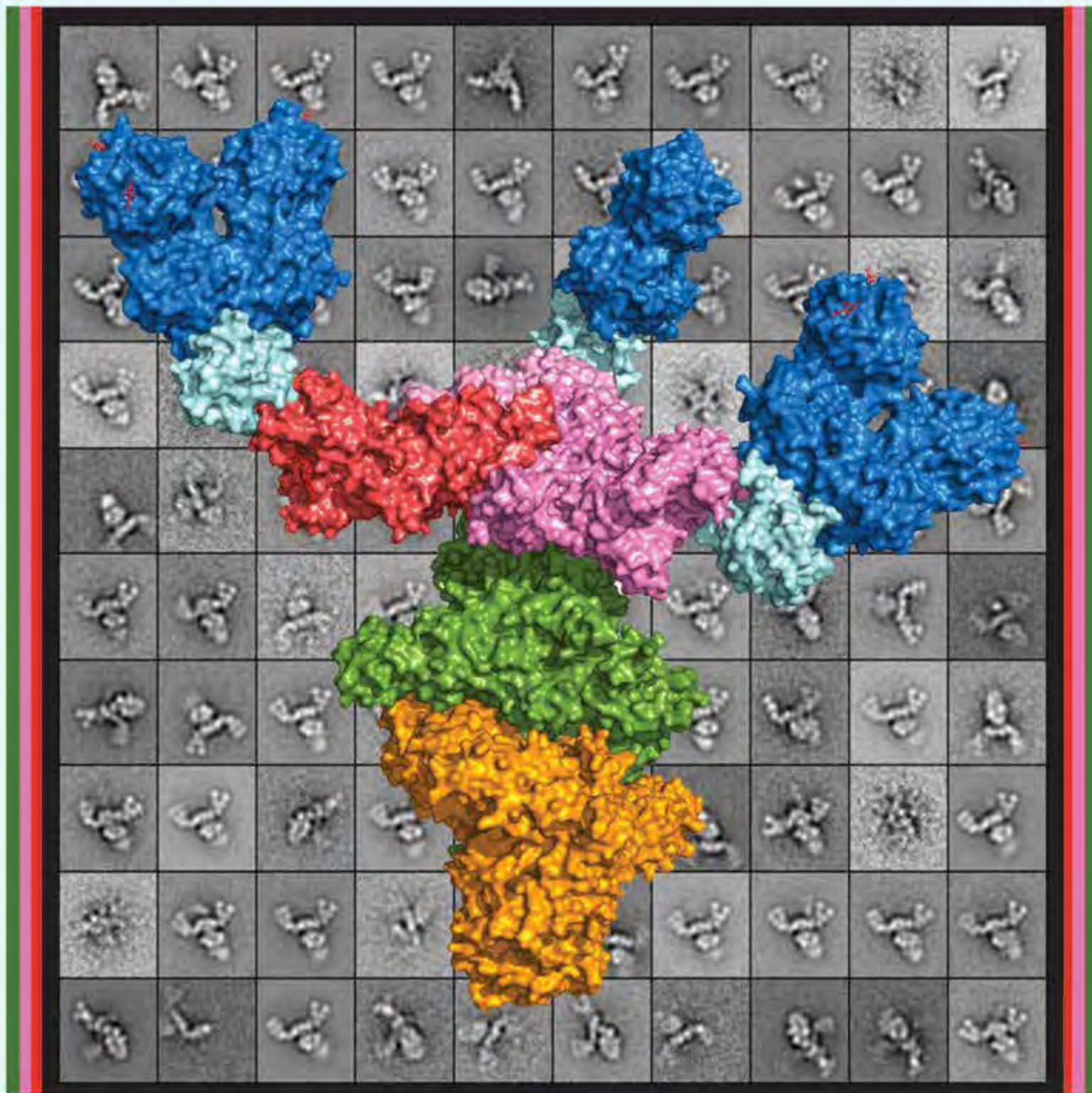


ACA Reflexions

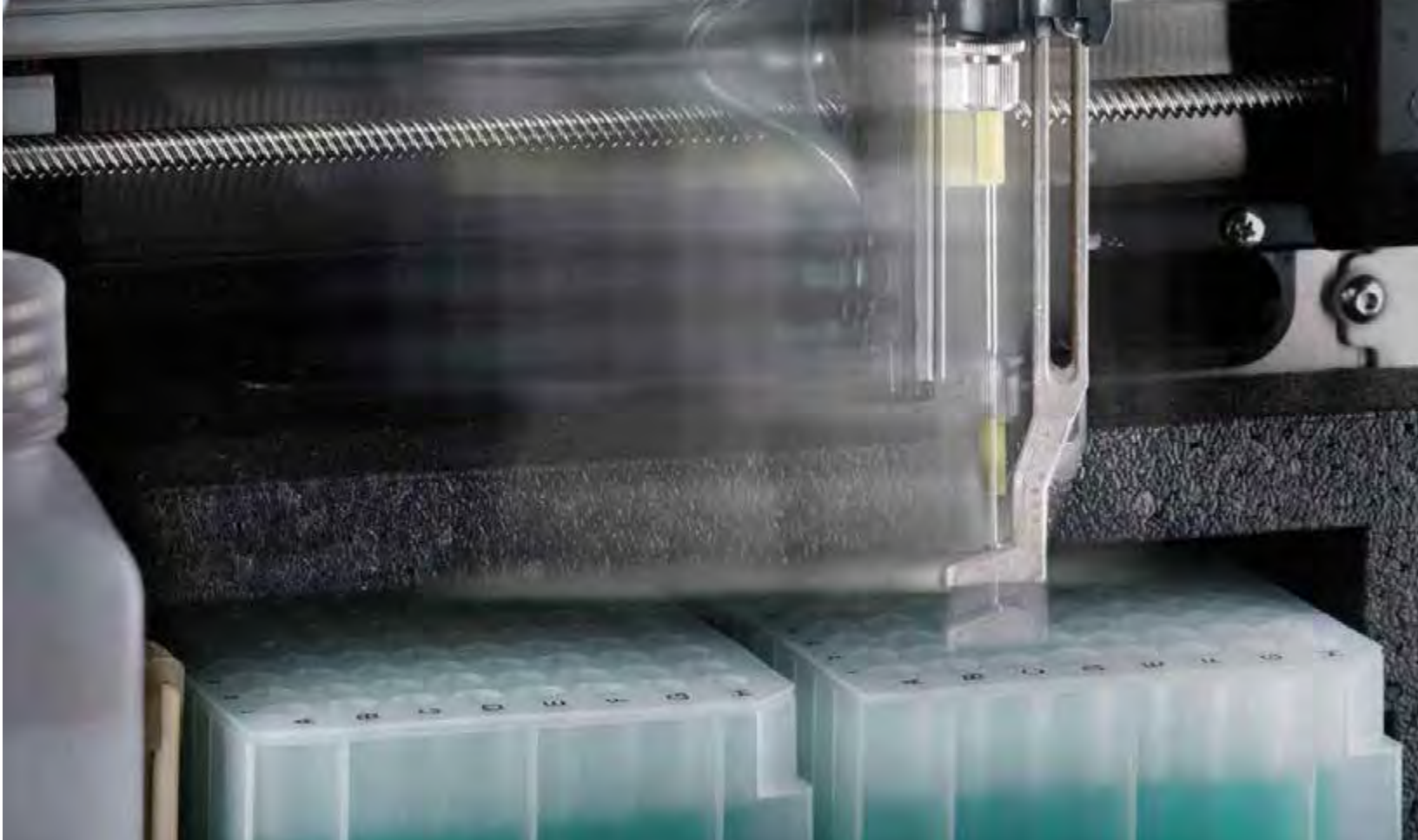
ACA
Structure Matters

Number 2

Summer, 2014



***Etter Early Career Award at
Albuquerque ACA Meeting***



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Presidents Column**Outreach and Education – Two New Thrusts:**

Going forward we have identified four key objectives for the ACA that can move us to a more vibrant society. Two of the four are outreach and education, but more of that in a minute.

Have you noticed students' excitement when they figure out a puzzling technology, or when they put the 'pieces' together for themselves the first time? That excitement is contagious.

The same excitement delights young children. As natural scientists, they love to explore. Just like Dorothy Crowfoot Hodgkins at age 9, fresh from trying to identify minerals she found close to where she lived in Africa, declared that she wanted to study chemistry and then crystallography so she could "see atoms." We can use crystallography to excite children about science and STEM fields in general. The International Year of Crystallography 2014 gives us just such an opportunity to start this outreach.

Outreach, you say. When do I have time for that in my busy schedule? Grants now often require a component of outreach. Furthermore, a student or scientist "knows what they know" better when they explain it to someone else. For example, I have played the viola since I was in 6th grade. But in college, I had the opportunity to teach a beginner how to play the viola. I listened differently after that. In fact, I played differently after that. Teaching indeed helps us "know what we know".

It's refreshing to see our YSSIG members sharing the joy of crystallography with high school students. Since they started at the Boston meeting in 2012, they have worked with local high school classes to grow lysozyme crystals (thanks to a generous donation of materials from Hampton Research). Classes often take their crystals to an x-ray facility where they can see how they diffract.

This was so exciting that the teacher who worked with the students in Boston repeated the experiment in 2013 without YSSIG support! YSSIG also worked on the project with high schools in Hawaii and in Albuquerque. They even went to the New Mexico Museum of Science to give live "grow your own crystals with lysozyme" demonstrations to draw museum goers into Doris Schattschneider's lecture on Escher and crystallographers.

Hands-on demonstrations based on experiments that students do and the conclusions they draw from them are close in spirit to the new science standards for K-12 education. So-called Next Generation Science Standards, based on guidelines from the National Academy of Sciences, involve students in discovery through experiments that they do themselves. Experiments such as growing crystals illustrate guiding principles and applications of these principles to technology, showing how the structure of materials determines their physical properties, and illustrating how function follows form.

But how can these isolated instances involve our membership as a whole. Through the diligent efforts of Danielle Gray (U of Illinois) and the support of Brian McMahon (IUCr), ACA's IYCr website has been launched (www.iycr2014.org/acal/home).

On it are links to educational handouts and experiments from elementary to university level. Further, there are resources such as downloadable posters and museum mineral and gem websites. And finally, there's a way to connect with classrooms in your area so that you can "know what you know" and ignite a spark in the classrooms. We provide a service where a school can request a crystallographer to assist in a crystal growth demonstration, a diffraction experiment and/or an exploration of symmetry.

OK. That's outreach (we hope it's here to stay, keeping us "young," so to speak). But what about more formal education? Since we lost the Department of Crystallography in Pittsburgh (two of our ACA Fellows – Helen Berman and Ned Seeman – were students there), fewer and fewer crystallography courses are being taught. Crystallography is sometimes viewed as a tool rather than a cutting edge technique to study the structure of matter. But we remember that 1/8 of all Nobel Prizes awarded in chemistry and physics involve crystallography! And we can be proud of that.

So how can crystallography education continue? Our Strategic Planning Committee (send suggestions for your long term view of the ACA to stratplanaca@gmail.com) has concluded that making our meetings a center for crystallographic education is one way to keep our membership excited and up-to-date, as well as to become a magnet for crystallographic continuing education. We are working with SIGs now to ensure that more educational sessions are offered at our national meetings. This will be a reason to attend. Not only to hear about the latest research in crystallography but to learn about the latest improvements in hardware and existing software and especially to become familiar with the tools and techniques used in new and emerging areas of research.

To underscore this need I mention that, among others, I have heard from Joseph Stanko, a former professor of mine and a 47-year member of the ACA. He wrote suggesting that we provide opportunities for ACA members to learn the newest methodologies and the latest tools in use today. We have already taken some steps in this direction: Andy Torelli and Ed Collins have run *Blackboard* sessions for the BioMac SIG for the past 5 years. The sessions have been aimed at updating macromolecular crystallographers in the use of software critical for data collection, reduction, structure solution, and refinement. We need to involve the other SIGs in offering similar educational sessions so that we can use our meetings to educate ourselves, to help each of us "know what we know."

So how do we start to revitalize our membership? First, excite and engage through public outreach. We excite children and their parents through crystallography. We invite local politicians to our celebrations in this year of crystallography. And second through education and training. We get back to our collective "black boards" to each one teach one. We train the next generation of crystallographers and use our meetings to do it. We can do it.

Martha Teeter

**AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2013 and 2012**

	CURRENT FUNDS (2013)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2013	2012
ASSETS				
Current Assets:				
Cash	129,807		129,807	180,374
Investments	576,272	447,165	1,023,437	985,436
Inventory	6,393		6,393	6,393
Accounts Receivable	0		0	30,214
Total Current Assets	712,472	447,165	1,159,637	1,202,417
Fixed Assets:				
Computers and Printers	0		0	0
Office Equipment	0		0	0
Accumulated Depreciation	0		0	0
Total Fixed Assets	0		0	0
TOTAL ASSETS	712,472	447,165	1,159,637	1,202,417
Liabilities:				
Unearned Revenues	49,023		49,023	56,432
Credit Card Liabilities	414		414	1,916
Total Liabilities	49,437		49,437	58,348
Fund Balance:				
Unrestricted	663,035		663,035	700,474
Restricted		447,165	447,165	443,595
Total Fund Balance	712,472	447,165	1,159,637	1,144,069
TOTAL LIABILITIES & FUND BALANCE	712,472	447,165	1,159,637	1,202,417

* Current Balances in individual restricted funds - *as of December 31, 2013*

Bau Neutron Award	35,641
Buerger Award	38,229
Etter Award	66,858
Fankuchen Award	70,086
Patterson Award	46,510
Pauling Award	36,571
Supper Award	12,243
Student Travel Fund	18,337
Trueblood Award	38,583
Warren Award	30,403
Wood Science Writing Award	53,524
 History Fund (unrestricted)	 4,520

A more detailed report on the ACA finances
may be obtained by sending a written request
to the ACA office in Buffalo, PO Box 96, Ellicott
Station, Buffalo, NY 14205-0906.

News from Canada



The third Annual Macromolecular Crystallography Data Collection (MXDC) School was held at the Canadian Light Source (CLS) in Saskatoon on June 10-14, 2013. There were 22 participants from across Canada and the USA who attended this hands-on data collection school. In addition to the data collection component of the school the participants had an in depth view of PHENIX, a program developed for structure solution by Paul Adams, Tom Terwilliger and others. Paul was the invited speaker for this tutorial, a favorite among the attendees of the school. As this issue of *Reflexions* goes to press, the fourth Annual MXDC School will have been held at the CLS on June 9 - 13, 2014. This year's invited speaker was Trevor Moraes (University of Toronto). He discussed molecular replacement, structure validation and the most effective way to use the graphics program COOT.

Following the Data Collection School, the Second Annual Meeting of Structural Biologists at the Protein Structure, Function and Malfunction was held at the University of Saskatchewan in Saskatoon (June 14-15, 2014), organized by David Sanders and Mirek Cygler.

A third meeting/workshop was also held in Vancouver (June 6-10, 2014): the 5th Canadian Chemical Crystallography Workshop was organized as a satellite to the 97th Meeting of the Canadian Society for Chemistry. The workshop was targeted towards chemistry graduate students and PDFs who wanted to learn the fundamentals of the theory and practice of structure determination using x-ray crystallography. More information can be found at www.canadiancrystallography.ca/5thccw/index.html.

The International Year of Crystallography (IYCr) is being celebrated at several places across Canada this year. Louise Dawe (Wilfred Laurier University) is the coordinator of the IYCr activities that will take place at the IUCr Congress in Montreal (August 5 - 12, 2014). Several other events are being planned at other locations in Canada. Marie Fraser (University of Calgary) and Masood Parvez (University of Calgary), will put on a demonstration and lectures at the University of Calgary in September. Michael James is organizing an event to be held at the Telus World of Science in Edmonton in September or October (telusworldofsciencedmonton.ca). The dates for this are not yet finalized.

The executive of the Canadian National Committee for Crystallography (CNCC) is about to change its current membership. Members of the present CNCC who will be replaced are: Marie Fraser (Treasurer), Stan Cameron (Member at Large) and Pam Whitfield (Vice Chair). We wish to thank each of them for their dedicated service to the advancement of crystallography in Canada. In addition to maintaining geographical, linguistic and gender parities as much as possible, the CNCC needs executive members with certain skills. Marie Fraser is a macromolecular crystallographer from Calgary who has served for several years as treasurer. Thus we need a treasurer to manage the Larry Calvert Travel Fund of the CNCC as well as to submit the annual registered charity information to the Canada Revenue Agency. Stan

Cameron (Dalhousie University) is a small molecule crystallographer, and Pam Whitfield is a powder diffraction specialist who recently has moved from the NRCC in Ottawa to the Spallation Neutron Source at the Oak Ridge National Labs in Tennessee. In addition to replacing these people it is also necessary that the CNCC have someone to serve as webmaster for their web site and as the editor of the annual *Newsletter*. If you are interested in any of these positions please contact the CNCC Secretary, Joe Schrag at: joe.schrag@cnrc-nrc.gc.ca.

Louise Dawe and Michael James will shortly be sending out a survey designed to shed light on the reasons why so few Canadians are members of the ACA. Approximately 46 members have renewed their memberships for 2014. This represents only 20% of those in Canada who claim to use crystallography as a research tool and are listed in the World Directory of Crystallographers published by the IUCr. Louise and I urge you to respond to this survey so that some positive action may be taken to alleviate this sorry and, I hate to say, apathetic situation.

The Canadian Division of the ACA, chaired by Louise Dawe, held their annual meeting at the ACA meeting in Albuquerque, NM. We had an outstanding turnout of 75% of those Canadians who were at the 2014 ACA Meeting. It was too bad that only 8 Canadian members of the ACA were at Albuquerque. I do realize that there was a conflict with the Montreal Meeting of the IUCr and that travel funds are short, but we would like to have a larger representation of Crystallographers to decide on the Canadian content of future ACA meetings. Among the several items that were discussed at this meeting was the Canadian participation at the 2015 ACA meeting in Philadelphia. There have been a few suggested sessions for this meeting. David Rose suggested a session on Structural Glycobiology. Pawel Grochulski has agreed to co-chair a session on Complementary Methods with someone from the BioMac SIG and Michael James suggested a session on the Thermodynamics of Ligand Binding to be co-chaired by Barry Finsel in the BioMac Sig. It would be encouraging to have someone from the Small Molecule SIG suggest possible Canadian sessions for future ACA meetings.

Mike James



Both Marcia and Rao celebrated 25 years with the ACA in Albuquerque.

Martin J Buerger Award

Greg Petsko, Arthur J. Mahon Professor of Neurology and Neuroscience at Weill Cornell Medical College, and Tauber Professor of Biochemistry and Chemistry, Emeritus, at Brandeis University, has been selected to receive the 2015 ACA Buerger Award.

Petsko started his impressive career with a BA degree from Princeton University (1970). He then moved across the pond as a Rhodes Scholar at Oxford University to pursue his doctorate with Sir David Chilton Phillips, which he completed in 1973. After a brief postdoc in Paris, he started his career at Wayne State University School of Medicine and in 1979 he moved to the MIT as an associate professor in chemistry, becoming full professor in 1985. He remained at MIT until 1990, when he joined the faculty of Brandeis University as the Lucille P. Markey Professor of Biochemistry and Chemistry. While at Brandeis he later became the Gyula and Katica Tauber Professor of Biochemistry and Chemistry, directed the Rosenstiel Basic Medical Sciences Research Center and served a term as chair of the Department of Biochemistry. In 2012 he moved to Weill Cornell Medical College in New York City, where he was appointed as director of the Helen and Robert Appel Alzheimer's Disease Research Institute and as the Arthur J. Mahon Professor of Neurology and Neuroscience in the Feil Family Brain and Mind Research Institute. He is also professor of biomedical engineering at Cornell University.

The list of awards and honors he received for his extraordinary research activity is too long to report here. Highlights include: the Siddhu Award for outstanding contributions to x-ray diffraction from the Pittsburgh Diffraction Society (1980); the Pfizer Award in Enzyme Chemistry from the American Chemical Society (1986); the Max Planck Prize, shared with Roger Goody (1991); and the Lynen Medal, shared with Janet Thornton (2001). He is member of the National Academy of Sciences, the Institute of Medicine, the American Academy of Arts and Sciences, and the American Philosophical Society and, he is a Fellow of the AAAS. He is currently President of the International Union of Biochemistry and Molecular Biology.

During his career he has extensively used x-ray crystallography, molecular biology, yeast genetics, organic synthesis, enzyme kinetics and molecular dynamics calculations to understand enzyme structure and function. With Dagmar Ringe, his long-time collaborator at Brandeis, he has developed new diffraction techniques that allow recording entire macromolecular datasets in milliseconds and which, combined with low-temperature experiments, can be used to capture snapshots of catalytic intermedi-

ates. Recently he has focused his attention on neurodegenerative diseases, such as Alzheimer's, Parkinson's and Lou-Gehrig's diseases, using structure-based drug design techniques to develop possible therapeutics against what he defined, in his 2008 TED talk, as the "coming neurological epidemic".

Greg Petsko is a keen science communicator and an engaging public speaker. He is very involved in the discussions of the social aspects of science; following his first TED talk, he gave a second thought-provoking talk at TEDMED in 2012, where he took the audience through the science of Alzheimer's disease and its genesis, and pointed out the urgency of acting against it in an increasingly aging world—and the present lack of investment (i.e. money) to do so. He also contributes comments to *BioMed* and *BMC Biology*, and for more than a decade he has maintained a monthly column on science and society in *Genome Biology*. These entries are now collected in a book entitled *Gregory Petsko in Genome Biology: The first ten years*. (When pressed, however, he admits that the columns guest-written by his two dogs, Mink and Clifford, have been much more popular than those he writes himself.)

Petsko is a strong advocate of teaching arts and humanities as part of the science curriculum. He started his brilliant biochemical career with a major in classic literature, and he has often stated that studying humanities helped him become a better scientist. As such, while professor at Brandeis, alongside his biochemistry and chemistry classes, he taught several liberal arts courses: *The Social History of the Detective Story*; *The Treatment of Science and Scientists in the Cinema*; and *Critical Thinking*.

B. E. Warren Award

Laurence Marks, professor of Materials Science and Engineering at Northwestern University, is the recipient of the 2015 ACA Warren Award, which recognizes an important recent contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques.

Marks began his scientific career in the UK, earning his BA and his PhD at the University of Cambridge. Among his most significant recognitions, he received a Sloan Foundation fellowship in 1987 and the Burton Medal from the Electron Microscopy Society of America for achievements in electron microscopy by a young researcher in 1989. He has been fellow of the American Physical Society since 2002.

Laurence Marks studies materials at the nanoscale. He uses both a theoretical and a practical approach to analyze their atomic structures and to tweak their properties, with the idea of making them better suited for practical applications. His laboratory uses a wide variety of techniques, such as x-ray crystallography, scanning electron microscopy, transmission electron microscopy, atomic force microscopy, and

single particle spectroscopy to name a few, to characterize different materials, from their surface structure to their frictional properties, and to corroborate models predicted with algorithms developed in house.

His research in particular focuses on: achieving more efficient catalysis using controlled oxide nanoparticles; improving solid oxide fuel cells, to produce electricity directly from hydrocarbons; understanding the characteristics of oxide surfaces, still largely uncharacterized, to design more desirable surfaces; studying the tearing-and-wearing process caused by friction of metallic surfaces, to improve, for example, prosthetic devices; and engineering a new type of concrete/cement with a cheaper energy production cost.

Etter Early Career Award



Yan Jessie Zhang, from the Department of Chemistry and Biochemistry of The University of Texas at Austin, is the recipient of the 2015 Etter Early Career Award. The American Crystallography Association established this annual award in 2002, to recognize the work of scientists at the earlier stages of their independent careers in crystallography.

Zhang received her Bachelor of Science from Tsinghua University in 1997, working in the field of medicinal chemistry. She moved to the USA to gain a Master's degree from University of Oregon, in 2000, where she trained in crystallography with Brian Matthews. She earned a PhD in 2004 from the Scripps Institute, working in the laboratory of Ian Wilson on structure-based drug design. She then moved to the Salk Institute for Biological Studies to carry out her post-doctoral research on enzymes involved in transcription and oncogenic pathways, under the guidance of Joseph P. Noel. In the fall of 2008 she joined the University of Texas at Austin, where her main focus is to understand the mechanisms of transcriptional regulation and their impact in neuronal stem-cell differentiation.

Yan Jessie Zhang has already achieved many impressive milestones. As a grad student, she solved the crystal structure of the glycinamide ribonucleotide (GAR) formyltransferase, a fundamental enzyme in the purine biosynthesis pathway that is the target of several anti-cancer drugs. Zhang herself used the structural information she obtained from her crystallographic studies to design several potent inhibitors of this enzyme, one of which is currently in phase-1 clinical trials. During her post-doctoral research she began her studies on the RNA Polymerase II C-terminal domain (CTD), the protein that regulates the assembly of the transcriptional apparatus in Eukaryotes. Now, as an independent investigator at the University of Texas, Austin, she continues this line of research. Assembly of the transcriptional apparatus is regulated by the so-called "CTD code", a shape-encoded

language linked to the conformational state of the RNA Polymerase II CTD and regulated through phosphorylation. Merging her broad expertise in eukaryotic transcription regulation, x-ray crystallography and structure-based drug design, Zhang is currently studying the phosphatases that act on RNA Polymerase II CTD, to understand how their activities affect transcription, in particular in the context of cancer and neurogenesis. The final aim of her research is to design small molecules that could interfere with the function of these phosphatases and appropriately tune gene expression. As an example, she solved the structure of the phosphatase Scp1, involved in neural gene silencing, with a peptide representing its biological target and with a specific inhibitor called rabeprazole, providing a model for the development of new drugs that could potentially promote neuronal growth in patients suffering from neurodegenerative diseases.

Crystallographer Elected to National Academy: Marius



G. Clore has been elected to the National Academy of Sciences. Clore is the director of the Protein Nuclear Magnetic Resonance Section in the Laboratory of Chemical Physics at the National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health. His group focuses on protein complexes involved in signal transduction and transcriptional regulation, as well as on proteins related to AIDS. He is also interested in developing novel NMR methods to study transient macromolecular complexes.

Protein Society - Carl Brändén Award: This Award,



sponsored by Rigaku Corporation, was created to honor a scientist for significant contributions to the development of the field of structural biology field, both as a researcher and as an educator. The 2014 awardee is ACA member Stephen White (Department of Physiology and Biophysics, University of California-Irvine) White has greatly contributed to the field of membrane protein folding, focusing in particular on the thermodynamics of the process, and is a well-respected educator and mentor to his students.

Membrane proteins require the assistance of a special auxiliary machinery—a protein complex called the translocon—to migrate from the ribosome, where they are synthesized, to the membranes. Here, a complex network of interactions between the proteins, the lipid bilayers, and water steer the protein to its functional fold. Stephen White has studied this process using a variety of techniques: x-ray and neutron scattering to characterize the structural changes occurring in the polypeptides and in the lipid bilayers, as well as physico-chemical techniques to measure the energy required for the proteins to adopt the correct fold. His lab also studies translocon-assisted membrane protein folding, and uses molecular dynamic simulations to model the process. Finally, he uses his results to develop web-based membrane structure prediction tools.

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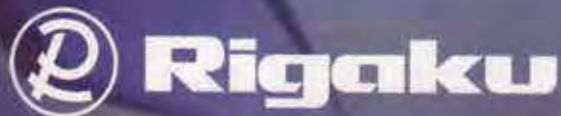
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White has had a quite extraordinary and eclectic career that has brought him many recognitions for his research, including: the Biophysical Society Distinguished Service Award in 1999; the Athalie Clarke Research Achievement Award from the UCI College of Medicine in 2000; a PhD *honoris causa* from Stockholm University in 2008; and the Avanti Award in Lipids from the Biophysical Society in 2009 “for his novel findings in the areas of membrane structure and protein insertion into membranes”.

ACS 2014 Gordon Hammes Biochemistry Lecture:



ACA Member Thomas Poulos (UC Irvine) is being recognized for his outstanding contributions in scientific research at the interface of chemistry and biology, particularly in the realm of biochemistry, biological chemistry and molecular biology. Poulos' research focuses on the structural biology of heme enzymes. He solved the first heme enzyme crystal structure, cytochrome c peroxidase, and the first cytochrome P450 crystal structure. Since then he

and his coworkers have solved the structure of other metallo-enzymes and related electron transfer proteins including nitric oxide synthase (NOS). These structural investigations coupled with protein engineering, enzymological, and spectroscopic approaches have sought to elucidate how these enzymes activate peroxide and molecular oxygen, a required step in many substrate oxidation reactions. A related area is the structure of redox protein complexes and how redox partner recognition is coupled to functionally important structural changes. In collaboration with Rick Silverman (Northwestern), the Poulos group also is working in the area of NOS structure-based drug design in an effort to develop therapeutic agents for neurodegenerative diseases. Poulos' Hammes Lecture will be delivered at the ACS national meeting in the fall of 2014.



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100 Years of Crystallography:

It was 1912 when Max von Laue and two of his colleagues,

Walter Friedrich and Paul Knipping, shot a beam of x-rays through a crystal of copper sulfate, discovering for the very first time the phenomenon of x-ray diffraction. An epoch-making discovery, in the words of G. Granqvist, the Chair of the Nobel Committee for Physics of the Royal Swedish Academy of Sciences, who awarded von Laue the Nobel Prize in 1914.

To commemorate the 100 years since the Nobel Prize to von Laue, the United Nations General Assembly has declared 2014 the International Year of Crystallography. During the course of the year, the IUCr has been coordinating the implementation of several educational initiatives to increase public awareness of the science of crystallography and to inspire young people, and has encouraged the organization of conferences and workshops all over the world, in particular in Africa, Asia and Latin America, to foster international collaborations and to advance research in the field. These initiatives are linked on the IUCr website. Among them, there are photography competitions to interpret “Crystallography in Everyday life” and crystal growing competi-

tions for secondary school students, open labs and workshops in many countries, lectures, seminars and meetings on crystals and crystallography.

Journals such as *Nature* and *Science* have published special issues to celebrate x-ray crystallography. *Nature's* January 29, 2014 issue focused on *Crystallography at 100*, and in July 2014 *Nature* will publish a second special collection entitled *Nature Milestones: Crystallography*. The collection will contain a series of short articles presenting key developments in the field, a chronology of events connected with each milestone, and a reprinted collection of landmark papers from *Nature* and other *Nature* titles. In March 2014 *Science* also published a “Crystallography at 100” special issue, which presented a well-balanced mixture of historical pieces and articles on technology development.

Update on the ACA History Portal: Work on the History Portal has been going full-speed since its inception. To help readers keep up-to-date with the latest additions, *RefleXions* will run a regular column listing what's new on the webpage.

The publication of the first five videos in the Nobel Prize section of the Portal is the highlight of this issue. The videos were recorded during the 1988 Nobel Laureates Symposium, during the ACA meeting in Philadelphia. The speakers were Sir John Kendrew, Dorothy Crowfoot Hodgkin, William N. Lipscomb, Herbert H. Hauptman, and Jerome Karle. In addition, there are also two videos of Linus Pauling giving the introductory and concluding remarks at the Philadelphia Symposium.

These historic videos are now available thanks to the joint effort of many people. Helen Berman converted the VHS tapes recorded at the 1988 meeting into DVDs; Ilia Guzei, from the Communications Committee, reformatted the digital files to be compatible for YouTube, split them into individual lectures and uploaded them; Virginia Pett took care of the titles and descriptions; Patricia Potter designed and implemented the Nobel Prize page and linked the videos to the individuals listed in the “People” tab of the History Portal. The result is a collection of invaluable talks by some of the most brilliant x-ray crystallographers of the 20th century.

Besides the Nobel chapter, two seminars from the 2013 meeting in Honolulu have also been uploaded on the Portal. Thomas C. Terwilliger's *Molecular Replacement and Model-building Using Distant Homology Models as Templates* celebrates his receipt of the Kenneth Trueblood Award. Alexander McPherson's presentation *Let Us Now Praise Famous Men* honors Richard E. Dickerson (recipient of the 2013 ACA Fankuchen Award) and other famous crystallographers of the 20th century.

Editors note: If you've enjoyed the “Living History” articles in *RefleXions* and online at the ACA History Portal, or if you've watched a video on the ACA YouTube Channel, perhaps you would like to volunteer for the newly established Ad Hoc History Committee (Chair, Virginia Pett; Members, Ilia Guzei, Judith Flippen-Anderson and Patti Potter). There are opportunities for varied talents: identifying authors, editing memoirs for the newsletter, recording videos at ACA meetings, making movies that combine speaker and slides. If you are interested in joining this Committee, please contact Virginia Pett, pett@wooster.edu.



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YSSIG News and Views



Los Alamos High School students, growing lysozyme crystals before their field trip to Los Alamos National Laboratory.

By all measures, this was an outstanding year for the YSSIG. Several of our officers were actively engaged in activities throughout the year including a trip to Paris for the opening ceremony of the IYCr. We not only continued our outreach activities, but expanded them to include additional events. The level of enthusiasm and participation at YSSIG events during the meeting in Albuquerque was extremely high, and we successfully recruited numerous volunteers to assist with events for next year.

YSSIG members chaired or co-chaired several scientific sessions including the *Etter Early Career Symposium*, *Exciting Structures*, *Blackboard Sessions: Data Processing with the Pros*, and *Industrial Research from Young Scientists*. We also hosted a young scientist orientation at the beginning of the meeting, an undergraduate symposium (in collaboration with the Society of Physics Students, SPS) and a *Career Development Panel*.

The YSSIG mixer was a hit! The event was held at the Andaluz rooftop bar in downtown Albuquerque. Both the atmosphere and refreshments provided were outstanding, and the feedback we received was overwhelmingly positive. There were greater than 100 individuals in attendance despite the rainy and cold weather. Several senior ACA members attended the mixer and interacted enthusiastically with the young scientists. Among them were the career odyssey panelists, and the President and Vice-President of the ACA.

We initiated a third High School Outreach with John Bacik and Javier Gonzalez at Los Alamos National Labs. We also held a crystal growth demonstration and educational information event at the New Mexico Museum of Natural History that was very well attended (> 30 non-scientists). This event, held in the atrium of the Museum on the Saturday preceding the meeting, accompanied the workshop and lecture by Doris Schattschneider.



Mariia Bauman (left) and Andy Torelli (right) interacting with young visitors to the New Mexico Museum of Natural History and Science during the YSSIG/Protein Data Bank crystal growing demonstration.

This was the first year that, together with the SPS, we organized an undergraduate symposium to promote undergraduate education. The undergraduate symposium started with welcoming remarks from ACA President Martha Teeter. This was followed by a lecture by Cora Lind-Kovacs, *Through the looking glass: A reciprocal space perspective*. SPS sponsored a reception for the students. The symposium also involved a poster competition (sponsored by SPS and MiTeGen). This year's winner was Eileen Brady.

All of this activity would not be possible without the generous support from our sponsors. We specifically would like to acknowledge Rayonix for funding the YSSIG mixer and Hampton Research together with Laboratory Product Sales (LPS) for its continuous support of the high school outreach. We are grateful to the SPS for supporting the first undergraduate symposium and to MiTeGen for its contribution to the first undergraduate poster award! We also acknowledge Bruker for its continuous support of young scientists and contribution to many YSSIG events! An additional note of thanks goes to Alkermes for sponsoring the *Industrial Research from Young Scientists* scientific session. And, of course, we would like to thank ACA for supporting YSSIG and subsidizing a variety of activities!



Yulia Sevryugina



Jarrod French



Protein Data Bank: 100,000 structures

The Worldwide Protein Data Bank (wwPDB) is proud to announce that it has released to the community its 100,000th structure on May 14, 2014. Established in 1971, this central, public archive of experimentally-determined protein and nucleic acid structures has reached this important milestone thanks to the efforts of structural biologists throughout the world.

This achievement coincides with another major cause for celebration: The International Year of Crystallography (IYCr). IYCr commemorates the centennial of x-ray diffraction, and providing an opportunity to commemorate the successes of our discipline and to examine how the sharing of structural information has been fundamental to enabling scientific discovery.



Function follows form: In the 1950s, scientists had their first real look at the structures of proteins and DNA at the atomic level. The determination of these early three-dimensional structures by x-ray crystallography inspired a new era in biology. The value of archiving and sharing these data was indisputable and, in 1971 the Protein Data Bank (PDB) was established as an international collaboration with sites in the US and the UK.

Beginning with just seven entries—carboxypeptidase A, chymotrypsin, cytochrome c, hemoglobin (lamprey), lactate dehydrogenase, subtilisin, and trypsin inhibitor—the PDB archive

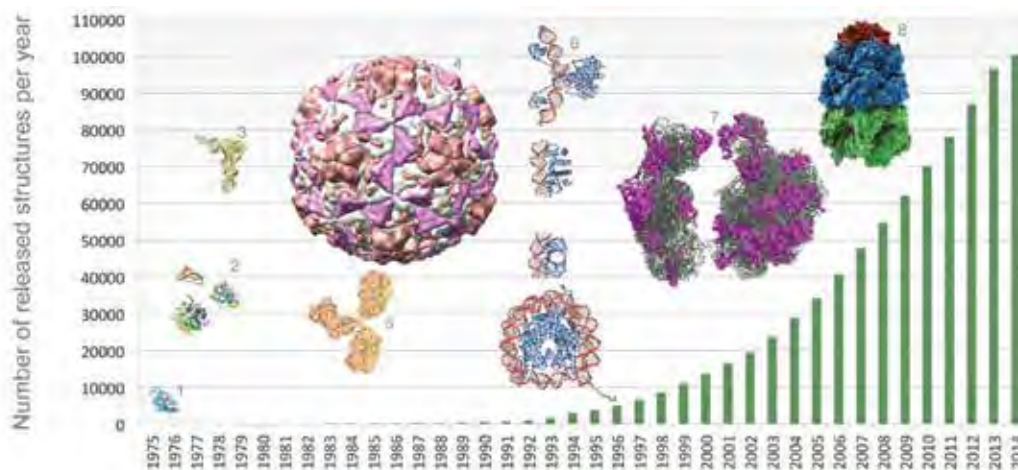
provides both a home and an access point to the world's output of biomacromolecular structures. The PDB is growing swiftly, doubling in size since 2008 and releasing around 200 new structures to the scientific community every week. The resource is accessed hundreds of millions of times every year by researchers, students, and educators wishing to explore how different proteins are related to one another, to clarify biological mechanisms and to develop new medicines.

“The PDB is a critical resource for the international community of working scientists which includes everyone from geneticists to pharmaceutical companies interested in drug targets,” said Nobel Laureate Venki Ramakrishnan of the MRC Laboratory of Molecular Biology in Cambridge, UK.

A growing community: Since its inception, the PDB has been a community-driven enterprise, evolving into a mission critical international resource for biological research. Since 2003 the Worldwide PDB (wwPDB) organization, a collaboration involving four PDB data centers in the US, UK, and Japan, has ensured that these valuable data are securely stored, expertly managed, and made freely available for the benefit of scientists and educators around the globe. wwPDB data centers work closely with community experts to define deposition and annotation policies, resolve data representation issues, and implement community validation standards. In addition, the wwPDB works to raise the profile of structural biology with increasingly broad audiences.

Each structure submitted to the archive is carefully curated by wwPDB staff before release. New depositions are checked and enhanced with value-added annotations and linked with other important biological data to ensure that PDB structures are discoverable and interpretable by users with a wide range of backgrounds and interests.

Future challenges: The scientific community eagerly awaits the next 100,000 structures and the invaluable knowledge these new data will bring. However, the increasing number, size and complexity of biological data being deposited in the PDB and the emergence of hybrid structure determination methods, which use a variety of biophysical, biochemical, and modelling techniques to determine the shapes of biologically relevant



Number of structures available in the PDB per year through May 14, 2014, with selected examples. Early structures included myoglobin (1; PDB ID 1mbn), the first structure solved by x-ray crystallography, and small enzymes (2; top: 4pti, bottom right: 2cha, bottom left: 3cpa). As technologies developed, the archive grew to host examples of tRNA (3; 6tna), viruses (4; 4rhv), antibodies (5; 1igt), protein-DNA complexes (6; top to bottom, 1j59, 1tro, 2bop, 1aoi), ribosomes (7; 1fjg, 1fka, 1ffk), and chaperones (8; 1aon).

molecules, constitute major challenges for the management and representation of structural data. wwPDB will continue to work with the community to meet these challenges and ensure that the archive maintains the highest possible standards of quality, integrity, and consistency.

About the wwPDB: The wwPDB (wwpdb.org) is the international partnership of four organizations that manages the PDB archive. Its mission is to maintain a single archive of macromolecular structural data that is freely and publicly available to the global community. It consists of: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; rcsb.org) at Rutgers, The State University of New Jersey and University of California San Diego and BioMagResBank (BMRB; bmrwisc.edu) at the University of Wisconsin in the USA, EMBL-EBI's Protein Data Bank in Europe (PDBe; pdbe.org) and the Protein Data Bank Japan (PDBj; pdbj.org).

The RCSB PDB receives funds from the NSF, NIH and DOE. The PDBe receives funding from EMBL, the Wellcome Trust, NIH, EU, BBSRC and MRC. PDBj is funded by the Japan Science and Technology Agency, and BioMagResBank by NLM.

Figure references: *Myoglobin* (PDB ID 1mbn): J. C. Kendrew, G. Bodo, H. M. Dintzis, R. G. Parrish, H. Wyckoff, D. C. Phillips. (1958) *Nature* 181: 662-666; J. C. Kendrew, R. E. Dickerson, B. E. Strandberg, R. G. Hart, D. R. Davies, D. C. Phillips, V. C. Shore. (1960) *Nature* 185: 422-427; *Enzymes* (top, 4pti): M. Marquart, J. Walter, J. Deisenhofer, W. Bode, W., R. Huber, (1983) *Acta Crystallogr B39*: 480; (bottom left: 3cpa): D. W. Christianson, W. N. Lipscomb. (1986) *PNAS, USA* 83: 7568-7572; (bottom right: 2cha): J. J. Birkoft, D. M. Blow. (1972) *J Mol Biol* 68: 187-240; *tRNA* (6tna): J. L. Sussman, S. R. Holbrook, R. W. Warrant, G. M. Church, S.-H. Kim. (1978) *J Mol Biol* 123: 607-630; *Virus* (4rhv): E. Arnold, M. G. Rossmann. (1988) *Acta Crystallogr A44*: 270-282; *Antibody* (1igt): L. J. Harris, S. B. Larson, K. W. Hasel, A. McPherson. (1997). *Biochemistry* 36: 1581-1597; *Protein-DNA complexes*, top to bottom (1j59): G. Parkinson, C. Wilson, A. Gunasekera, Y. W. Ebricht, R. E. Ebricht, H. M. Berman. (1996) *J Mol Biol* 260: 395-408; (1tro): Z. Otwinowski, R. W. Schevitz, R.-G. Zhang, C. L. Lawson, A. Joachimiak, R. Q. Marmorstein, B. F. Luisi, P. B. Sigler. (1988) *Nature* 335: 321-329; (2bop): R. S. Hegde, S. R. Grossman, L. A. Laimins, P. B. Sigler. (1992) *Nature* 359: 505-512; (1aoi): K. Luger, A. W. Mader, R. K. Richmond, D. F. Sargent, T. J. Richmond. (1997) *Nature* 389: 251-260; *Ribosome* (1fjg): A. P. Carter, W. M. Clemons, D. E. Brodersen, R. J. Morgan-Warren, B. T. Wimberly, V. Ramakrishnan. (2000) *Nature* 407: 340-348; (1fka): F. Schluenzen, A. Tocilj, R. Zarivach, J. Harms, M. Gluehmann, D. Janell, A. Bashan, H. Bartels, I. Agmon, F. Franceschi, A. Yonath. (2000) *Cell* 102: 615-623; (1ffk): N. Ban, P. Nissen, J. Hansen, P. B. Moore, T. A. Steitz. (2000) *Science* 289: 905-920; *Chaperone* (1aon): Z. Xu, A. L. Horwich, P. B. Sigler. (1997) *Nature* 388: 741-750.

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Structural Dynamics – News and Updates

Structural Dynamics is an online-only, open-access journal that provides a forum for the community of scientists working on the development, implementation, and use of new tools for the determination of static and time-evolving structures. *Structural Dynamics* is the first journal entirely devoted to this field, with a wide range of methodologies that interrogate, in “real-time”, not only the evolving geometric structure, but also the underlying electronic structure of assemblies of atoms, as well as correlations between them. The journal covers the following areas:

Structural dynamics of molecular systems, biological systems, solid materials, liquids and solutions, and surfaces and interfaces

Static structural determination, static imaging techniques and studies using highly coherent sources

Dynamical studies of systems both in and out of equilibrium, with a time resolution from femtoseconds to milliseconds

Spatial resolutions from 1 Å to 1 μm

Electronic structure studies connected to molecular/lattice/protein structure

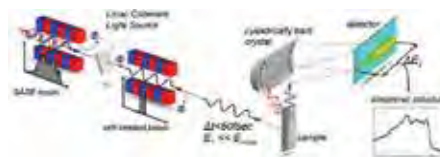
Structural Dynamics Editorial Board: The Board welcomes new Associate Editor Toshinori Suzuki (Professor of Chemistry at the Graduate School of Science of Kyoto University), a prominent scientist in molecular beam scattering and ultrafast photoelectron spectroscopies of chemical reaction dynamics in gas and liquid phases. Suzuki joins Editor-in-Chief Majed Chergui (Switzerland) and Associate Editors Thomas Elasser (Germany), Franz Pfeiffer (Germany), George Phillips, Jr. (USA), Gwyn P. Williams (USA) and Linda Young (USA) to complete an international editorial board whose expertise encompasses all areas of research covered by the journal.

Structural Dynamics Advisory Board: The two most recent additions to the Structural Dynamics Advisory Board are John Helliwell and Nobel Laureate Ahmed Zewail.

John R. Helliwell (University of Manchester, UK) is the recipient of the 2014 ACA Patterson Award for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography. His career has been dedicated to exploring new applications of synchrotron radiation as well as to improving synchrotron and neutron facilities worldwide. He also pushed forward the development of Laue methods for time-resolved studies.

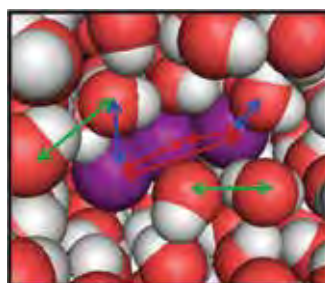
Ahmed Zewail (Linus Pauling Chair Professor of Chemistry and Physics, and Director of the Center for Physical Biology at Caltech) was the sole recipient of the 1999 Nobel Prize in Chemistry for his studies of the transition states of chemical reactions using femtosecond spectroscopy. He also pioneered ultrafast electron diffraction and microscopy of molecular, biological and materials systems. In 2009, President Obama appointed him to the Council of Advisors on Science and Technology.

Structural Dynamics is pleased to add Helliwell and Zewail to the impressive list of highly respected international scientists that have already voiced their support for the Journal by agreeing to serve on its Advisory Board (sd.aip.org).

Structural Dynamics - Editor's Picks

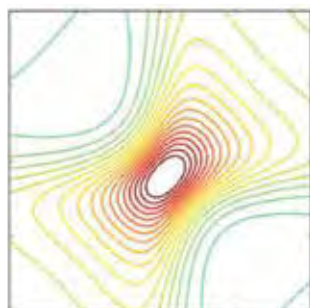
Communication: *The electronic structure of matter probed with a single femtosecond hard x-ray pulse*, J. Szlachetko, C. J. Milne, J. Hozowska, J.-Cl. Dousse, W. Błachucki, J. Sà, Y. Kayser, M. Messerschmidt, R. Abela, S. Boutet, C. David, G. Williams, M. Pajek, B. D. Patterson, G. Smolentsev, J. A. van Bokhoven and M. Nightegaal. *Struct. Dyn.* 1, 021101 (2014)

Abstract: Physical, biological, and chemical transformations are initiated by changes in the electronic configuration of the species involved. These electronic changes occur on the timescales of attoseconds (10^{-18} s) to femtoseconds (10^{-15} s) and drive all subsequent electronic reorganization as the system moves to a new equilibrium or quasi-equilibrium state. The ability to detect the dynamics of these electronic changes is crucial for understanding the potential energy surfaces upon which chemical and biological reactions take place. The paper reports on the determination of the electronic structure of matter using a single self-seeded femtosecond x-ray pulse from the Linac Coherent Light Source hard x-ray free electron laser. By measuring the high energy resolution off-resonant spectrum (HEROS), we were able to obtain information about the electronic density of states with a single femtosecond x-ray pulse. We show that the unoccupied electronic states of the scattering atom may be determined on a shot-to-shot basis and that the measured spectral shape is independent of the large intensity fluctuations of the incoming x-ray beam. Moreover, we demonstrate the chemical sensitivity and single-shot capability and limitations of HEROS, which enables the technique to track the electronic structural dynamics in matter on femtosecond time scales, making it an ideal probe technique for time-resolved x-ray experiments.



Topical Review: *Molecular reaction and solvation visualized by time-resolved X-ray solution scattering: Structure, dynamics, and their solvent dependence*. Kyung Hwan Kim, Jeongho Kim, Jae Hyuk Lee and Hyotcherl Ihee. *Struct. Dyn.* 1, 011301 (2014)

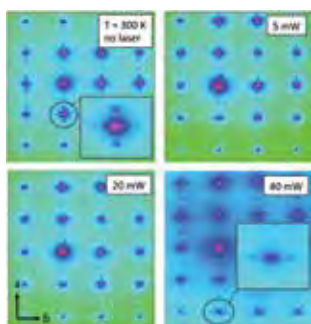
Abstract: Time-resolved x-ray solution scattering is sensitive to global molecular structure and can track the dynamics of chemical reactions. This article reviewed recent studies on triiodide ion (I_3^-) and molecular iodine (I_2) in solution. For I_3^- , we elucidated the excitation wavelength-dependent photochemistry and the solvent-dependent ground-state structure. For I_2 , by combining time-slicing scheme and deconvolution data analysis, we mapped out the progression of geminate recombination and the associated structural change in the solvent cage. With the aid of x-ray free electron lasers, even clearer observation of ultrafast chemical events will be made possible in the near future.



Two-dimensional x-ray correlation spectroscopy of remote core states. Daniel Healion, Yu Zhang, Jason D. Biggs, Weijie Hua and Shaul Mukamel. *Struct. Dyn.* 1, 014101 (2014)

Abstract: Nonlinear all-x-ray signals that involve large core-atom separation compared to the x-ray wavelengths may not be

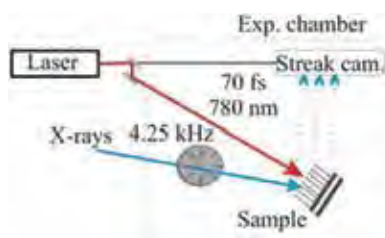
described by the dipole approximation since they contain additional phase factors. Expressions for the rotationally averaged 2D x-ray photon echo signals from randomly oriented systems that take this position-dependent phase into account for arbitrary ratio between the core separation and the resonant wavelength are presented. Application is made to the Se K-edge of a selenium dipeptide system.



Ultrafast structural and electronic dynamics of the metallic phase in a layered manganite. L. Piazza, C. Ma, H. X. Yang, A. Mann, Y. Zhu, J. Q. Li and F. Carbone. *Struct. Dyn.* 1, 014501 (2014)

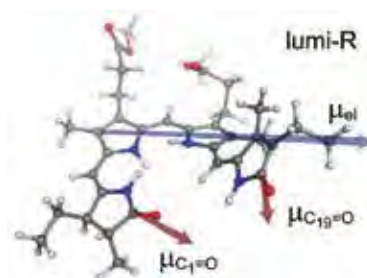
Abstract: The transition between different states in manganites can be driven by various external stimuli. Controlling these transitions with light opens the possibility to

investigate the microscopic path through which they evolve. We performed femtosecond (fs) transmission electron microscopy on a bi-layered manganite to study its response to ultrafast photoexcitation. We show that a photoinduced temperature jump launches a pressure wave that provokes coherent oscillations of the lattice parameters, detected via ultrafast electron diffraction. Their impact on the electronic structure is monitored via ultrafast electron energy loss spectroscopy, revealing the dynamics of the different orbitals in response to specific structural distortions.



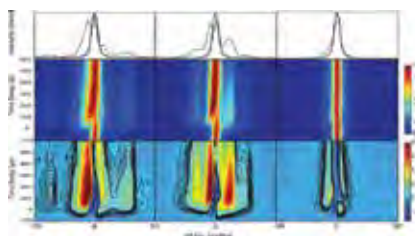
Measurements of light absorption efficiency in InSb nanowires. A. Jurgaitis, H. Enquist, M. Harb, K. A. Dick, B. M. Borg, R. Nüske, L.-E. Wernersson and J. Larsson. *Struct. Dyn.* 1, 014502 (2014)

Abstract: This paper reports on measurements of the light absorption efficiency of InSb nanowires. The absorbed 70 fs light pulse generates carriers, which equilibrate with the lattice via electron-phonon coupling. The increase in lattice temperature is manifested as a strain that can be measured with x-ray diffraction. The diffracted x-ray signal from the excited sample was measured using a streak camera. The amount of absorbed light was deduced by comparing x-ray diffraction measurements with simulations. It was found that 3.0(6)% of the radiation incident on the sample was absorbed by the nanowires, which cover 2.5% of the sample.



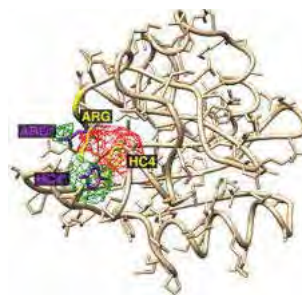
Active and silent chromophore isoforms for phytochrome Pr photoisomerization: An alternative evolutionary strategy to optimize photoreaction quantum yields. Yang Yang, Martin Linke, Theodore von Haimberger, Ricardo Matute, Leticia González, Peter Schmieler and Karsten Heyne. *Struct. Dyn.* 1, 014701 (2014)

Abstract: Photoisomerization of a protein bound chromophore is the basis of light sensing of many photoreceptors. We tracked Z-to-E photoisomerization of Cph1 phytochrome chromophore PCB in the Pr form in real-time. Two different phycocyanobilin (PCB) ground state geometries with different ring D orientations have been identified. The pre-twisted and hydrogen bonded PCB^a geometry exhibits a time constant of 30 ps and a quantum yield of photoproduct formation of 29%, about six times slower and ten times higher than that for the non-hydrogen bonded PCB^b geometry. This new mechanism of pre-twisting the chromophore by protein-cofactor interaction optimizes yields of slow photoreactions and provides a scaffold for photoreceptor engineering.



Transient crystalline superlattice generated by a photoacoustic transducer. A. Loether, Y. Gao, Z. Chen, M. F. DeCamp, E. M. Dufresne, D. A. Walko and H. Wen. *Struct. Dyn.* 1, 024301 (2014)

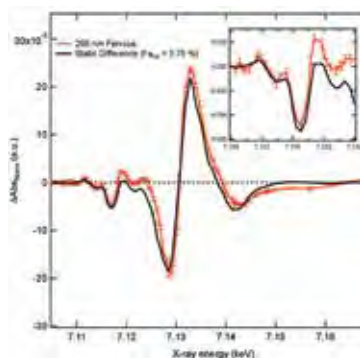
Abstract: Designing an efficient and simple method for modulating the intensity of x-ray radiation on a picosecond time-scale has the potential to produce ultrafast pulses of hard x-rays. In this work, we generate a tunable transient superlattice, in an otherwise perfect crystal, by photoexciting a metal film on a crystalline substrate. The resulting transient strain has amplitudes approaching 1%, wavevectors greater than 0.002 \AA^{-1} , and lifetimes approaching 1 ns. This method has the potential to generate isolated picosecond x-ray bursts with scattering efficiencies in excess of 10%.



Enzyme transient state kinetics in crystal and solution from the perspective of a time-resolved crystallographer. Marius Schmidt and Dilano K. Saldin. *Struct. Dyn.* 1, 024701 (2014)

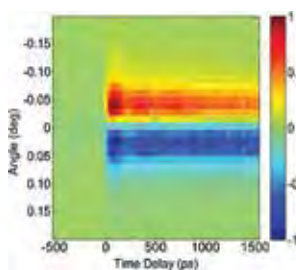
Abstract: With recent technological advances at synchrotrons [Graber et al., *J. Synchrotron Radiat.* 18, 658–670 (2011)], it is feasible to rapidly collect time-resolved crystallographic data at multiple temperature settings [Schmidt et al., *Acta Crystallogr. D* 69, 2534–2542 (2013)], from which barriers of activation can be extracted. With the advent of fourth generation x-ray sources, new opportunities emerge to investigate structure and dynamics of biological macromolecules in real time [M. Schmidt, *Adv. Condens. Matter Phys.* 2013, 1–10] in crystals

and potentially from single molecules in random orientation in solution [Poon et al., *Adv. Condens. Matter Phys.* 2013, 750371]. Kinetic data from time-resolved experiments on short time-scales must be interpreted in terms of chemical kinetics [Steinfeld et al., *Chemical Kinetics and Dynamics*, 2nd ed. (Prentice Hall, 1985)] and tied to existing time-resolved experiments on longer time-scales [Schmidt et al., *Acta Crystallogr. D* 69, 2534–2542 (2013); Jung et al., *Nat. Chem.* 5, 212–220 (2013)]. This article reviews and outlines steps that are required to routinely determine the energetics of reactions in biomolecules in crystal and solution with newest x-ray sources. In eight sections, we aim to describe concepts and experimental details that may help to inspire new approaches to collect and interpret these data.



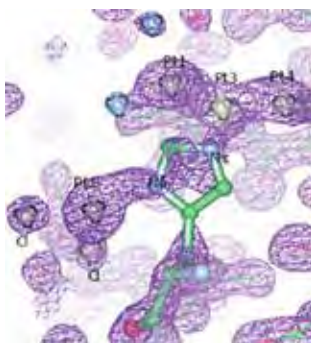
Photooxidation and photoaquation of iron hexacyanide in aqueous solution: A picosecond X-ray absorption study. M. Reinhard, T. J. Penfold, F. A. Lima, J. Rittmann, M. H. Rittmann-Frank, R. Abela, I. Tavernelli, U. Rothlisberger, C. J. Milne and M. Chergui. *Struct. Dyn.* 1, 024901 (2014)

Abstract: We present a picosecond Fe K-edge absorption study of photoexcited ferrous and ferric hexacyanide in water under 355 and 266 nm excitation. Following 355 nm excitation, the transient spectra for the ferrous and ferric complexes exhibit a red shift of the edge reflecting an increased electron density at the Fe atom. For the former, an enhanced pre-edge transition is also observed. These observations are attributed to the aquated $[\text{Fe}(\text{CN})_5\text{OH}_2]_3^-$ species, based on quantum chemical calculations which also provide structural parameters. Upon 266 nm excitation of the ferric complex, a transient reminiscent of the aquated species is observed (appearance of a pre-edge feature and red shift of the edge) but it is different from that obtained under 355 nm excitation. This points to a new reaction channel occurring through an intermediate state lying between these two excitation energies. Finally, 266 nm excitation of the ferrous species is dominated by the photooxidation channel with formation of the ferric complex as main photoproduct. However, we observe an additional minor photoproduct, which is identical to the 266 nm generated photoproduct of the ferric species, suggesting that under our experimental conditions, the pump pulse photooxidises the ferrous complex and re-excites the primary ferric photoproduct.



Measurement of transient atomic displacements in thin films with picosecond and femtometer resolution. M. Kozina, T. Hu, J. S. Wittenberg, E. Szilagy, M. Trigo, T. A. Miller, C. Uher, A. Damodaran, L. Martin, A. Mehta, J. Corbett, J. Safranek, D. A. Reis and A. M. Lindenberg. *Struct. Dyn.* 1, 034301 (2014)

Abstract: We report measurements of the transient structural response of weakly photo-excited thin films of BiFeO_3 , $\text{Pb}(\text{Zr,Ti})\text{O}_3$, and Bi and time-scales for interfacial thermal transport. Utilizing picosecond x-ray diffraction at a 1.28 MHz repetition rate with time resolution extending down to 15 ps, transient changes in the diffraction angle are recorded. These changes are associated with photo-induced lattice strains within nanolayer thin films, resolved at the part-per-million level, corresponding to a shift in the scattering angle three orders of magnitude smaller than the rocking curve width and changes in the interlayer lattice spacing of fractions of a femtometer. The combination of high brightness, repetition rate, and stability of the synchrotron, in conjunction with high time resolution, represents a novel means to probe atomic-scale, near-equilibrium dynamics.



Structural dynamics of cisplatin binding to histidine in a protein. S. W. M. Tanley and J. R. Helliwell. *In Press*

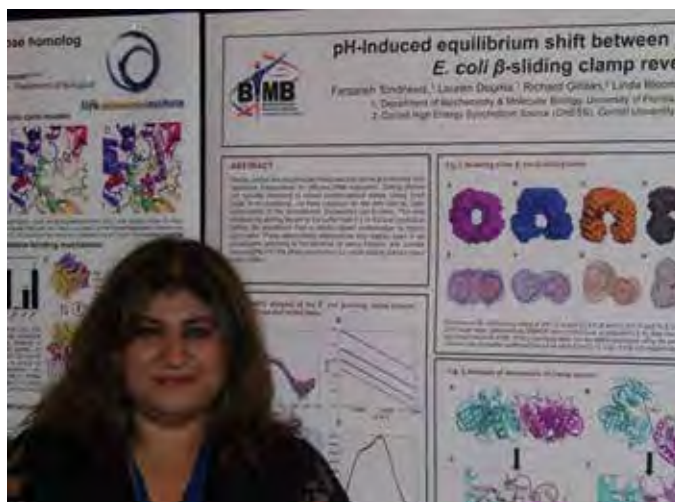
Abstract: The platinum anti-cancer agents cisplatin and carboplatin bind to the histidine 15 residue in the model protein hen egg white lysozyme (HEWL). By using temperatures either side of the protein glass transition state, ($\sim 180\text{K}$), several platinum binding modes are seen and it is shown that not all these platinum modes are stable. In particular the mean square displacement vibration amplitudes of the cisplatin and of the histidine to which it is bound are analyzed in detail. As well as the multiple platinum peaks, the electron density for the His-15 side chain is weak to absent at 150K and 200K, which points to the imidazole ring of the His side chain sampling multiple positions. Most interestingly the His-15 imidazole becomes more ordered at room temperature.



Ultrafast electron diffraction using an ultracold source. M. van Mourik, W. Engelen, E.J.D. Vredendregt, and O.J. Luiten. *Struct. Dyn.* 1, 034302 (2014)

Abstract: The study of structural dynamics of complex macromolecular crystals using electrons requires bunches of sufficient coherence and charge. We present diffraction patterns from graphite, obtained with bunches from an ultracold electron source, based on femtosecond near-threshold photoionization of a laser-cooled atomic gas. By varying the photoionization wavelength we change the effective source temperature from 300 K to 10 K, resulting in a concomitant change in the width of the diffraction peaks, which is consistent with independently measured source parameters. This constitutes a direct measurement of the beam coherence of this ultracold source, and confirms its suitability for protein crystal diffraction.

Featured in Physics Today: "Electron diffraction from an ultracold source", May 2014'



Farzaneh Tondevis was the recipient of the first Structural Dynamics ACA Poster Prize for her presentation entitled: PrizepH-Induced equilibrium shift between closed and open E. coli B-sliding clamp revealed by: Farzaneh Tondevis (1), Lauren Douna (1), Richard Gillilan (2), Linda Bloom (1) and Robert McKenna (1) - (1 - University of Florida, 2 - CHESS at Cornell)



Bridget D'Amelio and Judith Flippen-Anderson at the Structural Dynamics booth in Albuquerque

From the Editor of RefleXions: Since a significant number of ACA members are doing research that is supported, directly or indirectly, by public funds, they are acutely aware of the ongoing discussions related to government mandates (both the US and the UK) on public access to their results. On pages 40-41 of this issue Fred Dylla (CEO of the American Institute of Physics) presents an overview of the issue from

the perspective of all parties involved (the government, authors, publishers, and librarians) and describes a solution that he feels could satisfy all stakeholders.

Structural Dynamics, is a Gold open access publication in that while it will be based on an 'author pays' model it is up to the publisher to make the final form of the paper freely available, as opposed to Green open access where the responsibility will lie with the author. ACA members will be entitled to a significantly lower submission fee than will be available to non-members. **However, a fee is a fee so this would be a good time to point out there will be no charge for the first 50 accepted articles - now would be a great time to submit your paper !**

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Puzzle Corner

In this issue, we have the solution to the last DISORDERED puzzle, a new DISORDERED puzzle, the solution to the Cubes Within Cubes puzzle, and a new crystallographic poetry puzzle. Ideas for future issues are always welcome.

Frank Fronczek

Solution to Cubes Within Cubes Puzzle In the Spring issue, we posed the following: Consider a stack of unit cubes, four on an edge. How many cubes of various sizes are contained in it?

Answer: There is one 4x4, eight 3x3, 27 2x2 (8 at corners, 12 on edges, 6 on faces, and one at center), and 64 1x1, for a total of **100**. (I expect that crystallographers, being comfortable with cubic symmetry, found this one less challenging than most people would.)

Poetry Puzzle Following are a few lines from a poem. What is the title, and who is the author?

*A crystal assembles itself out of its own constituent disarray:
the puzzle puts itself together, each piece falling as though by
chance into its correct location.*

*A crystal is nothing more than a breeze blowing sand into the
form of a castle or a film played backwards of a window being
smashed.*

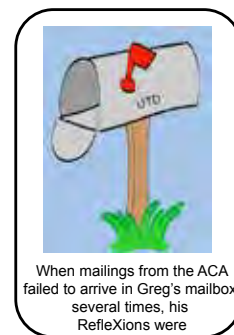
DISORDERED

Reorder these words to find the missing answer.

TIREMYBUT Y T T E R B I U M
TILESTAC L A T T I C E S
GREENCINT C E N T E R I N G
YELSIN L Y S I N E
ACRAPISIT A S P A R T I C

Answer:

S Y S T E M A T I C A L L Y A B S E N T



DISORDERED

Realign the letters to achieve a collimated answer.

GELDINISH ○ ○ ○ ○ ○
FOTFAKE ○ ○ ○ ○
SILKVLOOT ○ ○ ○ ○
MUCUVA ○ ○
LIMPLASM ○ ○ ○ ○

Answer:

○ ○ ○ ○ ○ ○ ○ ○ ○



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M. Gary Newton (Feb 18, 1939 – Feb 22, 2013)

Gary Newton and I met when I first interviewed at the University of Georgia 20 years ago. He had already been a full Professor of Chemistry for more than 10 years. During our meeting he showed me his Nonius Kappa diffractometer and told me about its history. I was surprised to learn that he had one of the very earliest models of the unit in this country. It was almost one year older than the one in the Department of Crystallography at the

University of Pittsburgh where I was a faculty member.

Gary was born on a farm near the city of Millen, GA (~ 80 miles NW of Savannah). He obtained his PhD in Chemistry from Georgia Tech in 1966 and joined the University of Georgia in 1967. The obituary published by the local newspaper shared that he liked classical music. Later he became a fan of Pink Floyd, REM, and other rock bands. He read extensively, played bridge, photographed wildflowers, kept beloved dogs, collected depression era glassware and crystal, and liked wine and gourmet foods.

Gary was a very resourceful mentor for many students, and participated in various crystallographic activities at the University of Georgia during a career that spanned more than 45 years. He and I became very close friends after I joined the faculty in 1995. He was a wonderful colleague and provided tremendous help to John Rose and myself when we first relocated to Georgia, and then throughout the 18 years we worked together. He helped us greatly from 1997-2002 by managing the UGA's ACA Summer School of Crystallography, and participated in the formation of SER-CAT's consortium and the UGA's structural genomic program. He became Professor Emeritus around 2004, and enthusiastically took on the role of Editor of *The SER-CAT Spectrum* in 2008.

Gary loved his friends and colleagues in the crystallographic community and participated in almost all of the ACA and IUCr meetings before his death. His dynamic and helpful spirit will be greatly missed by all of us who knew him. His full obituary may be found at www.legacy.com/obituaries/onlineathens/obituary.aspx?pid=163637870.

B.C. Wang

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The Crystallographic Roots of DNA Nanotechnology

Nadrian C. Seeman has received many awards and honors, notable among them the 2010 Kavli Prize in Nanoscience. The Kavli Prize is awarded in Oslo by The Norwegian Academy of Science and Letters, The Kavli Foundation (US) and The Norwegian Ministry of Education and Research: "Seeman invented structural DNA nanotechnology when he realized the building blocks of the genetic blueprint of living organisms could be harnessed to create the raw materials for new, nanoscale circuits, sensors and medical devices." Ned and other winners of the 2010 Kavli Prize were received by President Obama at the White House in 2011. In 2014 Ned was recognized by the ACA as an ACA Fellow.



I was born in Chicago at the end of 1945 as an only child in a middle-class Jewish family. My father sold fur garments in Chicago (from 1953 in his own store), but after my birth my mother did not return to teaching

until my grandmother died in 1963. In 1951, we moved to the suburb of Highland Park, where we remained until I went to college in 1962. I was a quiet child who preferred reading over sports, a characteristic that has persisted. Sputnik was launched in October, 1957; a year later, I became a "Sputnik Kid" who was brought daily to the high school in the early morning, where I took a special algebra class, before spending the rest of the day at my middle school. As a nocturnal person, I didn't do all that well, but I was set on a path of advanced math and science courses from then until the end of high school. A year earlier, my father had begun a campaign to convince me that I wanted to be a physician. The math and science that I liked were not incompatible with my father's goal, so he gave me no flack about them. At about the time I got to high school, I lost whatever faith I might have had, and I've been an atheist ever since.

The most important scientific influence in my early life was my high school freshman biology teacher, John E. Broming. The school year was divided into six 6-week segments, and he devoted the first of these to teaching the class the rudiments of chemistry and physics as they applied to the structure of matter; this emphasis instilled in me the sense that life is a physico-chemical phenomenon, and that's where my intellectual center has been ever since, on the cusp of the physical and biological sciences, at the edge of life. In addition, when we did get to biology, I found it was pretty neat, with lots of nifty structures and shapes and an apparently logical nature that appealed to me. I got a high school diploma at the end of my third year and went off to the University of Chicago as a pre-med. At the time, I didn't yet know that my job as a professor of science existed: I thought a university professor did the same thing as a high school teacher, only teaching more advanced material. I had no idea

that I could spend most of my day having fun doing research and *also* get paid to do it. That was the most important thing I learned at Chicago.

It was damn near the only thing I learned. As Mark Twain put it, I didn't let college interfere with my education. I was a poor student, getting grades that were mediocre on a good day, and there weren't many of those. The only things I remember from my undergraduate science courses are the Watson-Crick pairing rules, that A pairs with T and G pairs with C. My grandmother died during my first year in college, and I recognized both the inevitability and finality of death. The notion of spending my life keeping other people alive for a few extra years lost any appeal it might have had for me. When I learned that a university career offered the pleasures of doing research, I announced to my parents that I wanted to become a biochemist, which I thought was the area closest to my interests. My father greeted my decision to become a scientist instead of a physician much as I imagine he would have welcomed a career choice of mobster.

Biochemistry at Chicago in the middle 1960s turned out to be a great disappointment. The field as taught at that time treated little of the information content of molecular biology, which I sensed was really neat. Rather, it had been developed by organic chemists, and was basically the study of the metabolic transformations of small molecules, not the study of the macromolecules whose information content made biology special. When the realization of what biochemistry seemed to be all about sank in, I switched to physical chemistry, where I didn't do well, either. In the end, I was rejected by all the chemistry graduate schools to which I applied. I went to the Chemistry Department's advisor to present my predicament: I asked, "Nobody wants me. What can I do?" His reply was, "That's not true. Uncle Sam — he wants you!" This remark was uttered in the middle of the Vietnam War, to which I was staunchly opposed, both because of my left-wing politics, and also because I didn't want to return from Southeast Asia as a putrefying corpse in a body bag. I stumbled out of his office and had no idea what to do with my life.

Nevertheless, I managed to stay draft-resistant by fast-talking my way into Chicago's graduate Biochemistry Department, where I didn't do much better in the basic biochemistry courses the second time around. During my spring vacation that year one of my roommates and I took a drive-away to San Francisco; the 46 hour continuous drive to Reno (as far as the car was going — we rode a bus the rest of the way) with minimal sleep gave me hallucinations without drugs, and cleared a lot of cobwebs from my brain. I spent the week walking around Golden Gate Park, and decided that perhaps there were interesting things to be done in science, even though Watson & Crick and Monod & Jacob seemed to have solved all the big problems of which I was aware. I did a lot better the following quarter, but my performance was still inadequate. The key difference this time was the graduate student advisor in biochemistry, John H. Law. He saw that I was probably talented, but was not really interested in what was offered there. At the end of the year, he told me I should leave, and managed to get me into the new crystallography/biochemistry training program at the University of Pittsburgh. This was the single greatest favor anybody did for me before I left Chicago.

Pittsburgh was a totally different experience. I was immedi-

ately engaged in crystallography research, which turned out to be a lot of fun. Between Bryan Craven's crystallography course, Bob Rosenstein's tutelage and Helen Berman's friendly advice, I learned how to do crystallography, and more importantly how to think about 3D structure and symmetry. The laboratory was run by G.A. Jeffrey (Jeff), whose gentle directing hand kept us fairly happy and adequately funded. Bob Stewart's Friday afternoon seminars at the Craig Street Inn taught me that one could learn, discuss and think productively about Science over beers. I have probably never done anything that I enjoy as much as solving high-resolution small molecule crystal structures, both in Pittsburgh and later, but deep down the purely analytic nature of crystallography left me unsettled. Nevertheless, I was having fun and I was doing well, so I figured that I could deal with whatever problems there were at a later time.

The world was never far from us in those days; I solved my first crystal structure in 1968, presented it at the August American Crystallographic Association meeting in Buffalo, and returned to find a notice from my draft board that I had been re-classified 1A (prime candidate for drafting) and was soon called for my physical examination. Knowing a little about physiology, the morning of the exam I ate a quarter pound of butter (absorbed into garlic bread — could halitosis get me out of the army?) and a quart of soft ice cream; I was able to urinate sugar for them, enabling me to fail the physical. During my second year in Pittsburgh, I finally came to terms with my father, whom I convinced I was not a bum, even though I wanted to become a scientist. We had a tolerable relationship for the remaining 20 months of his life: I handed him my thesis and he dropped dead the following day.

I got my degree in August, 1970, my self-confidence restored (arguably over-restored), and went off to Columbia University as a postdoc to work on the protein-folding problem, which I then believed to be important, interesting and (foolishly) tractable. I went to the laboratory of a prominent pompous person who turned out to be of lightweight intellectual heft. Within four months, I realized I had made a serious mistake, and started trying to leave for what had been my primary other postdoctoral possibility, Alex Rich's laboratory at MIT. To do so entailed getting fellowships, so I suffered in the Columbia laboratory for over a year until they kicked in. In the meantime, I was instrumental in the solution of the first dinucleoside phosphate structure, and I garnered a little notoriety that way.



Nadrian C. Seeman and John Rosenberg with the ApU structure showing Watson-Crick base pairing (1973).

After the unpleasantness of my Columbia experience, I really enjoyed Alex's lab. During my first years there, I was central in solving three more dinucleoside structures, including one that showed A-U Watson-Crick base pairing at high resolution for the first time. This resulted in more recognition, and times were good. Alex always devoted a lot of energy to making the lab a fun and exciting place to pursue science; I really enjoyed the intellectual environment he created, mixing crystallographers with molecular biologists. Among other things, this atmosphere stimulated me to write my most highly cited early paper, on protein-nucleic acid recognition. Although we all joked about how Alex availed himself of the fruits of our labor, Alex really made serious intellectual contributions to that work, pointing out how I was fooling myself about certain aspects of base pair symmetry, and suggesting that a paired amino acid-base interaction might be involved in the recognition of adenine.

It's worth pointing out that I had crystallized none of the dinucleoside structures myself - I had just used my structure-solution skills in their determination. The structure containing the Watson-Crick A-U base pairs was a lucky punch. I hadn't designed the crystal; it just happened. The final dinucleoside structure I solved contained an intercalating drug, 9-aminoacridine, but it was an unlucky punch; I didn't find the intra-helical intercalation I had sought, and it was the hardest of all to solve. It left a somewhat bitter taste in my mouth to have so little control over the structure of the crystal, a problem I would ultimately address. I have a Chinese fortune cookie strip taped to my refrigerator, "Failure teaches success". The failure I experienced with the 9-aminoacridine crystal reminded me of the analytical nature of crystallography, with no control over the structure. I began to think about ways to control crystalline structure, thinking that ultimately led to my thinking up DNA nanotechnology.

By 1974 the crystallographic game was changing. Solving small molecule structures was becoming less and less important, and the key skill transformed from being good at solving structures to being good at crystallizing important macromolecules, usually proteins. I was totally unskilled at generating crystals, never absorbing the subtleties of the trial and error ("pee in a pot and pray") approach. I also had become unenthusiastic about proteins: nucleic acids are very general, but every protein seems to be unique. I am just not suited to devoting years of my life (which it took in those days) to isolating, producing, and teasing out the structure of one of thousands of different proteins. Furthermore, my experiences with tRNA in Alex's lab made me somewhat uncomfortable with the lower resolution of macromolecules. This placed me in a bit of a quandary. In addition, the mid-1970s were a bad time to be seeking an independent position as a biological crystallographer: We were considered expensive, and those of us competing for jobs were often vying with non-crystallographers, whom the hiring departments preferred. Despite my postdoctoral successes, I had to spend two years seeking an independent position, and was turned down by all the desirable and most of the undesirable departments where I interviewed. I used to kick the wall in my bedroom from frustration: I had spent almost a decade at my work, was widely recognized (at least at ACA meetings), and still I could not get a job. The hole in the wall wound up with a diameter over half a meter.

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Eventually, I landed a position in the Biology Department at SUNY/Albany. The only thing worse than looking for a job was finding this one, because Albany was in many respects a scientific death sentence. Unlike MIT, many of my colleagues seemed far more interested in their families than in their science. In my generation, many of the students in biology/biochemistry departments had the same appreciation of the importance of chemistry and physics that I did, but that tradition had died out by the time I got to Albany. The graduate student complement in Albany consisted largely of mathophobic failed pre-meds, and during my first seven years I recruited no graduate students, and as a beginner at an undistinguished institution, I attracted only ineffective postdocs. Without a full-time labor force, I was unable to grow crystals of anything interesting to me or to anybody else, and thus was unable to get my crystallographic act in gear.

The good thing that happened in Albany was that in the fall of 1978 Bruce Robinson (a postdoc with Leonard Lerman at the time) came into my office and asked if I could build a model of a Holliday Junction, a DNA branched junction structure that is an intermediate in genetic recombination. When we looked at the model, we discovered some asymmetries that we thought might have some impact on the kinetics of branch migration. I had nothing else working for me, but as a crystallographer, I had learned to write programs; I wrote some code that simulated the process, and I started thinking about branched DNA. One of the problems with what Bruce and I were doing was that any hypotheses we might generate were untestable. This was because the symmetry of naturally-occurring branched molecules led to branch migration, whereby the branch point migrates all over the place, producing a polydisperse solution that ultimately resolves to duplex DNA. Thus, our project started off as a scholastic enterprise, rather than a scientific one. In the spring of 1979, I flew with Greg Petsko to the ACA meeting in Honolulu. During the flight, Greg mentioned that it might be possible to crystallize structures resembling intermediates in the hemoglobin oxygenation pathway by mixing iron-containing hemoglobin with cobalt-containing hemoglobin. This comment planted a seed in my head that one could use tricks to prepare analogs of intermediates like the Holliday junction. About a month later, that seed grew into the notion that by using synthetic DNA one could eliminate the symmetry inherent in naturally-occurring branched molecules, resulting in immobile branched junctions. This would enable us to test hypotheses, and also perhaps allow structural characterization.

I was elated with this idea, and started building physical models; I showed one to a visitor who asked if it were possible to make junctions with more arms than the four in a Holliday junction. I had no idea, but soon worked out that an evident structural constraint would permit up to eight arms in an immobile junction, although that is no longer the limit. In September, 1980, I went to the campus pub to think about 6-arm junctions. Because it was easy to draw them with hexagonal symmetry, I had thought about them that way, before entering the bar. While drinking a beer, I suddenly thought of Escher's woodcut "Depth" containing fish with three orthogonal axes (a head and tail, two vertical fins and two horizontal fins), making them topologically isomorphous with six junctions. Furthermore, the fish in that woodcut are organized periodically in 3D, just like the molecules in a molecular



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crystal. However, thinking of the fish as nucleic acids, I imagined their contacts being programmed by sticky ends; these are single-stranded intermolecular interactions that occur between the overhangs that arise when one strand of a DNA duplex is a little longer than the other. Sticky ends were familiar, because they had been used by genetic engineers since the early 1970s. Thus, I had the idea of self-assembling crystals with pre-defined intermolecular contacts, rather than using trial and error.

I've had a number of insights in my life, but this was my major epiphany. I realized that branched DNA molecules could be self-assembled into N-connected objects, lattices and other networks using the specificity of sticky ends; this was thinking that remained with me from my days in Jeff's clathrate hydrate lab, although I had only kibitzed on those projects. The idea felt great — it still entailed working with nucleic acids, it still involved symmetry and crystallography, but now I imagined that I would have a target for my creative urges, designing DNA objects and lattices. I re-oriented my research direction towards implementing this idea, even though it was extremely dangerous to do so in the fourth year of my five-year assistant professorship. Nevertheless, this notion has grown into the field of DNA nanotechnology.

It took a long time. I started collaborating with Neville Kalenbach, then at Penn, who taught me how to work with DNA in solution. He also bought the DNA that made the first immobile junctions, although I eventually learned how to make it myself. The biggest favor Neville did for me was to hire me in 1988 at New York University's Chemistry Department, where he had become chair. After 4000 days (OK, 3983, but I round off), I was rescued from the uncomfortable small-town milieu of Albany.

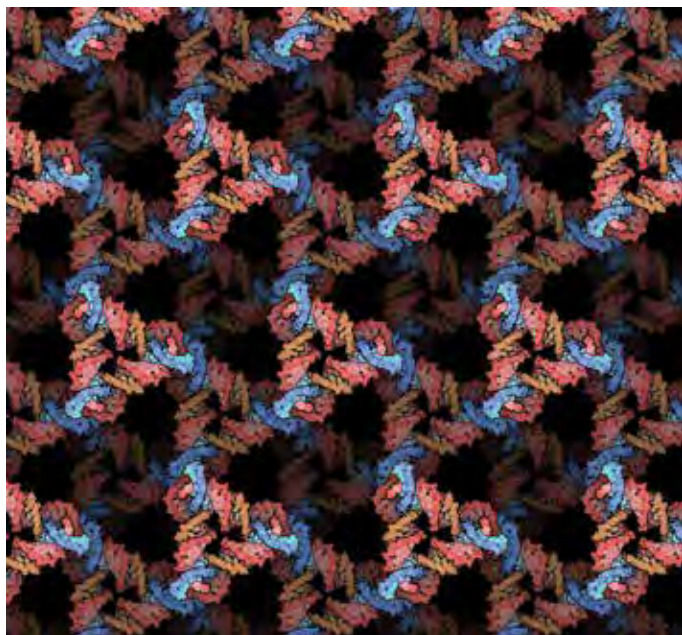


Nadrian C. Seeman and Junghuei Chen with DNA cube-like catenane (1990).

As a friend of mine put it, "It is one thing to be a big fish in a little pond and another to be a little fish in a big pond: It is something entirely different to be a fish out of water." On the scientific front, the move solved my labor problem: Rather than being a person on the fringes of a Biology Department, my interests were relatively mainstream in a Chemistry Department, and I rapidly attracted students.

The very first thing I did in my NYU laboratory was to synthesize the strands for a DNA cube-like catenane, built in 1990 by my first Ph.D. student, Junghuei Chen. This was the key founding experiment of structural DNA nanotechnology. This is DNA nanotechnology, where the DNA sequence is used to program the structure assumed by the DNA molecules, and is not just the use of DNA whose complementarity allows it to be used as smart glue. John Mueller, my second Ph.D. student, built a deliberate knot a year later, thereby establishing the area of synthetic single-stranded DNA topology. Tsu-Ju Fu first built small DNA double crossover (DX) molecules (analogs of meiotic intermediates) in 1993, and a year later, in a rotation exercise, Xiaoping Yang showed that these were rigid motifs that could be used in DNA nanotechnology to build both lattices and nanomechanical devices.

In the spring of 1995, I attended the first meeting on DNA-based computation, where I met Len Adleman, Erik Winfree and Paul Rothemund. In his talk, Erik proposed that he could use our system, 4-arm branched DNA molecules with specific sticky ends, as cellular automata. We hadn't yet published the



Self-assembled DNA triangle crystal structure (November 2009 PDB Molecule of the Month by David Goodsell).

rigidity of DX molecules, so I suggested that he use them instead of 4-arm junctions, which we had shown were flexible. After I visited Caltech, Erik and I began a collaboration, which resulted in the first 2D DNA crystalline arrays. In addition, I became a member of the DNA-based computation community, which has been the source of many of the people who have moved into DNA nanotechnology. In the ensuing years, we extended DNA nanotechnology to include robust nanomechanical devices, walkers, and ultimately an assembly line.

So what about 3D crystals? As soon as the 2D arrays were produced, we started trying to self-assemble 3D crystals. We had a lot of crystals, but we did not get crystals with adequate resolution. We were using 2D motifs that we converted to 3D motifs by connecting them with a non-half-integral twist; these

worked very poorly. However, my former student, Chengde Mao, now in his own lab, developed what he called the “tensegrity triangle”, a robust motif whose helix axes are oriented in linearly independent directions. When we made the edges short enough, the crystals diffracted to 4 Å resolution, and our crystallographic team, led by Jens Birktoft, was able to determine the structure through SAD, using iodinated nucleotides. It had been only 29 years since my afternoon in the Albany campus pub.

From the foregoing, it should be clear that I regard the entire field of DNA nanotechnology to be an outgrowth of crystallography and crystallographic thinking. In work we plan soon to publish, we have shown that it is possible to improve the resolution of crystals held together by sticky ends just by fiddling with the sticky ends. We now have 3 Å or slightly better resolution of the same crystals. We have not yet developed good crystals whose cavities are large enough to act as hosts for other macromolecules, a key part of my original proposal for DNA nanotechnology. I'm glad all the problems aren't solved yet, and it's exciting to have major goals stretching before me, particularly when they are crystallographic goals.

Ned Seeman

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Eddy Arnold: Eddy Arnold is a Board of Governors Professor of Chemistry and Chemical Biology at Rutgers University, and a resident faculty member of the Center for Advanced Biotechnology and Medicine. He is an outstanding structural biologist who has done pioneering work determining the structure of viruses and viral enzymes. Some of his most notable accomplishments include the structure determination of the

HIV reverse transcriptase enzyme and the discovery of inhibitors of this enzyme, which have proven instrumental to the development of new and improved treatments for HIV infection. He has also made important contributions to the crystallographic community, including serving as the co-editor of *Volume F* of the *International Tables of Crystallography*.



Abraham Clearfield: Abraham Clearfield currently holds the position of Distinguished Professor of Chemistry at Texas A & M. He bears impressive credentials as a researcher in inorganic chemistry, with over 600 papers to his name, and an *h*-index that places him among the top 250 chemists world-wide; he has also published a key text in the field of powder diffraction. He is

widely respected as an educator as well, having mentored many students who have gone on to become luminaries in diffraction science, and has served as Director of the Materials Science and Engineering program at Texas A & M. He has provided great service to the crystallographic world, including serving as ACA President, chair of several SIGS, and a member of the US National Committee for Crystallography.



Larry Dahl: Larry Dahl currently holds the R.E. Rundle Chair at the University of Wisconsin, where he is also a Hilldale Professor. He and his group have conducted pioneering work in the synthesis and characterization of a broad range of metal complexes; these have included high-nuclearity homometallic and heterometallic carbonyl clusters, many of which posed daunting crystallographic problems. He is a member of the US National Academy of Sciences and has received many awards, including the ACS F. Albert Cotton Award in Synthetic Inorganic Chemistry. He has trained nearly 100 PhD students, thereby influencing generations of scientists, and has also been active in outreach activities that bring presentations on symmetry and crystallography to general audiences.



George Phillips: George Phillips is the Ralph and Dorothy Looney Professor of Biochemistry and Cell Biology at Rice University. He is a renowned crystallographer and biophysicist, who has worked for decades to relate the three-dimensional structure and dynamics of proteins to biological function, productively occupying the interface between experiment and computation. His research accomplishments include methodological advances such as improved ways to model protein motion, refine protein structures, and interpret maps, as well as significant chemical and biological contributions in fields as diverse as muscle function, natural product synthesis, and oxygen transport. He is a leader in crystallographic education, having developed multiple curricula in structural biology, molecular biophysics, and computer science, as well as producing widely used educational software. He recently served as President of the ACA and was instrumental in the creation of the new ACA journal *Structural Dynamics*.



Nadrian Seeman: Nadrian (Ned) Seeman holds the Margaret and Herman Sokol Chair in Chemistry at New York University. He has conducted pioneering work in the area of DNA nanotechnology, and indeed is widely credited with being a founder of this field. His laboratory has designed and produced elaborate nanoscale structures of nucleic acids, including both two- and three-dimensional self-assembled lattices. His work has been featured in hundreds of peer-reviewed publications, as well as in the popular science press. Ned has received numerous awards and accolades including the Kavli Prize in 2010, and is a fellow of both the AAAS and the Royal Society of Chemistry; he recently delivered a plenary address at the annual meeting of the ACA (see Ned's autobiography on pages 19-23).



John Spence: John Spence is Regent's Professor of Physics at Arizona State University and a visiting Professor at Lawrence Berkeley Lab. He has made significant contributions to a variety of fields relating to electron diffraction, including convergent beam methods, crystallography of high-Tc superconductors, and the development of the ALCHEMI method. Most

recently, he has played major roles in pioneering both femtosecond protein nanocrystallography and coherent x-ray diffractive imaging, both of which exploit the newly available free-electron laser x-ray sources. These new approaches hold the promise of completely revolutionizing the crystallography of macromolecules. He has served as a co-Editor of *Acta Crystallographica*, Chair of the IUCr Commission on Electron Diffraction, and a member of the US National Committee on Crystallography. He is the recipient of the 2012 Buerger Award of the ACA.



Ron Stenkamp: Ron Stenkamp is a Professor in the Departments of Biological Structure and Biochemistry at the University of Washington. He is accomplished in both small-molecule and macromolecular crystallography, and has made important contributions both to methodology and to expanding our knowledge of chemical and biochemical structures.

He is best known for determining structures of a wide variety of important proteins, including streptavidin, several metalloproteins, different blood-clotting proteins, and rhodopsin, the receptor for light that is found in the eyes of all animals and the first G-protein-coupled receptor for which a structure was ever published. In addition to his research accomplishments, Ron has been a stalwart supporter of the ACA, serving on the Continuing Education and Publications committees, acting as Program Chair for the 1993 Annual Meeting, and co-editor for the *ACA Newsletter*.



Winnie Wong-Ng: Winnie Wong-Ng is a Senior Research Chemist and Project Leader at the National Institute of Standards and Technology. She is a world expert in the crystal chemistry and phase equilibria of high Tc superconductors, and has developed the most reliable phase diagrams of these complex systems through a combination of innovative experimental

designs and modeling. In addition, she has done important work with the International Centre for Diffraction Data to help make powder diffraction data available to the community. Her service to the ACA has been extensive, and includes being a member of multiple committees, organizing four symposia or sessions at ACA meetings, and acting as local chair of the 1998 national meeting in Crystal City, Virginia.



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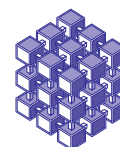
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The Theory that Would Not Die: How Bayes' Rule Cracked the Enigma Code, Hunted Down Russian Submarines & Emerged Triumphant from Centuries of Controversy: Sharon Bertsch McGrayne, Yale University Press, New Haven, CT, 2011, 336 pp, ISBN 978-0-300-18822-6.

"It was a matter of applying Bayes' Theorem to estimate the conditional probabilities. Giving due weight to the prior probabilities and ..." No, this is not from a lecture by Gerard Bricogne, but rather from a Robert Ludlum novel, *The Ambler Warning* (2005). I thought this would be a good way to demonstrate how pervasive Bayes' Theorem has become.

McGrayne's book starts with a short biography of Rev. Thomas Bayes and a simple statement of the theorem that bears his name: prior times likelihood is proportional to the posterior. In the 1st chapter we learn that Bayes made some errors in convincing others of the validity of the theorem, because the prior must often be a guess and scientists did not like the subjective nature of this starting point. The 2nd chapter covers the re-derivation of Bayes' Theorem by Pierre Simon Laplace and how Laplace used it to resolve the issue of the stability of the solar system, among many other problems. In the 3rd chapter, readers learn how Bayes' Theorem almost died at the hands of the frequentists yet managed to survive.

Next the author fast-forwards to World War II, in which Alan Turing and his team at Bletchley Park used Bayes' Theorem to decode Enigma. We are then introduced to Arthur Bailey, an insurance actuary, who used the theorem to predict the probability of airplane accidents, and Jerome Cornfield, a researcher at NIH, who used it to show the correlation between smoking and lung cancer in the 1950s.

One of the strengths of Bayes is its ability to predict probabilities when there is no frequency data. So, Jimmie Savage used Bayes to help the Air Force come to terms with the very real probability that something bad could happen with all the bombs flying around in B-52s in the 50s and 60s. To his credit, Gen. Curtis LeMay changed Air Force operations in accordance with Bayes. There are many examples of how Bayes has solved difficult problems that frequency-based statistics could not: finding Russian submarines that went missing, finding a lost atomic bomb after a mid-air refueling accident, determining the author of *The Federalist*, helping Google Translate translate, and finding the final resting place of Air France 447.

This is one of those books that I probably wouldn't have found without perusing stacks at a bookstore. It is a real gem and reads with the speed of a spy novel. The history and application of Bayes' Theorem is brought out in clear, easy-to-understand language, with detailed footnotes and an extensive bibliography. A humorous piece on religion and Bayes by Michael J. Campbell and some simple, real life examples are provided in the appendices.

Buried Glory; Portraits of Soviet Scientists: Istvan Hargittai, Oxford University Press, Oxford, UK, 2013, 368 pp, ISBN 978-0-199-98559-3.

Istvan Hargittai's *Buried Glory* describes the lives, scientific work, and personalities of 14 brilliant male scientists from the former Soviet Union. Seven were Nobel Laureates who made crucial discoveries in physics and chemistry. At certain times of their lives, many were also victims of terror or persecution simply as a result their Jewish heritage, or their support for ideas that ran counter to Stalin or the Communist Party's paranoid and isolationist agenda. More than half are buried in the Novodevichy Cemetery in Moscow. Hargittai personally interviewed some of his subjects and did extensive research with many annotations for each chapter.

The author did an insightful analysis of the wrenching conflicts between many of the subjects' love of country and their deep dismay at some of the actions of their political leaders and their ideology. Some of the men described were involved in development of Soviet nuclear weapons. As such, they had the same desire to succeed mixed with the recognition of the horror of the actual use of the weapons that western scientists had at the end of WWII. We have all heard of Andrei Sakharov, but he was only one of many who suffered for dissidence. Each character was also depicted as intensely human, with all the associated flaws, intrigue, and large egos that often go with immense intellect. Of course they experience the same fun and wonder as all of us do in the lab or in theoretical discovery. The experience of reading this book was difficult at first, because for me the writing was a bit rambling and seemed disconnected, but I found it worthwhile for what I learned. An example that will appeal to crystallographers is A.I. Kitaigorodskii, who predicted the distribution frequencies of the space groups based on favorable molecular close packing using wooden, arbitrarily-shaped molecular 'models'.

As a scientist I have always enjoyed the international aspect of our connections, and I have had many colleagues who grew up in the Soviet Union. The excitement of scientific discovery often seems to transcend our other more 'tribal' affiliations. Reading this book made me ask myself whether I would have spoken up or stayed silent at some of the atrocities witnessed by these men. The author also made a perceptive and ironic observation that the conditions that led to some of their great discoveries may not be present in the more materialistic Russia of today.

Laurie Betts

The Sixth Extinction: An Unnatural History: Elizabeth Kolbert, Henry Holt and Co, New York, 2014, 321 pages, ISBN: 978-0805092998

I heard an interview with the author in late December (2013) and preordered my copy and finally got around to reading it - just in time - as the latest IPCC report is due out soon.

The author paints a pretty bleak picture of the future. Kolbert spends considerable time studying several extinct species and the cause of their demise in the first part of the book. The extinction timeline is interspersed with species undergoing extinction now and species long gone. Some like mastodons seem to have died a slow death at human hands while the great auk was clearly wiped out by humans. Species that died out a long time ago, like the ammonites and dinosaurs, are given their due.

Next Kolbert explores the Anthropocene, the modern era. She looks at the acidifying of the oceans, which has an impact on shelled creatures and reefs. She spends a couple of chapters looking at how deforestation is changing the climate and causing "relaxation of species" - polite term describing the reduction of the number of species in an area as it is cut off from larger areas by man-made structures such as roads. Kolbert then looks at the Columbian exchange that has had the effect of flattening the earth once again into one supercontinent exchanging species between places in a manner that could not have happened at such great speed without man.

She also describes how humans have been trying to save species like the Sumatran rhino through breeding programs and takes a look at how homo sapiens did in the Neanderthals, and finally at saving the DNA of species for posterity.

I tend to be an optimist. I would like to think, "Don't worry. As long we keep exploring [other planets], humanity is going to survive," but I think the quote by Richard Leakey, "Homo sapiens might not only be the agent of the sixth extinction, but also risks being one of its victims" is more appropriate.

On the lighter side

Life by Keith Richards and James Fox, Little, Brown and Co., New York, 2010, 576 pages, ISBN: 978-0316034418.

Sex, drugs and rock-n-roll in no particular order other than chronological. I recommend having an iPod with Forty Licks on it so you can listen to the songs as the author describes the creation of the music.

Dance of the Reptiles: Rampaging Tourists, Marauding Pythons, Larcenous Legislators, Crazy Celebrities, and Tar-Balled Beaches: Selected Columns by Carl Hiaasen, 2014, Vintage, New York, 416 pages, ISBN: 978-0345807021.

This book contains classic columns by Hiaasen from the Miami Herald on various topics as time progresses over the last couple of decades. I now know where Mr. Hiaasen gets his ideas for his fiction. The adage, "truth is stranger than fiction," applies here.

*Note: Unless otherwise indicated - all reviews by
Joe Ferrara*

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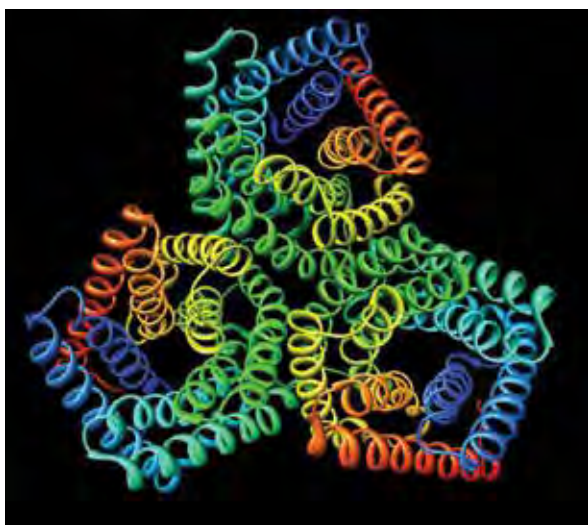
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The Joint Mid-Atlantic Macromolecular Crystallography Meeting - SER-CAT Symposium, April 23-26, 2014

This year the annual SER-CAT Symposium was held jointly with the 44th annual Mid-Atlantic Macromolecular Crystallography Meeting at the University of Maryland's Institute for Bioscience and Biotechnology Research (IBBR) located on the Shady Grove Campus. Following the welcoming remarks from Roy Mariuzza and Peter Sun the meeting began with a Keynote Address by Wayne Hendrickson (HHMI/Columbia University) that provided an overview of the structure and action in transmembrane ion channels determined by the New York Consortium on Membrane Protein Structure. Wayne described the key features of a variety of ion transport channel structures including the 1.2 Å structure of a *H. influenza* homologue of the plant SLAC1 anion channel responsible for closing stomata in leaves. The number and variety of structures described was impressive, especially considering the challenging nature of membrane protein structure determination. The meeting began in earnest the following morning.



Homologue structure of the SLAC1 anion channel for closing stomata in leaves (PDB entry 3M71).

Session 1: Immunity/host-pathogen interactions was chaired by Roy Mariuzza (University of Maryland, IBBR). Scott Walsh (University of Maryland, IBBR) presented some recent structure/function studies related to interleukin-7 signaling including the structure of an unliganded form of the IL-7 receptor that is important to understanding the mechanism of normal and aberrant IL-7 signaling. Tengchuan Jin, (NIAID/NIH) (Co-winner of the HKL Research Prize for the best oral presentation) presented an informative talk on the structural basis of cytosolic DNA recognition by the PYHIN family innate immune receptors AIM2 and IFI16 including the first structure of an inflammasome in complex with its ligand. The work is important to understanding the molecular mechanism of DNA mediated inflammation during infection or under autoimmune conditions. Beatriz Trastoy-Bello (University of Maryland School of Medicine) (Co-winner of the HKL Research Prize for the best oral presentation) described the crystal structure of EndoS from *Streptococcus pyogenes*. EndoS is an immunomodulatory endoglycosidase specific for human IgG antibodies and is a potential therapeutic target for autoimmune diseases. The structure presented and a model of

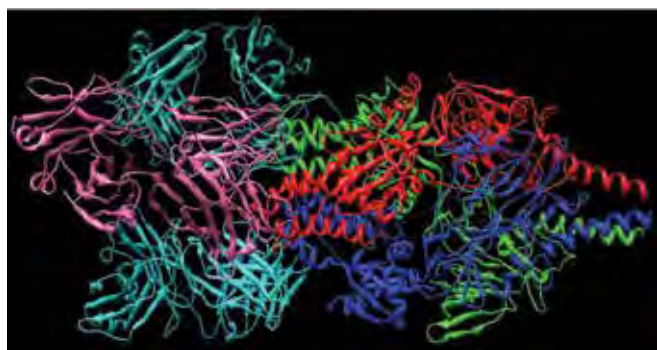
the enzyme substrate complex with IgG1 suggest that concerted structural changes in both enzyme and substrate are needed for antibody deglycosylation. Konstantin Korotkov (University of Kentucky) presented his recent work on key proteins involved in the bacterial ESX or type VII secretion system. The ESX secretion system plays an important role in the virulence of pathogenic mycobacteria such as *M. tuberculosis* but little is known about ESX membrane transport. The structures presented form a starting point for understanding the mechanism of ESX protein transport. Nicholas Noinaj (NIDDK/NIH) gave an interesting talk on the BAM complex, an outer membrane multi-component β barrel protein assembly machine. Using both the Bam A crystal structure and MD simulations, a mechanism for Bam A folding and membrane insertion was proposed that included a lateral opening of the Bam A β barrel and a substrate exit pore positioned above the lateral opening site.

SESSION 2: Enzymes was chaired by Osnat Herzberg (University of Maryland, IBBR). Jacob Morgan (University of Virginia) presented his work on the structure of the cyclic-di-GMP-activated cellulose synthase BcsA-B complex that is involved in the synthesis of bacterial cellulose. The structure of the complex provided new mechanistic insights into how cyclic-di-GMP allosterically modulates enzymatic function. Greg Buhrman (North Carolina State University) described the crystal structure of the biotin carboxylase subunit of 2-oxoglutarate carboxylase from *Hydrogenobacter*. The structure represents an important step in understanding its enzymatic mechanism and how it can be adapted to renewable biofuel production. Liudmila Kulakova (University of Maryland, IBBR), gave an informative talk on the crystal structure of carbamate kinase from the human parasite *Giardia lamblia* in complex with disulfiram. The crystal structure revealed that the disulfiram thiocarbamoylated Cys-242 inhibits enzymatic function. Since disulfiram is already an FDA-approved drug for chronic alcoholism, it is a promising candidate for anti-giardial therapy. Elsa Garcin (University of Maryland Baltimore County) presented a multifaceted study on the mechanism of guanylate cyclase (sGC) catalytic activity. Using crystal structures of isolated catalytic domains, key structural elements that modulate the dimer interface were identified and, together with other studies, a novel regulatory mechanism was proposed in which distinct domain interactions fine-tune the catalytic activity. Kasia Rudzka (Johns Hopkins University School of Medicine) reported crystallographic studies of CuH variants of peptidylglycine α -hydroxylating monooxygenase (H107A and H108A) aimed at investigating the interaction between the enzymes' CuM and CuH copper centers. Interestingly, the H108A crystal structure showed a large inter-domain conformation change compared to the wild-type and H107A structures that may have mechanistic implications.

SESSION 3: Viruses was chaired by Jeff Boyington (Vaccine Research Center, NIAID, NIH). Hua Yang (Centers for Disease Control) described her work related to characterizing the newly emerging H7N9 influenza virus, which is of public health concern because of its high (31%) fatality rate. Crystallographic and other studies of H7N9 hemagglutinin mutants reveal a weak human receptor preference, suggesting that these viruses require further adaptation in order to adapt fully to humans. Gordon Joyce (VRC, NIAID, NIH) presented an interesting talk on Respira-

tory Syncytial Virus (RSV), which is a health concern for both infants and the elderly. Using a variety of approaches coupled with the crystal structure of RSV F glycoprotein stabilized in the prefusion state, F glycoprotein variants having increased physical stability, expression levels and antigenicity have been developed, that show promise for RSV vaccine development. Ravikiran Yedidi (NCI/NIH), reported on his work related to understanding the structural basis of HIV protease inhibitor drug resistance. The crystal structures of HIV protease from wild type and from a multi-protease inhibitor-resistant strain of HIV-1 in complex with ritonavir and a novel protease inhibitor GRL008 were presented. The structures provided structural basis for ritonavir resistance and for GRL008 potency against both wild type and multi-protease inhibitor-resistant strains. Julia Greenfield, (University of Maryland IBBR) gave an informative presentation on the crystal structure of the Viunlikevirus tail spike protein, a 2300 residue trimeric structure solved by Se-MET MAD. The structure is a 3-face β -helix similar to many tail spike proteins, but other structural features suggest a different and novel mode of catalytic action. Paulina Dziubanska (University of Virginia) presented her work on the C-terminal domain of the Ebola virus nucleoprotein (NP), which is thought to serve as a hub for protein-protein interactions important for NP incorporation into virus-like particles and for NP interaction with the matrix protein VP40. The crystal structure of the NPC-terminal domain revealed a novel fold, with topology distantly related to the β -grasp fold, which may provide a template for drug design.

Plenary: Peter Kwong (VRC, NIAID, NIH) spoke on the progress in determining the full atomic-level structure of the HIV-1 Env spike and the role that the NIAID VRC Structural Biology Section and SER-CAT played in the project. The Env spike is a type 1 fusion protein that facilitates attachment and entry of HIV-1 into host cells. Thus it is a target for vaccine development and has been the focus of structural studies for the past 30 years. Using crystal structures, cryo-EM and other techniques, a picture of the trimeric gp120-gp40 spike complex has been slowly revealed over the past decade. The structures have in turn yielded new insights into structure-based vaccine design, which is beginning to show promise.



The crystal structure of the prefusion-stabilized RSV F glycoprotein protein variant in complex with a neutralizing antibody (PDB entry 4JHW). The F protein trimer (right) is colored red, green and blue while the corresponding bound antibodies are colored pink, light green and cyan. The structure was used to design better RSV vaccine candidates.

The SER-CAT Session was chaired by John Rose (University of Georgia, SER-CAT). Sam Wilson (National Institute of Environmental Health Sciences, NIH) was honored with the 2014 SER-CAT Outstanding Science Award based on his publication *Observing a DNA polymerase choose right from wrong* (*Cell* 2013 **154**:157-68). He described the time-lapsed crystallographic study of DNA polymerase beta, which revealed that the enzyme changes its shape depending on whether it incorporates the correct complementary nucleotide or an incorrect noncomplementary nucleotide that results in a mistake, or a mutation. The study also revealed the requirement of a third metal ion-binding site during the reaction. Edward Pryor (University of Virginia), was honored with the 2014 SER-CAT Young Investigator Award for his publication *Structure of the integral membrane protein CAAX protease Ste24p* (*Science* 2013 **339**:1600-4). He presented the crystal structure of Ste24p, a zinc metalloprotease that catalyzes two proteolytic steps in the maturation of yeast mating pheromone α -factor. The structure can be described as a ring of seven transmembrane helices enclosing a voluminous cavity that houses the active site and substrate-binding groove. Gaps between splayed transmembrane helices allow substrate access and, a processive mechanism of substrate insertion, translocation, and ejection was proposed.

George Srajer (Advanced Photon Source) reported on the plans for the APS Upgrade, which includes rebuilding the storage ring to accommodate a multi-bend acromat (MBA) magnetic lattice. The MBA will increase X-ray beam brightness by a factor of 100 to 1000 and provide for 1-micron X-ray beams. Several examples of the science that the new lattice will enable were presented. John Chrzas (SER-CAT) focused on where SER-CAT is today and where we hope to be post MBA. Highlights include the new Rayonix MX300HS CCD detector capable of recording 10 images per second (78 micron pixel) in shutterless mode. Improvements are planned to (1) the sample-mounting robot, (2) crystal alignment, (3) computing infrastructure and (4) data storage needed to support 10 Hz data collection.

SESSION 4: DNA/RNA Enzymes was chaired by Xinhua Ji (NCI, NIH). Shuishu Wang (Uniformed Services University of the Health Sciences) reported the crystal structure of the response regulator PhoP from *M. tuberculosis* in complex with a direct-repeat DNA sequence. PhoP regulates the expression of more than 100 genes. The crystal structure revealed the mode of PhoP dimerization and how PhoP recognizes the direct repeats of its DNA partner. Smita Kakar (NCI/NIH), presented his recent work on the SAXS studies of the RapA protein, a 110 kDa ATPase involved in RNA polymerase recycling, and its RNA complex. The studies show that the RapA structure opens up in solution compared to the structure observed in the crystal and that this solution conformation is the structure that binds RNA polymerase. Andrea Moon (NIEHS/NIH) described the crystal structure of a catalytically inactive mutant (H148A) of Nuclease A (GBS_NucA) from *S. agalactiae*, a potential virulence factor. The study identified residues on the surface of GBS_NucA that are thought to influence DNA substrate binding and catalysis, as well as increased our understanding of the role played by GBS_NucA in bacterial virulence and persistence. Scott Bailey (Johns Hopkins University) gave an interesting talk on the crystal structure of *E. coli* Cascade bound to its ssDNA target. Cascade

is a surveillance complex of five CRISPR-associated proteins (CasA1, CasB2, CasC6, CasD1 and CasE1) and a 61 nt CRISPR-RNA used to protect prokaryotes from foreign genetic elements, such as phage and plasmids. The crystal structure provides insights into Cascade assembly and mechanism. Katherine Warner (NHLBI, NIH) introduced a novel concept for RNA targeted drug discovery aimed at inhibiting thiamine pyrophosphate (TPP) riboswitches. Using crystal structures of small molecule “drug like fragments” bound to TPP riboswitches, it was observed that ligands bound in the TPP aminopyrimidine binding site in some cases (confirmed by SAXS and SHAPE analyses) introduced a conformational change in the TPP pyrophosphate binding site that may prove to be an useful avenue for drug discovery.

SESSION 5: Methods was chaired by Albert Fu (SER-CAT). Alexander Wlodawer (NCI, NIH) presented an interesting talk on the Protein Data Bank and how to use its structures for your research. He noted that not all structures are created equal in terms of quality and warned that including a low-quality structures in your analyses might bias the results. Several examples of such structures were presented as well as how to identify them. Jinghua Lu (NIAID/NIH) presented his work on the systematic determination of heavy atom reactivity profiles with peptide ligands as a rational approach for identifying possible heavy atom derivatives needed for phasing macromolecule diffraction data. The structure of mouse serum amyloid A2, was determined by heavy atom phasing using heavy atom salts identified from the reactivity profile, was presented as an example of this technique. Marcus Mueller (Dectris Ltd.) gave an informative talk on data collection strategies to fully exploit the advantages of hybrid pixel detectors. Data was presented that showed that a fine ϕ - slice data collection strategy was best suited to these fast readout, low noise detectors in terms of data quality and anomalous signal. The audience was also cautioned about data collection at high frame rates and its impact on data quality if the experiment is not designed properly. John P. Rose (University of Georgia) presented the initial testing of the Rayonix MX300HS CCD detector at SER-CAT. The 30 X 30 cm detector can collect 10 images per second with a pixel size of 78 microns. Initial tests show that data collected in shutterless mode gave high data quality based on frame width (0.1, 0.2, 0.5, 1.0 degrees), frame rate (1, 2, 5, 10 Hz) or data reduction program used. The S-SAD structure determination of Trypsin using 1 Å X-rays ($\Delta F''_{(s)} = 0.25$) was presented. Xinhua Ji (NCI, NCI) described an eight-year effort to determine the structure of IraP, one of the small anti-adaptor proteins that regulate the response of bacteria to various stress conditions. The crystals exhibit pseudo-merohedral twinning and initial structures gave only the N-terminal half of the molecule. The structure was finally determined using the N-terminal fragment and molecular replacement using Phenix – Rosetta.

SESSION 6: Regulatory Proteins was chaired by Peter Sun (NIAID, NIH). Matthew Cuneo (Oak Ridge National Laboratory) presented his work on a dimeric periplasmic binding protein (PBP) involved in active transport of metabolites in bacterial ABC transport systems. Alpha helices at the dimer interface undergo conformational change upon ligand binding, resulting in ligand bound monomers that are involved in ligand transport. It is thought that this allosteric switch may represent an additional unidentified regulatory mechanism in PBP mediated ABC transport. Jennifer

Kavran (Johns Hopkins University School of Medicine) presented her recent biochemical and biophysical studies of Insulin-like Growth Factor Receptor (IGF1R). The studies showed that the IGF1R ectodomain maintains the receptor in an autoinhibited state where the transmembrane regions of the receptor are held apart. Ligand binding was shown to activate the receptor allowing the transmembrane regions to come together allowing tyrosine autophosphorylation. This suggests that autophosphorylation is the key allosteric step regulated by ligand binding. Yili Li (University of Maryland) gave an interesting talk on the C-type lectin-like receptors that govern natural killer (NK) cell activity. The crystal structure of human NKp65 in complex with the keratinocyte-associated C-type lectin (KACL) was reported. The structure explains the exceptionally high affinity of the NKp65–KACL interaction ($KD = 6.7 \times 10^{-10}$ M) and provides a binding topology template that can be applied to other NKC-encoded receptor–ligand pairs. Eric Toth (University of Maryland School of Medicine) reported the 2.55 Å crystal structure of human quinolinic acid phosphoribosyltransferase (QPRT) bound to its inhibitor phthalic acid (PHT). QPRT sits at the junction of the *de novo* NAD⁺ biosynthesis and the kynurenine pathway of tryptophan degradation making it a potential therapeutic target. The crystal structure provides a view of the conformational change in the QPRT hexamer upon inhibitor binding that will aid in fully understanding QPRT function and mechanism. Matthew Lau (NHLBI, NIH) focused on his work with the glmS ribozyme, a catalytic RNA, which differs from other self-cleaving ribozymes in that it requires an exogenous small-molecule GlcN6P for catalysis. Crystal structures of both wild type and mutant ribozymes show that in the mutant structure the GlcN6P binding pocket has been disrupted. Interestingly, the addition of metal ions to the mutant ribozyme restores activity suggesting that glmS ribozymes may have evolved from a metalloribozyme.

Poster Session: The poster session was both lively and informative. Yuqian (Roger) Shi's (Duke University) poster describing his structural investigation of Human Exonuclease I was named the winner of the HKL Research Best Poster presentation prize.

Phenix Workshop: The meeting ended with a Phenix workshop on Saturday, which was well attended. Workshop instructors were Paul Adams and Nathaniel Echols (Lawrence Berkeley National Laboratory) and Tom Terwilliger (Los Alamos National Laboratory). Topics covered included automated structure determination, structure solution from weak anomalous data (Terwilliger), molecular replacement (Adams), new tools for automated model completion and refinement (Echols).

John P. Rose

Acknowledgements: Special thanks to the meeting organizers Roy Mariuzza (Univ. of Maryland, IBBR), Peter Sun (NIAID, NIH), John Rose (SER-CAT, University of Georgia), Osnat Herzberg (Univ. of Maryland, IBBR), Jeff Boyington (VCR, NIAID, NIH) and Zheng-Qing (Albert) Fu (SER-CAT, Univ. of Georgia); the meeting sponsors (Agilent Technologies, Art Robbins Instruments, BioLegend, Bruker, Dectris, GenScript, Hampton Research, HKL Research, Microlytic, Molecular Dimensions, Rayonix, Rigaku, TPP Labtech, the NIH, the Southeast Regional Collaborative Access Team and Vaccine Research Center) who helped support the workshop; the Univ. of Maryland IBBR and its staff for providing an outstanding meeting site; the Phenix team “Paul Adams, Nathaniel Echols and Tom Terwilliger for providing a wonderful and informative workshop.

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Vice-President
Bill Royer



Professor of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA.

Education: BS, Penn State University (1976); PhD in Biophysics at Johns Hopkins University (1984) with Warner Love; postdoc at Columbia University Medical School with Wayne Hendrickson (1984-1990), which was a superb experience.

Professional Activities: ACA BioMAC SIG (Chair, 2007 - Chair-elect, 2006), Board of Governors, Consortium for Advanced Radiation Sources (2003-1012), Editorial Board Member: *Journal of Biological Chemistry* (2000-2005, 2007-2012), *Protein Structure, Function and Bioinformatics* (1998-2010). Reviewer for numerous NIH and NSF grants and journals including *Science*, *Acta Cryst. D*, *Biochemistry*, *PNAS*, *Protein Science*, *J. Mol. Biol.* and *Structure*, among others.

Research interests: I have been intrigued by the ability of x-ray crystallography to reveal the structure of molecules, particularly biological macromolecules, for over 35 years. As a graduate student, I became fascinated with hemoglobins for several reasons. I was initially motivated to understand the molecular basis for sickle-cell disease and to possibly use structural information to design inhibitors that would disrupt fiber formation. I was also intrigued by the ability of hemoglobins to sense their environment by exploiting structural transitions that permit communication between subunits and facilitate efficient oxygen transport. The vast diversity of hemoglobins among invertebrates, with cooperative hemoglobins ranging in size from simple dimers to megadalton assemblages with over one hundred subunits, suggests that nature has found mechanisms on multiple occasions that promote efficient delivery of oxygen. Investigating the structure and function of many such hemoglobins over the years has permitted us to learn fundamental principles for intersubunit communication, self-limited assembly of megadalton complexes and evolution of diverse solutions to the problem of efficient oxygen delivery in multicellular organisms. Our latest efforts have involved time-resolved crystallographic experiments on a

Candidates for ACA Offices in 2015

The Nominating Committee (George Phillips, Carrie Wilmot and Victor Young) proposes the following candidates for the 2014 elections for ACA offices in 2015.

Officers:

Vice-President: William Royer & Tom Terwilliger

Committees:

Communications: Katrina Forest & Jack Tanner

Data, Standards & Computing: Stephen Burley & Wladek Minor

Continuing Education: Andy Howard & Mark Wilson

To nominate write-in candidates for any office, write to the ACA Secretary: **Patrick Loll, Dept. of Biochem. & Molecular Biol., College of Medicine, Drexel Univ., Philadelphia, PA (pat.loll@drexel.edu)**. Letters must be received by September 15, 2014 and must be signed by 5 ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in **October 2014**.

cooperative dimeric hemoglobin to follow allosteric transitions as they occur. These experiments have uncovered unexpected features of the allosteric transition, including a contribution of interface water molecules within 5ns following ligand release and a linkage through a tight interface contact where E and F helices cross each other that permits direct communication across the dimeric interface.

For a number of years, we have investigated the structural transitions involved in the activation of interferon regulatory factors (IRFs), work pioneered by our fantastic UMass colleague Kai Lin whose career was tragically cut short by colon cancer. Our structure of a phosphomimetic mutant of IRF5 revealed dramatic structural transitions that couple phosphorylation with dimerization and assembly with other factors. These structural transitions are central for the transmission of signals initiated by pathogen detection to trigger the expression of proteins involved in the innate immune response. We are continuing our investigation of structural transitions and working to expand into full-length IRF molecules. IRF5 has been shown to be correlated with a number of autoimmune diseases, especially Lupus; our goal is to obtain insight into the activation at a level that will inform the design of inhibitors that could become useful in the treatment in Lupus and other autoimmune diseases.

In our other major project, we are working to identify inhibitors of the co-transcriptional repressor C-terminal binding protein (CtBP), a potentially useful cancer target. CtBP 1 and 2 have been shown to be overexpressed in many human cancers where they act to inhibit apoptosis and promote metastasis. Unusual among transcription factors, CtBP harbors an essential dehydrogenase catalytic domain that enables CtBP to be a redox sensor and provides an attractive target for small molecule inhibition. By investigating the details of the active site, we have identified reasonably high affinity inhibitors and are working to identify even higher affinity inhibitors and, through our collaborations, to

investigate the effectiveness of these inhibitors in tumor models. While we are only playing a small part, this is especially satisfying as an extension of my first interest in sickle-cell disease and also, of course, as a response to the devastation of cancer on friends and relatives that so many of us have experienced.

I have been very lucky to have the support of colleagues at UMass, particularly that of Celia Schiffer, that has allowed me to continue active research even as my success in obtaining external funds has waned, hopefully just temporarily. The support we receive and give, both in our own institutions and through societies like the ACA, is essential to the continuing progress of research.

Statement: I am honored to be nominated for the office of Vice-President of the ACA. Although I have not been able to attend the 2013 and 2014 ACA meetings, I have considered the ACA as my home scientific organization since the very first ACA meeting that I attended as a young graduate student in East Lansing, Michigan (following a ride from Baltimore in the back of a VW Bug with baby Jeffrey Hanson and his parents Jonathan and Louise Karle Hanson in the front seats). I have gained immensely from the rich mixture of presentations on techniques and results at every ACA meeting that I have attended.

During decades of involvement in protein crystallography, I have seen spectacular advances that have revolutionized our field. As a graduate student, we were generally limited to working on naturally abundant proteins and accepted that it may take many months or years to determine a crystal structure once suitable crystals were obtained. This has completely changed to the point that we can now apply macromolecular crystallography to address the most biologically important questions. Assuming suitable crystals can be obtained (not necessarily guaranteed but the odds are much better given the available tools) structures can often be determined rapidly. Thus, this is a wonderful time to be a structural biologist. On the flip side, there is little stability in funding these days, making it more difficult to take on long-term research projects.

I would particularly like to work in two areas to assist the ACA to respond to these difficult funding times: promoting public understanding of the importance of fundamental research in our society and helping young scientists navigate their careers in this new era. I will be especially interested in listening to the ideas from all ACA members about how to make progress in these areas.

I think the ACA is in a very good position to play a role in education of the public to foster greater support for the scientific enterprise. Unlike many other scientific disciplines, the inherent beauty of macromolecular and small molecule structures that we generate can often be appreciated without extensive scientific sophistication. (This was recognized by Irving Geis over 50 years ago and is evident every time you see a DNA double helix model in ads to sell drugs and much less related stuff.) In the case of protein crystallography, the idea of designing drugs to fit into naturally occurring cavities does not require knowledge of the complex signaling pathways in which such proteins carry out their function. Rather, knowing that a protein is involved in deciding a cell's fate is sufficient to appreciate the approach of using its structure to design inhibitors that can fit like a key into a lock to turn an enzyme off.

Visual effects in education can have a profound impact. This has been evident to me when growing crystals of ammonium phosphate at elementary schools, running sizing columns that separate red hemoglobins from blue hemocyanins with high school students, and growing lysozyme crystals with graduate students. Such simple experiments can dramatically change how students view science and scientists. I am alarmed at anti-science attitudes of many politicians and am convinced that such attitudes would not be as prominently represented at the highest levels of government if we did a better job educating the public about science and its value. As crystallographers, we have an invaluable product in the images that we obtain and the resulting understanding that we gain into chemistry and biology. I applaud the recent efforts, as part of the 2014 International Year of Crystallography, to increase public understanding of the spectacular power of crystallography, and I would like to see the ACA expand these efforts in schools, museums and the media. Public education should also be directed at policy makers, particularly members of Congress. I would like to explore ways to facilitate such discussions and would work with other organizations, such as FASEB, that are already heavily involved in advocacy.

Young scientists entering our profession have more choices, but probably less security, in this new environment. Many of us who have been in academics for our entire careers are ill equipped to advise young scientists about careers other than academics. We therefore need to look elsewhere to be sure that students have the information and resources they need to navigate through career opportunities in this new era. At UMass Medical School, like other institutions, we have begun efforts to help young scientists prepare for alternate career paths, which can help inform efforts at national societies. The YSSIG is already involved in many wonderful activities, including excellent high school outreach projects like those alluded to above. I would like to support and expand what is available to support young scientists. For instance, other scientific organizations run active career blogs and career development sessions. I would like to investigate some of these efforts and work with the YSSIG to see what can be productively incorporated within the ACA.

I recognize that I have not had as much experience in the governance of the ACA as many who have been nominated for this position. I did, however, gain greater appreciation of the inner workings of the ACA during my time as Chair of the BioMAC SIG and I have thoroughly enjoyed the many ACA meetings that I have attended over the years. Therefore, if elected, I will work to become more familiar with all aspects of the ACA to learn how I can work to make it a better organization that serves the interest of all its members, both young and not-so-young. I will also work to be an effective voice for the ACA to help us contribute to an appreciation of science by society at large.

Vice-President
Tom Terwilliger



Laboratory Fellow, Los Alamos National Laboratory, Los Alamos, NM

Education: AB Physics, Harvard College (1978); PhD Molecular Biology, UCLA, (1981); Helen Hay Whitney Postdoctoral Fellow (with Daniel E. Koshland, Jr.) UC Berkeley (1982-1985)

Professional activities: Co-editor, *Acta Cryst. F* (2005-); Co-editor, *Journal of Structural and Functional Genomics* (2005-); Faculty of 1000 Section Head (Structural Genomics) (2011-); IUCr Diffraction Data Deposition Working Group (2011-); ACA Data, Standards & Computing Committee (2013-2016). web site: solve.lanl.gov/terwilliger

Research interests: Methods development for macromolecular crystallography; structural genomics, macromolecular structure determination and analysis.
Statement: The ACA plays a crucial role in the promotion and development of the field of crystallography along with its sister organizations around the world and with the IUCr. As one of the leaders of the ACA I would endeavor to maintain the current vitality of the ACA and also to help the ACA develop and promote a vision of the future of crystallography. The annual ACA meetings are major events that provide a forum for a wide range of science benefiting from crystallography. These meetings also have a strong emphasis on methods and the nuts and bolts of structure determination and analysis that I feel is essential to the strength of the field. Continuing these

strong traditions would be a top priority of mine. The standing committees and interest groups of the ACA play an important role in communicating the vision of the ACA, assisting members with continuing education, and setting standards for data and reporting, and helping young scientists, all while helping maintain continuity in the ACA. Continuing the roles of these standing committees and interest groups and helping to invigorate them will be another important priority. Supporting the outstanding ACA staff in their continuous maintenance of the ACA organization will be a third. In addition to these vital current functions of the ACA, it will be important to continue the development of a vision of where crystallography should go. There are many new developments both in crystallography and in other structural fields that affect the work and future of crystallographers. In macromolecular crystallography the change from crystallography as a profession to structural biology as a profession has changed the training of students and the research focus of nearly all in the field. It will be important to ensure that there is sufficient training in crystallography available, and that there are sufficient researchers who continue to develop the field, as the methods that exist today are far from optimal. Also in macromolecular crystallography it will be important to recognize the developments in all technologies for structural biology and to bring together complementary methods. There has been a long and productive past for crystallography and there will be a long and productive future as well. I would be honored to be able to help the ACA continue to lead in developing this future.

Communications Committee
Katrina T. Forest



Professor, Bacteriology Department, University of Wisconsin-Madison,

Education: BS Applied Biology, MIT (1987); PhD Molecular Biology, Princeton (1993); postdoctoral work at the Scripps Research Institute (1993-1997).

Professional Activities: ACA member since 1988; NIH Prokaryotic Cellular and Molecular Biology study section chairperson; *Journal of Bacteriology* editorial board member; reviewer for *JACS*, *Mol Micro*, *J. Bact.*, *PNAS*, *Nature Biotechnology*, *Nature*; LS-CAT advisory board member; 2016 Photoreceptors Gordon Conference co-chair; ACA Continuing Education Committee member (2011-2012).

Research Interests: My group focuses on structural microbiology, which we think of as applying x-ray crystallography as well as many other biochemical and microbiological techniques that will help us to understand how bacteria interact with the world. In particular, we study the assembly and retraction of Type IV Pili, and the structure/function relationships and biotechnology applications of the red light photoreceptor Phytochrome. In the past five years we have increasingly worked with several colleagues at UW-Madison on crystal structure determinations of molecules that fall in a "twilight zone" between small and protein-sized. Some of these include non-natural amino acids and several have been analyzed using quasiracemic crystallography.

Statement: Student membership in the ACA was fundamental to my training as a crystallographer and to my sense of belonging in this community. During my academic career, I have been the lone structural biologist in a microbiology department; connecting with colleagues at other universities and staying current on crystallographic methodologies have been important benefits of ACA membership. I would be honored to serve on the Communications Committee as a way of giving something back to the ACA.

While we may live for those fleeting moments in which we realize we have discovered something about the natural world that no one else is yet aware of, our findings are only fully realized when they are explained to others. Our responsibilities as scientists include communicating our results with colleagues, funding agencies, students, and the general public. I have



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enjoyed opportunities during my career to discuss our research with local newspapers and television stations, to present it to interested citizens at public outreach events, and to share our science during campus workshops for middle school students. My lab has also expanded our definition of science communication by hosting Artists in Residence whose own artistic output, influenced by the experimental goings on in the lab, serves as a novel way for us to communicate the beauty in science to the general public.

If I am elected to the communications committee I will work with my colleagues to maximize exposure of the annual ACA meetings, coordinate videotaping of and special volumes dedicated to plenary lectures, solicit contributions for *RefleXions*, serve as an ambassador for the value of crystallography to funding agencies, and seek additional opportunities to communicate the importance of crystallography to the general public.

Communications Committee

Jack Tanner



Professor, Depts of Biochem and Chemistry, University of Missouri-Columbia

Education: BS Chemistry, University of Missouri-Columbia (1983); PhD Chemistry, Brown University (1988); Postdoctoral research in computational chemistry (University of Houston, J.A. McCammon, 1988-1991); Postdoctoral research in protein crystallography (University of Houston, K.L. Krause, 1991-1997).

Professional Activities: BioMAC SIG Secretary/Treasurer (2007-2008); ACA-session Co-Chair (2005); Judge, Oxford Cryosystems poster contest (2005) Contributor to ACA *RefleXions* (2004-2005).

Research Interests: Protein structure and function, x-ray crystallography, SAXS, computational biology. Current projects include flavoenzymes, proline catabolic enzymes, and aldehyde dehydrogenases.

Statement: It is an honor to be nominated again for a position on the Communications Committee. I have been an ACA member for about 20 years. I attend the meeting every few years and encourage my graduate students to join the ACA. I believe that the ACA must play a leading role in setting and maintaining the high standards of x-ray crystallography. I am deeply concerned with the shoddy protein crystallography that I have encountered with increasing frequency over the past several years as a manuscript reviewer and user of the PDB. Like many of you, each year I review a few manuscripts that have obvious errors such as ligands and side chains with no density and bizarrely chosen asymmetric units that don't represent the solution oligomer. As a member of the Communications Committee I will support educational workshops and sessions at the ACA meeting designed to educate graduate students and postdocs about our craft. I believe that service is an important part of professionalism and I look forward to serving ACA members in this capacity, if elected.

Data, Standards & Computing

Stephen K. Burley



Distinguished Professor, Rutgers University; Director, RCSB Protein Data Bank; Director, Center for Integrative Proteomics Research, Rutgers University; Member, Rutgers Cancer Institute of NJ; Adjunct Professor, UC San Diego

Education: BSc Physics, University of Western Ontario, Canada (1980); DPhil, University of Oxford (1983); MD, Harvard Medical School (1987)

Professional Activities: Not-for-profit – current: Advisory boards: INSTRUCT: An Integrated Structural Biology Infrastructure for Europe (2008-); SickKids Res. Inst. (2013-). Editorial advisory board: *Journal of Functional and Structural Genomics* (2000-); *Molecular Cell* (1997-); *Scientific Data* (2013-); *Structure* (1995-); *Nature Scientific Data* (2013-). **Completed:** Worldwide Protein Data Bank (wwPDB) Foundation (Chair, Board of Directors); RCSB PDB (Chair, Scientific Advisory Board); wwPDB (Chair, Scientific Advisory Board); Structural Genomics Consortium (Member, Board of Directors—Eli Lilly and Co. Representative); RIKEN Cluster of Life Science Platform (Member, Advisory Board); ACA (Chair, Industrial & Synchrotron Radiation SIG); DIAMOND CEO Search Committee (Member, Wellcome Trust Representative); Int. Structural Genomics Org. (ISGO; Member, Exec. Comm.); Cancer Res. Foundation Fellowship Advisory Panel (Member); Chemistry in Cancer Res. Task Force, AACR (Member, Steering Comm.); DIAMOND Synchrotron Scientific Advisory Comm. (Member); Life Sciences Res. Foundation, Postdoctoral Fellowship Advisory Panel (Member); NAS Study on Intellectual Property in Genomic and Proteomic Research and Innovation (Committee Member); NIGMS/NCIAPS X-ray Beamline (Member, Scientific Advisory Board); Nucleic Acids Data Base (Member, Scientific Advisory Board); Royal Society of Canada, Life Sciences Fellowship Committee (Member); *Genome Biology and Genes and Development* (Member, Editorial Advisory Board).

For-Profit Founder, Board of Directors, Scientific Advisory Boards, and Consultancies – completed: Prospect Genomics, Inc. (Co-Founder); Oncocyte, Inc. (Member, Board of Directors); Eclonion, SA; GENSET, SA; Gryphon Pharmaceutical Science, Inc.; Scriptgen Pharmaceuticals, Inc.; Gryphon Pharmaceutical Sciences, Inc.; and Structural GenomiX (Member, Scientific Advisory Board); Protein Solutions, Inc. (Chair, Scientific Advisory Board). Coferon, Inc., Amgen, Inc. Novagen, Inc., Tularik, Inc. (Consultant)

Research Interests: X-ray crystallography, structural bioinformatics, biological databases, structure-guided drug discovery, cancer genomics and proteomics, antibiotic resistance, scientific and medical education.

Statement: As an educator and Director of the Center for Integrative Proteomics Research at Rutgers University (proteomics.rutgers.edu) I am currently leading efforts to create new outreach and instructional vehicles describing the best practices for using data resources and tools in structural biology to broader audiences in biology, life sciences and physical sciences. I see great potential for the Data Standards and Computing Committee (DSCC) and the ACA working to identify exemplar curricula and materials to support such instructional programs for both scientific and general audiences.

As the former Chair of both the RCSB Protein Data Bank (PDB, www.rcsb.org/pdb) and wwPDB (www.wwpdb.org) Advisory Committees, I have been actively involved in the PDB efforts developing community-based standards for deposition, publication, and archiving of macromolecular structural models and underlying experimental data. I believe the DSCC and ACA can play an important role in promoting and strengthening the progress from these efforts, and in playing an active role with continuing challenges of developing standards for new diffraction, hybrid experimental, and integrative methodologies.

The crystallographic community benefits from the availability of structure data hosted in a variety of data repositories. I believe an important role of the DSCC and ACA can be to increase community awareness of the sustainability challenges faced by these repositories, and to promote successful models of sustainability that ensure continued availability and high level service that these repositories provide. There are also the opportunities to extend successful models of sustainability to other communities developing repositories for experimental data complementary to crystallographic data.

Data, Standards & Computing

Wladek Minor



Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA

Education: MSc, physics, Warsaw University (1969); PhD, physics, Warsaw University (1978)

Professional activities: Member of the www.mcsg.anl.gov and the www.nkysgrc.org (both centers of the NIH Protein Structure Initiative), and www.csgid.org (a project of the NIAID) and www.enzymefunction.org (an NIH Glue Grant).

Research Interests / Statement: In the last fourteen years, my laboratory has developed sophisticated database systems for tracking and extracting information from experimental data from all phases of the macromolecular protein crystallography pipeline. These systems have been used to track millions of experiments on tens of thousands of proteins for multiple large-scale structural biology centers, including two high-throughput enabled PSI: Biology centers (NYSGRC and MCSG), Center for Structural Genomics of Infectious Diseases (CSGID) and Enzyme Function Initiative (EFI). Along the way, my laboratory has produced numerous tools and protocols to address specific problems in macromolecular crystallography, including validation of metal-ion binding sites and identification of potential ligands via cocktail screening. I also have been very active in the ongoing discussions in the crystallographic community regarding standards of data collection, validation and deposition, and I have co-authored several review articles and book chapters on this topic. In addition, I have multiple decades of experience in crystallographic data

reduction and processing that led to over 150 publications and 30,000 citations. If elected, I will have an opportunity to serve the crystallographic and scientific community in a new capacity. I would be able to use all my knowledge and experience to make data more complete, reproducible, uniform and accurate.

Continuing Education

Andy Howard



Associate Professor, Biological & Chemical Sciences Dept, College of Science, Illinois Institute of Technology, Chicago, IL.

Education: BA Biophysics, Pomona College (1975); PhD Physics, UC San Diego (1981); Postdoc, crystallography, Molecular Biology Institute, UCLA, (1981-83) with David S. Eisenberg; Postdoc, Toxicology, Inhalation Toxicology Research Institute (1983-84) with Charles E. Mitchell

Professional activities: Member of ACA since about 1981, Director, ACA Summer School in Macromolecular Crystallography (2002-2008), ACA Data Standards & Computing Committee, (2006-2008 - I think), Treasurer, IIT Branch of Sigma Xi, Member, AAAS and ACS, At-large member, Illinois Board of Higher Education's Faculty Advisory Council, Secretary, University Faculty Council, IIT (2002-2010), First Chair, CAT Directors' Council, Advanced Photon Source (1997-1999), Faculty Member, Center for Synchrotron Radiation Research & Instrumentation, IIT.

Research interests: Crystallographic methods development, particularly data processing software; beamline automation; crystallographic education; crystallographic standards and curation; structures of bacterial hemoglobin, cholera toxin, dystrophin components, alcohol dehydrogenase.

Statement: Small-molecule and macromolecular crystallography have become increasingly de-professionalized over the last three decades in the sense that non-specialists can participate in and use crystallographic structure determinations. This de-professionalization is a good thing in that it increases the size of the community that can capitalize on the utility of crystallographic techniques, but it comes at a price: many of the practitioners of these techniques have only a meager understanding of the physics and chemistry that underlie these techniques. The result is that if our hardware and software do not yield answers on the first try, these users have no way of diagnosing problems and working around them, and they frequently have an inadequate understanding of what parts of our analyses are reliable and what parts are not. The task of crystallographic educators should be to provide this community of users with enough knowledge and wisdom about the fundamentals of the subject, and the ways that the field is advancing, that these non-specialist users can solve their own problems and have a deeper appreciation for its principles. Educators should also help practitioners to recognize the strengths and weaknesses of crystallographic analyses, and in particular to know what the confidence limits are for the conclusions that they derive from their data.

The ACA Continuing Education Committee should involve itself in in-reach to specialists so that they can keep up with the latest theoretical and experimental approaches. But its charge should, increasingly, involve outreach to the wider scientific community so that those non-specialists will know how to overcome roadblocks and understand the advantages and limits of crystallographic methods. I would be honored and excited to work with other members of the Committee to explore ways to accomplish both these in-reach and outreach goals.

Continuing Education

Mark A. Wilson



Associate Professor, Department of Biochemistry and Redox Biology Center, University of Nebraska, Lincoln, NE.

Education: BS Biochemistry and BA History, University of Rochester (1995); PhD Molecular Biophysics and Biochemistry, Yale University (2001)

Professional Activities: Co-chair of the *New Structures* session, ACA Annual Meeting (Knoxville, TN, 2008), Secretary of the Biomacromolecules ACA special interest group (2009-11), Co-Director of the Macromolecular Crystallography Laboratory at the University of Nebraska (since 2008), Synchrotron beamtime proposal reviewer for the Advanced Light Source (2009-2013).

Research Interests: Macromolecular crystallography; structural biology of redox-active proteins; biochemical basis of neurodegeneration; atomic and ultra-high resolution crystallography; protein disorder

Statement: I am honored to be nominated for election to the Continuing Education Committee of the ACA. The creation and dissemination of knowledge is the defining occupation of a scholar and the Continuing Education Committee provides an opportunity to participate in the dissemination portion of that mission on a national level. It would be a privilege to serve.

The Continuing Education Committee has a variety of responsibilities that share a common goal of encouraging a greater mastery of this complex discipline by

both students and experienced crystallographers alike. This is a challenging climate in which to emphasize the mastery of foundational concepts. Crystallography is often viewed as a fairly routine, albeit complex, method whose result is an essentially technical rather than intellectual accomplishment. I strongly feel that educational opportunities in crystallography should help rectify this misinformed view of what we do. While outreach to better inform our non-structural colleagues is important, I believe that the education of the next generation of crystallographers must emphasize the importance of a thorough mastery of crystallographic concepts and the often non-trivial challenges involved in solving and interpreting x-ray crystal structures. If elected to the Continuing Education Committee, I would work to have the value of conceptual aspects of crystallography reflected in the choice of some of the workshop topics at ACA meetings.

X-ray crystallographers have consistently made the fruits of their intellectual labor as widely accessible as possible. The Protein Data Bank is one of the most visible examples of an early, sustained, and far-sighted commitment to free access to models and, later, data on a global scale. The whole of the molecular life sciences would have been much diminished had the macromolecular crystallographic community not committed to the principles of open access data archiving decades before it became widely accepted in other fields. Similarly, the quality and power of modern crystallographic software that is made easy to use and freely available to academic users is remarkable and exemplifies an abiding community spirit in crystallography. Transparent methodology, freely available tools, and centrally archived results that can be scrutinized by colleagues around the world are values that set macromolecular crystallography apart from many other disciplines. As education involves not simply the transfer of knowledge, but the inculcation of values, I believe that the Continuing Education Committee can help ensure that workshops and training opportunities pass these values on to the next generation of crystallographers.



Image courtesy of Desirée Benefield and Borden Lacy.

What's on the Cover: D. Borden Lacy (Dept of Pathology, Microbiology, and Immunology, Vanderbilt U School of Medicine) was the winner of the **2014 Margaret C. Etter Early Career Award**. She presented her plenary lecture on Tuesday, May 27th preceding the *Etter Symposium* at the Albuquerque ACA meeting. Borden kindly supplied the cover image from a paper recently published in *PNAS* (Molecular Assembly of Botulinum Neurotoxin Progenitor Complexes, Desirée A. Benefield, Scott K. Dessain, Nancy Shine, Melanie D. Ohi & D. Borden Lacy, *Proc Natl Acad Sci*, (2013) **110**, 5630-35.)

Botulinum neurotoxin (BoNT) is produced by *Clostridium botulinum* and associates with nontoxic neurotoxin-associated proteins to form high-molecular weight progenitor complexes (PCs). The PCs are required for the oral toxicity of BoNT in the context of food-borne botulism and are thought to protect BoNT from destruction in the gastrointestinal tract and aid in absorption from the gut lumen. Organisms that produce BoNT also produce one or more neurotoxin associated proteins (NAPs) that noncovalently associate with the neurotoxin to form progenitor complexes (PCs). Borden and her colleagues determined 3D structures for each serotype using electron microscopy and the random conical tilt approach. Crystal structures of the individual proteins were placed into the BoNT/A1 and BoNT/B PC electron density maps to generate unique detailed models of the BoNT PCs. The hemagglutinin proteins (HAs) bind a variety of sialo- and asialooligosaccharides; sugars are depicted in the model as red sticks. These sugar binding sites could represent points of contact between the BoNT PC and mucins, glycolipids, or glycoproteins within the intestine. Additionally, it was observed that the complex has significant flexibility, which may be important for multivalent binding interactions on the intestinal surface.

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A Harmonious Balance for Public Access



The issue of public access to scholarly publications is becoming increasingly discussed among the physical sciences community, because of its complexity and the contentious debate surrounding it. Access is good for science and it's good for scholarship; that much all stakeholders can agree upon. Nearly a decade after the appearance of the first open access

journals whereby journals are published online outside of subscription paywalls—usually because of an author-paid fee—most journals are still funded through library subscriptions. Since much of basic research is funded by public funds, there has been increasing demand for some means of providing the public with access to publications that report on research that was publicly funded. But if not implemented pragmatically, public access can do more harm than good. This latter assertion is where the controversy comes in, and where our community must apply its most astute communication skills to make it universally understood.

Scientific progress occurs within a cycle as interconnected and self-sustaining as the spokes of a wheel, each relying on the others to carry its share so that the carriage it supports can continue to advance. When one spoke is compromised, the burden is felt throughout. Looking at the incubator for science, it's clear that there are many facets that rely on each other to thrive. Researchers and scholars need reliable information on which to base future research. The more of this information they have, the more effective they will be in advancing science. This information largely comes in the form of scholarly publications that have gone through peer review and which are fed content by researchers themselves. Scholarly publications are produced by publishers, which manage the peer review and invest heavily in improving, making discoverable, preserving, and delivering articles to the research community and the public. The result is improved productivity in science and science education and advanced interdisciplinary research. Scientific associations relying on journal revenue further support the community, bringing members together for collaboration and engagement.

The ability of publishers to recover their investments incentivizes innovation and the development of industry-wide interoperability standards and infrastructure. If all content were free, publishers could not deliver the value they bring to the process (broken spoke), and scholarly manuscripts would diminish in substance and discoverability (another broken spoke); those non-profit associations that support their constituencies with revenues from their journals would falter, with negative impacts on the science community (yet another compromised spoke). Ultimately, science itself suffers (broken wheel).

The trick is in devising the greatest possible public access while maintaining the added-value that publishers bring to

the process and keeping in mind the financial pressures put on libraries and research institutions. Publishers have for the last several years been working to diversify their business models to respond to the increased demands for public access, but not quickly enough, as governments in the United States and Europe are pursuing measures to hasten the public access movement.

In 2011, the government of the United Kingdom accepted the Finch Commission report, advising unfettered open access to all scholarly publications resulting from government-supported research either through direct funding of open access journals or after an embargo period for articles behind subscription pay walls. Although the report was hailed as revolutionary, widespread discourse continues over how to implement the recommendations. On February 22, 2013 the White House Office of Science and Technology Policy (OSTP) issued a memorandum on “increasing access to the results of federally funded scientific research.” This directive is the result of the America COMPETES Reauthorization Act of 2010, one section of which directed OSTP to work with the federal agencies that fund science and their stakeholders (such as publishers) to develop and implement policies that promote access to the results of agency-funded research.

In late spring, the Professional and Scholarly Publishing Division of the Assoc. of American Publishers offered to the US federal funding agencies and other stakeholders an initiative of the scholarly publishing community to help them meet the OSTP public access requirements. CHORUS, or the Clearinghouse for the Open Research of the United States, is a public-private partnership that aims to greatly increase public access to peer-reviewed publications resulting from federally funded research. Since then, CHORUS has incorporated as a non-profit organization.

CHORUS had its origins almost a year ago when a small group of publishers began a pilot project with four funding agencies to solve the initial problem of identifying those articles that resulted from federal research funding. This project, called FundRef, was done under the aegis of CrossRef, a nonprofit organization formed by publishers in 2000 to promote electronic access to scholarly literature by establishing identification standards. Widespread adoption of these standards interlinks the world's online publication platforms—4300 publishers use CrossRef's methodology, and more than 2000 libraries can access key identification information for nearly 60 million manuscripts from 27,000 scholarly journals. With the simple addition of metadata fields to reveal funding sources for all of these articles, federal agencies can easily track the bulk of published literature that results from their agency's funding. This is important to the agencies, and to us, because it will help demonstrate the value of their investment in research.

CHORUS builds on the FundRef protocols and provides a straightforward means of public access for the entire community of researchers, institutions, funding agencies, and the public. Using FundRef for identification and CrossRef to link to the publisher's site—where a free, full-text article will be available, and preserved and archived—the CHORUS board estimates that 80% of necessary infrastructure is already in place. The publishing community will provide the remainder of the build-out costs. The system is paid for by standard charges that publishers pay to CrossRef as we deposit articles and associated identification data into the CrossRef database.

CHORUS puts no additional demands on the researcher; the author is in communication with the publisher from submission to publication. Publishers will be responsible for complying with the agreed-upon terms. By directing readers to the publisher's site where the manuscript is first published, updated as necessary, and archived, publishers are compelled to preserve the value of their platform and the integrity of the record.

The publishing community is developing CHORUS as a public service to all stakeholders: funding agencies, the academic community, and the interested public. It is being offered to the government agencies at no cost, allowing them to maintain their focus on funding research and research management. Publishers are willing to shoulder the cost of CHORUS because it relies largely on existing infrastructure built up by the publishing industry through years of collaboration.

Publishers are willing to underwrite the additional costs required to develop CHORUS because it is the most pragmatic and least costly public access solution that can be widely adopted. CHORUS provides free access to content that is produced and supported via two basic publishing models: author-paid and (usually library-paid) traditional subscriptions. With the former, a publication's costs are paid upfront by the author or the author's sponsor, and full access is granted upon publication to all; CHORUS will provide links to this content. With the latter, CHORUS

will grant full access after an embargo period imposed by the funding agencies. For the near term, publishers will continue to depend on a mixed economic model to support their industry and sustain their contributions.

The CHORUS organization must remain neutral on embargos to remain credible to all collaborators. Nevertheless, controversy persists about the length of such embargo periods. Since 2008, the NIH has imposed a 12-month embargo for NIH-funded research works, largely biomedical in nature. However, the publishing community has argued that biomedicine is a well-funded, fast-moving field of scholarship; other fields cannot conform easily to a single embargo period. When properly implemented, embargos can be long enough for publishers to recover publication costs.

H. Frederick Dylla

*Executive Director and CEO of the
American Institute of Physics (AIP)*




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THANK YOU ALBUQUERQUE EXHIBITORS



***Congratulations to the recipients of the
2014 ACA / IUCr Travel Awards******Canada***

Mridula Swayampakula - University of Alberta

Cameroon

Patrice Kenfack Tsobnang - University of Yaounde

Hungary

Margit Fabian - Centre for Energy Research – Budapest

New Zealand

Franziska Huschmann - University of Otago

Yi Tian-Ting - University of Auckland

United Kingdom

Rajni Bhardwaj - University of Strathclyde

USA

Brian Dolinar - University of Wisconsin-Madison

Christopher Durr - The Ohio State University

Paulina Dziubanska - University of Virginia

Alisa Glukhova - University of Michigan

Travis Hayden - Texas Christian University

Katarzyna Jarzemska - University at Buffalo

Jaime Jensen - North Dakota State University

Kinberly Lincoln - Texas Christian University

Brian Mahon - University of Florida

Kimberly Maize - University of Minnesota

Krystle McLaughlin - Lehigh University

Jie Qiu - University of Notre Dame

Peter Randolph - University of Virginia

Katherine Sippel - Baylor College of Medicine

Mohammed Taha - University of Texas at Dallas

Andrey Yakovenko - Argonne National Laboratory

Each SIG peruses the submitted abstracts and selects one paper submitted by a student to give a lecture that represents the area of research covered by the SIG. Those selected also receive a certificate and a check for \$250.00. Congratulations to the following 2014 SIG Etter Lecturers

BioMac

Yusong Guo - Rice University

Fiber Diffraction

R. S. Madhurapantula - Illinois Inst. of Technology

Industrial

Jacob Trotta - Alkermes, Inc.

Light Source

Igor Petrik - University of Illinois Urbana Champaign

Materials

William Kerlin - University of Nevada Las Vegas

Neutron Scattering

Patricia Langan - Los Alamos National Lab

Powder

Vicky Doan-Nguyen - University of Pennsylvania

Small Angle Scattering

Jesse Hopkins - Cornell University

Small Molecule

Jordan Cox - University at Buffalo

Young Scientist

Brian Mahon - University of Florida

The USNCCr will be sending 5 delegates to represent the US at the IUCr Congress and General Assembly in Montreal in August.

Our delegates are:

Brian Toby (Chair) Argonne National Laboratory

Chris Cahill – George Washington University

Katherine Kantardjieff – California State Univ. San Marcos

Brian Matthews - University of Oregon

Joe Ng – University of Alabama Huntsville

Alternates:

Claudia Rawn – University of Tennessee

Joe Reibenspies – Texas A&M

Amy Sargent - Northwestern

Stephen K. Burley – RCSB PDB Rutgers Univ.

The USNCCr has also made some funds available to support students to attend the Congress. Congratulations to the following recipients of USNCCr travel grants:

Raul Castaneda -New Mexico Highlands U

Jesse Clark- Stanford / SLAC

Jordan Cox - University at Buffalo

Vicky Doan Nguyen - University of Pennsylvania

Benjamin Frandsen - Columbia University

Allyson Fry - Johns Hopkins University

Leighanne Gallington - Georgia Inst. of Tech.

Bradley Hintze - Duke University

Kirsten Jensen - Columbia University

Tiffany Kinninbrugh - Argonne National Lab

Josephine Leung - Scripps Research Institute

Justin Newman - Purdue University

Taryn Palluccio - Tufts University

Gregory Rohde - University of Minnesota

Silvia Russi - SSRL

Isha Singh - Indiana University School of Medicine

Anastasiya Vinokur - University of Wisconsin

Cody Webb - Syracuse University

Xuan Zhang - Texas A&M

Heping Zheng - University of Virginia

Contributors to this issue: Laurie Betts, Stephen Burley, Mike James, Grace Chik, Bridget D'Amelio, Louise Dawe, H. Frederick Dylla, Jeanette Ferrara, Joe Ferrara, Katrina Forest, Jarrod French, Frank Fronzcek, Andy Howard, D. Borden Lacy, Pat Loll, Wladek Minor, Eric Montemoyer, Chiara Pastore, John Rose, Bill Royer, Yulia Sevryugina, Jack Tanner, Martha Teeter, Ned Seeman, Tom Terwilliger, B. C. Wang, Kraig Wheeler, Mark Wilson, Christine Zardecki.

Cover: Images provided by D. Borden Lacy; production by Connie Rajnak.



No question about it - the Albuquerque meeting was enjoyed by one and all. Top row (left to right): Virginia Pett, Abe Clearfield, Ruth Clearfield, Ilia Guzei. Second row (left to right): Mike James, Connie Rajnak, Jenny Glusker, Miriam Rossi. Third row (left to right): Ron Hamlin, Haruko Hamlin, Jessica Addiss, Marcia Colquhoun. Bottom row (left to right): Brian Toby, Mary Ann Wu, Sue Byram. All photos courtesy of Dick Bromund.

American
Crystallographic
Association

$$\int e^{2\pi i \mathbf{q} \cdot \mathbf{r}} \sum_j$$



$d\mathbf{q} =$



Philadelphia, PA

July 25-29, 2015



Program Chair - Louise Dawe
ldawe@wlu.ca



Program Chair - Kraig Wheeler
kawheeler@eiu.edu



Photographer - Peter Müller
pmueller@mit.edu



Poster Chair - Ilia Guzei
iguzei@chem.wisc.edu



Session Photos - Jeff Deschamps
dechamps@nrl.navy.mil

July 25-29, 2015

Philadelphia, Pennsylvania

Sheraton Philadelphia Downtown

DEADLINES

Abstracts: March 31, 2015

Travel Grant Applications: March 31, 2015

Advance Registration: May 31, 2015

Hotel Reservations: June 18, 2015

Abstracts accepted online only

at least 40% of all talks will be from contributed abstracts

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Practical Crystallization (Blackboard Session)

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Undergraduate Reception

Career Development

Engaging Undergraduates with Crystallographic Research

AWARD SYMPOSIA

Buerger Award in honor of Greg Petsko

Warren Award in honor of Laurence Marks

Margaret C. Etter Early Career Award in honor of Yan Jessie Zhang

MICROSYMPOSIA

From Fingerprint to Full ID: PXRD

Molecular Machines

Crystal Engineering: Form and Function

Structural Dynamics

Advances in Serial Crystallography

Structural Glycobiology

Ambient and Cryogenic Approaches

Porous and Meso-Scale structures

Meeting logo designed by

Jason Mercer (Memorial University of Newfoundland)

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Crystallographic
Association

$$\int e^{2\pi i \mathbf{q} \cdot \mathbf{r}} \sum_j$$



$d\mathbf{q} =$



Philadelphia, PA

July 25-29, 2015

Transactions Symposium
Crystallography for Sustainability

Organizers: Cora Lind-Kovacs (University of Toledo; cora.lind@utoledo.edu); Robin D. Rogers (University of Alabama; rdrogers@ua.edu)

This multidisciplinary symposium will be focused on the cutting edge impact of crystallography-based research on global aspects of the sustainability of world resources, including green chemistry, the globalization of chemistry, and responsibilities and opportunities to serve the broader public. In particular, the symposium will cover such aspects as the lead role of crystallography in the design of materials and in the design of processes that reduce energy consumption, protect clean water supplies, provide unique environmental benefits, enable new medicines, or provide new greener routes to chemicals and materials. The *Transactions Symposium* will highlight the unique roles of crystallography in achieving major societal goals. Special attention will be given to providing international perspectives related to both areas of critical need, such as the supply of medicines and clean water and energy to all citizens of the world, and to overcoming the limitations or restrictions of raw materials for products that lead to improved quality of life. Possible topics are:

Crystallography in the design of sustainable materials

In situ characterization of materials and analysis to reduce waste

Crystal engineering

Energy-related materials (batteries, fuel cells, solar cells)

Crystallography in the design of sustainable processes

Design of catalysts for reduced chemical consumption

Photosynthesis as alternative production methods

Water purification

Catalysis

CO₂ capture

Crystallography used for a sustainable society

Food

Energy

Medicines

Drinking water

Learning lessons from nature about sustainability

Photosynthesis / the artificial leaf

General Meeting Information



The US Declaration of Independence was signed in Philadelphia in July 1776, and Pennsylvania was the second state to join the Union in 1787. It is a very walkable city. You will not need a car to visit the Liberty Bell (Independence Hall), the Franklin Institute, the Philadelphia Museum of Art and many other local attractions.

Philadelphia is also a 'foodie' town, and you will find palate pleasing repasts in all price ranges. The lower end need not be fast food, not with the myriad of eclectic food trucks that you will find all over the city. Sadly, the legendary Le Bec Fin is no more but upper end appetites will find restaurants like Alma de Cuba and a variety of tastes and prices featured in restaurants by Jose Garces and other celebrity chefs.

Obtaining a VISA: Advanced planning by foreign travelers is critical. For those travelers who will require a VISA: **applications should be made at least 90 days in advance of the travel date.** For further information contact: the US Department of State (travel.state.gov/visa/visa_1750.html).

Staying Green: All attendees will receive a hardcopy of the Program Schedule but the full set of abstracts will only be available online. We are not planning on having a meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Info: FREE WI-FI is included in the sleeping rooms, so bring your laptops and stay connected to home and office. 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 this commitment, which also brings with it free meeting space that helps keep registration fees affordable.

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

Financial support: Travel support will be available for young scientists. Applications should be made by the abstract deadline on the meeting web site.

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

SEPTEMBER 2014

14-17 **2nd International Conference on Science at Free Electron Lasers.** Villigen, Switzerland. science-at-fels-2014.eurofel.eu/

17-20 **15th International Conference on the Crystallization of Biological Macromolecules – ICCBM15.** Hamburg, Germany. www.iccbm15.org

OCTOBER 2014

26-28 **72nd Annual Pittsburgh Diffraction Conference.** University of Georgia, Athens, GA. pdc14.bmb.uga.edu/Home.html



26-31 **12th International Conference on X-Ray Microscopy.** Melbourne, Australia. www.xrm2014.com

JANUARY 2015

14-16 **BioXFEL STC Annual Conference.** Ponce, Puerto Rico. www.bioxfel.org/events/details/6

JUNE 2015

7-11 **International Conference on Structural Genomics 2015: Deep Sequencing Meets Structural Biology.** Rehovot, Israel. www.weizmann.ac.il/conferences/ICSG2015

JULY 2015

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



AUGUST 2015

23-28 **19th European Crystallographic Meeting, ECM29.** Rovinj, Croatia. ecm29.ecanews.org



DECEMBER 2015

5-8 **AsCA2015 Science City.** Kolkata, India. asca.iucr.org

The AIP State Department Science Fellowship

Most of the foreign policy issues faced by the US Department of State have a scientific or technical component. This fellowship is intended to enhance the S&T capacity of the Department by enabling at least one scientist annually to work at the Department's Washington, DC headquarters for a one-year term.

This is a unique opportunity for a scientist to contribute scientific and technical expertise to the Department and raise awareness of the value of scientific input. In turn, scientists broaden their experience by interacting with policymakers in the federal government and learning about the foreign policy process.

Application deadline: November 1 of the year prior to the fellowship term of the year applied for.

The AIP Congressional Science Fellowship Program

The American Institute of Physics, in partnership with the Acoustical Society of America (ASA), annually sponsors one scientist to spend a year providing analytical expertise and scientific advice to Congress. A second fellowship is sponsored by the American Physical Society. The program enables scientists to broaden their experience through direct involvement with the legislative and policy processes.

Fellows gain a perspective which, ideally, will enhance not only their own careers but also the physics community's ability to more effectively communicate with its representatives in Congress.

Benefits: Stipend of \$70,000 - \$72,000 per year. Relocation allowance. Allowance for in-service travel for professional development. Reimbursement for health insurance premiums up to specified maximum.

Application deadline: January 15 of the year of the fellowship term. Fellowships are for one year, usually running September through August.

Scientists at all career stages, including mid- and late-career professionals, are encouraged to apply. Although the fellowship is a full-time position, arrangements to supplement the stipend by continuing to receive a salary from a current employer while taking a sabbatical or leave of absence during the fellowship term may be worked out on a case-by-case basis.

www.aip.org/gov/fellowships/both_apply.html

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