography. In celebration of the Year of Chemistry and Philip's 80th Birthday, the 2011 ACA *Transactions* Symposium will include presentations by Philip and his former students, postdocs and collaborators in the areas of time-resolved photo-crystallography and charge density. The images were arranged by Jason Benedict. Starting at the upper left and proceeding clockwise the images are:

1. A typical setup for a photocrystallography experiment. A laser strikes a single crystal during a simultaneous x-ray data collection.

2. Progress in solid-state single-crystal to single-crystal photochemical reactions: *Kinetics of the single-crystal to single-crystal two-photon photo-dimerization of α -trans cinnamic acid to α -truxillic acid*, J. B. Benedict and P. Coppens, *J. Phys. Chem. A* **113**, 3116-3120 (2009).

3. Experimental deformation density map of a photoactive zinc complex: *Charge density analysis of the ground state of the photochromic 1,10-phenanthroline zinc (II) bis(thiolate) complex*, S. Scheins, S.-L. Zheng, J. Benedict and P. Coppens, *Acta Cryst. B* **66**, 366-372 (2010).

4. A new ultrafast shutter for time-resolved synchrotron experiments designed by Milan Gembicky and Philip Coppens.

5. Image of crystal and landmark results of monochromatic time-resolved x-ray diffraction experiments illustrating the

rhodium-rhodium contraction observed in the excited-state: *A very large Rh-Rh bond shortening on excitation of the $[Rh_2(1,8\text{-diisocyano-}p\text{-menthane})_4]^{2+}$ ion by time-resolved synchrotron X-ray diffraction*, P. Coppens, O. Gerlits, I. I. Vorontsov, A. Yu. Kovalevsky, Y.-S. Chen, T. Graber and I. V. Novozhilova, *Chem. Commun.* 2144 - 2145 (2004).

6. Background: Single pulse Laue diffraction image from time-resolved experiments on the [bis(4-chloro-thiophenyl)-1,10-phenanthroline]zinc(II) complex.

Nominations for 2012

ACA Awards: Nominations for the **B. E. Warren, M. J. Buerger, Charles Supper, and Etter Early Career** Awards are due by May 1, 2011.

ACA Offices and Committees: In the fall of 2011 we will elect a new Vice-President and Secretary and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 1, 2011.

Full details describing the criteria for all ACA awards and offices can be found on the website (www.AmerCrystalAssn.org). All Nominations should be sent the ACA office (marcia@hwi.buffalo.edu)

2011 Dues are Due

Please renew promptly and remember to support your favorite ACA Award Funds. **NOTE: It is now possible to renew online at www.AmerCrystalAssn.org**

TRAVEL FELLOWSHIPS for XXII IUCr Madrid Congress, 22-31 August 2011

The US National Committee for Crystallography, in cooperation with the ACA, will provide partial support for travel to the IUCr Congress in Madrid, Spain. Graduate students, post-doctoral fellows, or untenured faculty members in any of the crystallographic, diffraction, and imaging Sciences affiliated with the IUCr are eligible to apply. Undergraduate students will be considered in exceptional cases. Applicants must be training at a US institution. Applications from underrepresented minorities will be especially welcome. Recipients are expected to submit a short report (*) in return for their support after the meeting.

An application should include the following:

1. Cover page indicating name, address, telephone number, fax, and e-mail address of the applicant and name and address of mentor;
2. A current Curriculum Vita for the applicant;
3. Abstract including title and authors, with applicant as presenter, submitted for presentation at the 2011 IUCr Congress;
4. A paragraph by the applicant describing where they are in their career and why they want to attend the Madrid meeting;
5. A letter of recommendation from the mentor detailing the group's travel funding and explaining why funds from the USNCCr are needed.

Send applications to:

Cora Lind
 Department of Chemistry, MS 602
 The University of Toledo
 Toledo, OH 43606
 (419) 530-1505
 fax: (419) 530-4033

cora.lind@utoledo.edu


Deadline: 1 March 2011

(*)The amazing part of an IUCr congress is the great opportunities to interact with scientists from all over the world. The participants represent their national science and technology, and I believe that the intellectual communications and exchanges at such congresses are most beneficial for each scientist. Therefore, it is extremely important that young scientists in the US attend such conferences and broaden their network internationally. The travel fellowship program makes these opportunities possible for students and postdocs from many scientific institutions.

MARCH 2011

5-9 **Biophysical Society 55th Annual Meeting**, Baltimore, MD www.biophysics.org

APRIL 2011

25-29  **MaThCryst School on Fundamental Crystallography**, Mahdia, Tunisia. www.crystallography.fr/mathcryst/meetings.php

MAY 2011

10-14  **2011 International Conference on Structural Genomics** - Toronto, Canada www.icsgo2011.org

21-26 **ACA 2011, Sheraton Hotel New Orleans, New Orleans, LA** *Program Chair: Chris Cahill; Local Chairs: Cheryl Klein-Stevens & Ed Stevens*

23-27  **MaThCryst-Workshop on Crystallographic Software**, Tokyo, Japan

JULY 2011

11-15 **62nd Annual Applied Microscopy Conference**, Chicago, IL www.mcri.org

AUGUST 2011**OCTOBER 2011**

24-28  **MaThCryst-Workshop on Mathematical Crystallography**, Manila, Phillipines

JULY 2012

28-2 **ACA 2012, Westin Waterfront Hotel, Boston, MA**

SEPTEMBER 2012

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

2011 ACA Summer Small Molecule Course

The 10-day intensive course will be offered tentatively July 18st through July 27th, 2010 at the Indiana University of Pennsylvania located in the town of Indiana about 80 miles east of Pittsburgh, PA. The course will cover both single crystal and powder diffraction and each day will consist of lectures in the morning, hands-on workshops in the afternoon and computer tutorials at night. While some advanced topics will be introduced (Structure solution from powder data, advanced probability methods, solving difficult structures), the curriculum will mostly emphasize fundamental crystallography and no prior crystallographic experience will be assumed. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection and are expected to have completed at least undergraduate courses in chemistry, physics and mathematics and are advised to read in advance "Crystal Structure Analysis: A Primer", by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 24 attendees, who in past years have come from the U.S. and abroad from academia (students and faculty), government and corporate institutions. There will be at least 12 experienced teaching faculty present. Tuition will be \$300 (or \$800 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for an additional \$450 (\$750 or \$1,250 for corporate labs). Approximately 12 student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a waiver of tuition and living costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments at IUP will include two Bruker-Nonius CAD4 single crystal diffractometers, a Bruker D8 Advance and a Rigaku Miniflex powder diffractometer. In the past, Rigaku-Americas brought a SCXmini X-ray Crystallographic System and Bruker AXS brought a Smart X2S Benchtop Diffractometer to the IUP laboratory. Students will also have access to the Duquesne University X-ray Facility which has a Bruker APEX II single crystal diffractometer and a PANalytical X'Pert Pro powder diffractometer. The IUP computer facilities are excellent and each student will have access to an individual computer during the nightly tutorials. Access will also be available to the Cambridge structural data base and the ICDD powder diffraction data base. The software used in the course will be Bruker-Nonius SHELXTL, Rigaku Americas CrystalClear, GSAS/EXPGUI, FullProf, CRYSFIRE and CRYSTMOL.

The Course registration form can be obtained from the ACA web site at www.hwi.buffalo.edu/ACA/. Completed forms must be received before May 27th, 2011 by Charles H. Lake, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically lake@iup.edu for full consideration. Further information will be updated on the web site or can be obtained from lake@iup.edu or craven@icubed.com. Foreign students may be accepted early to provide extra time to process visas

Charles H. Lake and Bryan M. Craven, Organizers.



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