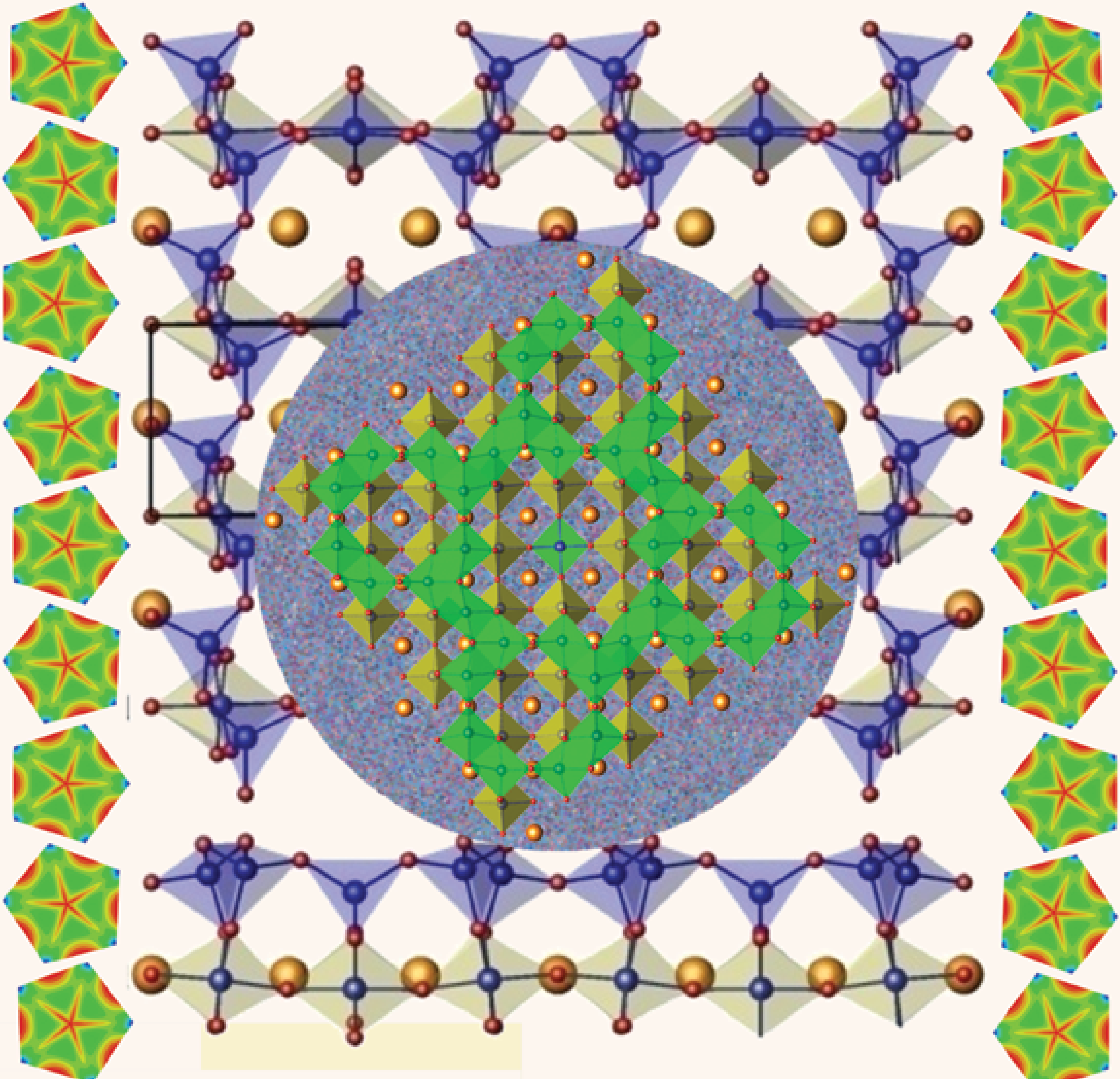
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 2 Summer 2015



Warren Award at Philadelphia ACA Meeting

ACA RefleXions
ACA - Structure Matters
Summer 2015

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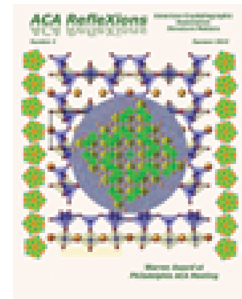

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President's Column

Greetings from Washington DC, where summer has rushed in without delay. The Cherry Blossoms have long gone, along with the tourists, soon to be replaced by interns! We had a productive spring Council Meeting in Buffalo this past April, and we look forward to meeting with the SIGs and Standing Committees in July in Philadelphia.

Many topics got covered, yet I'd like to draw your attention to our new *ad hoc* Committee on Outreach and Education. Council has decided that we need a more formalized mechanism for evaluating proposals for activities that fall between the duties of the current standing committees. Further, as I will expand upon below, we clearly need a more formal mechanism to coordinate and fund outreach activities that have impact beyond our membership and that serve to create more public awareness of crystallography.

Along this line, you may have noticed a new and improved membership renewal invoice. If not, keep your eyes peeled for a new category for donations called 'Outreach.' Whereas we, of course, welcome contributions to all of our funds and awards, some are at fully funded levels (such as the Buerger, Fankuchen and Patterson), meaning they generate enough interest to support the payout for the awards. Contributions to our new Outreach fund will be particularly helpful considering its novelty and importance. We wish to develop a capacity for a combination of regularly funded outreach activities (e.g., demonstrations at museums or expos, crystal growing contests, etc.), yet also to ensure a degree of flexibility and nimbleness to respond to opportunities as they arise. I trust you will agree that this is an important effort.

Like me, I am sure you are looking forward to our annual meeting in Philadelphia this July. I already drew your attention (in the Spring issue of *RefleXions*) to the outstanding program the SIGs have assembled (and the Program Chairs corralled!). Workshops are filling up, and a plenary Speaker has been announced for the open Wednesday morning slot. Juan Manuel Garcia-Ruiz of the National Research Council of Spain and Univ. of Granada will be presenting on research in the area of crystal growth, and his work in public outreach and engagement. Some of you who attended the 2014 IUCr Congress might remember his documentary *The Mystery of The Giant Crystals* (***www.trianatech.com/index.php?option=com_content&view=article&id=148&lang=en***), and public exhibition of *Cristales*, which he will be bringing to display at our meeting in Philadelphia. Finally, the *Transactions Symposia on Crystallography and Sustainability* stands to highlight some new relevance and broadening reach of our discipline to a diverse range of fields.

Despite our sound trajectory to the Philadelphia meeting, I would like to take moment to reflect on a challenging state of affairs for not only the ACA, but for scientific societies in general. Let's be realistic for a moment: our membership numbers are declining, we have shortened our meeting format by one day and we face some stiff PR challenges when the American Chemical Society refers to crystallography as a "tool." Moreover, in an age of unprecedented online resources such as social media and instant access to scientific publishing, some could rightly argue that the value of a scientific meeting or indeed a society in general has diminished over the years. Moreover still, as many of our respective disciplines evolve into cross-disciplinary pursuits, many of us are faced with the need to pick and choose which meetings to attend. These issues are by no means unique to the ACA, yet they are particularly impactful considering our modest size and lean infrastructure. I think you get the point here: Time for some reflection and strategizing.

What does this mean for the ACA and membership going forward? Well, for starters, I am a bit more optimistic than the previous paragraph might suggest. I think we have to face a *grand challenge* of demonstrating relevance. Or perhaps more importantly, making the relevance explicit, and I have a suggestion for doing so: we need to convey our relevance to society in general, and our students at all levels in particular. While critical, it is not enough to communicate the impact and contributions of crystallography to other scientists alone. We need to be able to articulate the value of crystallography to a broader audience, and although amorphous at present (pun intended), I have high hopes for our Outreach committee to at least partially address this. Considering our IYCr involvement and the recent successes of our crystal growing contests, I say there is real momentum here. Moreover, our engagement with the Council of Scientific Society Presidents (CSSP) provides a forum for broader impacts as well in terms of access to legislators and science advocates. As a scientific society, I argue there is an infrastructure and network that needs to be better tapped and leveraged.

So what are our action items on this? And what is the mechanism? How do we respond to this 'call to arms?' Beyond all of the wonderful science you do year round, I think we have a tremendous capacity within the *Transactions Symposia* at the annual meetings. In some ways, I look at Philadelphia's sustainability program as an ideal example of conveying relevance beyond our typical research areas and seeing the broader impacts of our work. Admittedly most people in attendance will indeed be the choir to whom we preach, yet there will, of course, be media outlets covering the meeting and related press releases. That said, the real value may be in educating *ourselves* as to crystallography's broader reach, which in turn empowers our individual communication efforts. Looking down the road to future meetings, the *Transactions Symposia* could serve as powerful forum in this regard. Let's keep thinking about this.

More on the theme of challenges facing the ACA: by the time you read this, you will have received an e-mail survey soliciting input on our current and future functions/roles/services etc. The above paragraphs highlight the dynamic nature of our scientific landscape, and the ACA must evolve along with some stark realities. As such, I hope you will have responded thoughtfully.

I am going to close with a few personal developments, if I may be so bold. It turns out I am due for a sabbatical for the next ('15-'16) academic year. I have decided to spend it here in DC for a number of reasons, one of which just turned two and is insufferably cute, yet others include a desire to tap further into the science policy community. My comments above about communication notwithstanding, I have strong desire to know more about the impact of science beyond the laboratory, as well as the drivers responsible for its funding. As such, I applied for a number of fellowships to place me inside the federal government as a science advisor. Yours truly was fortunate enough to be selected as an American Institute of Physics State Department Science Fellow. I start Sept 1 at the Bureau of International Security and Nonproliferation, Office of Weapons of Mass Destruction and Terrorism (ISN/WMDT- all Googleable). Needless to say I am thrilled at this opportunity and am eager for some exposure to the policy world. I may have shared with some of you some details about the other hat I wear in that I have a joint appointment in the Elliot School of International Affairs here at GW. For the past several years, I have developed and taught courses on the nuclear fuel cycle aimed specifically at non-technical students pursuing policy studies degrees. I have long been passionate about developing scientific literacy in non-technical arenas, and now it is time to develop some policy literacy in myself. Even more exciting is that I join the ranks of other ACA members who have received AIP Fellowships. Matthew McGrath (AIP- State Department Fellow) and Caitlin Murphy (AIP-Congressional Fellow) have been describing their experiences with regular contributions to *RefleXions,* and I look forward to crossing paths with them (You can read updates from Matthew and Caitlin on pages 34-35 of this issue). Not to worry- I can still handle the Presidency and we've got a fantastic VP to take over come January 1!

Chris Cahill

excillum
REDEFINING THE X-RAY TUBE

MetalJet sources – dream or reality

Over the last years, many of you may have heard about the new promising x-ray source technology based on a liquid-metal-jet anode developed by Excillum in Sweden. As it is a new technology, some may wonder if these sources are merely an exotic curiosity or actually stable work-horses in the lab. Here is at least the words of one of the many users around the world.

In February 2014, a Bruker Venture D8 diffractometer equipped with a MetalJet x-ray source was installed at the Department of Chemistry, University of Montreal.

Frank Schaper shares his thoughts on the installation: *Six months after its installation, performance of the MetalJet system has by far exceeded our expectations. The new metal-jet source coupled with the optimized multilayer optics is around 20 times brighter than current technology, and around 40 times brighter than our Cu rotating anode, when operated at less than maximum voltage. As a consequence, since the arrival of the MetalJet, our laboratory did not have to classify a single sample as "too weakly diffracting*

The smallest crystal employed so far in data collection had a maximum diameter of 20 µm. In addition to increased sensitivity, required measurement time reduced significantly. First structure solutions can be obtained from fast scans after 5-10 min, and even for the smallest crystals full sphere datasets were collected in less than 6 hours. In our hands the MetalJet thus easily replaces two conventional Cu-based diffractometers.

We re-gained the speed of data collection of Mo-based diffractometers with a sensitivity unparalleled even by Cu rotating anode sources and orders of magnitude above standard sealed tube Mo systems. In the few months since its installation the instrument quickly became essential for the success of research programs here at the University of Montreal.

Emil Espes

Editors note: *Excillum became a new Corporate Member in time to have been listed as such in the spring issue of RefleXions but we forgot to include them. We will be sure to include them from now on and, since they are new to us, asked them to provide a short introduction on who they are and what they offer.*

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2014 and 2013

	CURRENT FUNDS (2014)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2014	2013
ASSETS				
Current Assets:				
Cash	128,727		128,727	129,807
Investments	570,598	459,592	1,030,190	1,023,437
Inventory	6,393		6,393	6,393
Accounts Receivable	0		0	30,214
Total Current Assets	1,165,310	459,592	1,165,310	1,159,637
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	1,165,310	459,592	1,165,310	1,159,637
Liabilities:				
Unearned Revenues	12,400		12,400	49,023
Credit Card Liabilities	0		0	414
Total Liabilities	12,400		12,400	49,437
Fund Balance:				
Unrestricted	693,318		693,318	663,035
Restricted		459,592	495,592	447,165
Total Fund Balance	1,030,190	459,592	1,030,190	1,159,637
TOTAL LIABILITIES & FUND BALANCE	1,165,310	459,592	1,165,310	1,159,637

* Current Balances in individual restricted funds - *as of December 31, 2014*

Bau Neutron Award	36,192
Buerger Award	38,855
Etter Award	68,517
Fankuchen Award	71,146
Patterson Award	48,299
Pauling Award	38,172
Supper Award	12,509
Student Travel Fund	20,934
Trueblood Award	40,047
Warren Award	30,772
Wood Science Writing Award	54,159

History Fund (unrestricted) see page 13

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.

2016 ACA Trueblood Award to Axel Brunger

The 2016 Trueblood Award of the American Crystallographic Association for "exceptional achievements in computational or chemical crystallography" will be bestowed on ACA member Axel Brunger, Professor of Molecular and Cellular Physiology, Neurology and Neurological Sciences, Structural Biology (by Courtesy), and Photon Science Investigator, at the Howard Hughes Medical Institute at Stanford University.

Brunger carried out his undergraduate studies in Germany, between Hamburg and Munich, where he received a PhD in biophysics from the Technical University. He then moved to Harvard, to work as a post-doctoral researcher in the group of Martin Karplus. He very quickly became Associate Professor in Biophysics at Yale and progressed steadily in his academic career. In parallel, he also became investigator at the Howard Hughes Medical Institute, to which he has been affiliated since 1995.

Axel's contribution to computational crystallography has been invaluable for the development of modern macromolecular crystallography. It was very early in his career, when he was only a post-doctoral fellow, that he developed algorithms based on simulated annealing and molecular dynamics to refine protein structures. With John Kuriyan and Martin Karplus, he implemented these methods into the program *XPLOR*, which he later expanded into the widely used *CNS*, a freely available software that includes optimized tools for structure refinement, phasing and molecular replacement.

To prevent the possibility of over-refinement of crystallographic structures using simulated annealing, Brunger borrowed a cross-validation approach from statistics and adapted it to protein crystallography: the free R factor. This is now the standard criterion to judge agreement between observed and calculated structure factors. Also, in collaboration with Michael Levitt, Axel developed the *DEN* method (for Distortable Elastic Network), a refinement strategy that uses flexible adjustable restraints and that allows low-resolution refinements. His powerful computational tools revolutionized structural calculation, moving it towards automation and allowing non-experts to gain access to protein crystallography.

His brilliant contributions were all born as solutions to complex structural problems at the forefront of scientific investigation. Today Brunger is still pushing the limits of structural biology. He carries out cutting-edge research on the structural mechanisms of synaptic neurotransmitter release, complementing x-ray crystallography with single molecule microscopy and is exploring the new possibilities that x-ray free electron laser techniques offer for the structural determination of large macromolecular assemblies.

Chiara Pastore

2016 ACA Fankuchen Award to Elspeth Garman

The ACA will bestow the 2016 Fankuchen Award on Elspeth Garman, from Oxford University, UK. The award, which has been created "to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography," honors Elspeth's absolute dedication to teaching crystallography in seminars and workshops all over the world, and her great contributions to improve cryo-methods in crystallography.

Elspeth graduated in nuclear physics from Oxford University in 1979 and switched to biochemistry only later in her career, in 1987, when she joined the research staff at the Laboratory of Molecular Biophysics in Oxford. Since 1999 she has been faculty at the biochemistry department at Oxford University, where she now holds a position as Professor of Molecular Biophysics and as Director of the Systems Biology Programme at the Doctoral Training Centre. She is also Nicholas Kurti Senior Research Fellow in Macromolecular Crystallography and Tutor for Graduates at Brasenose College.

Elspeth's research on cryo-cooling and radiation damage has had a profound impact on crystallography. Armed with a rigorous approach inherited from her physics background and her natural inventiveness, she optimized cryogenic tools and cooling parameters, introducing a methodical approach to cryo-cooling that greatly improved diffraction data. Since radiation damage emerged as a serious problem in crystallographic structure calculation in 2000, she has spearheaded the studies dedicated to the issue, introducing mitigating measures such as the use of small molecules as radical scavengers. She experimentally determined the maximum x-ray dose that can be delivered to a macromolecule before compromising its structure—a parameter that is now called "the Garman" limit—and presented a method to predict the lifetime of proteins exposed to certain radiation doses. She also pioneered the use of an online UV-visible spectrometer to detect the early signs of radiation damage. Besides these studies, she developed the proton induced x-ray emission (PIXE) technique, which allows precise identification of trace metal elements within a protein structure, and she determined the structure of many proteins involved in infectious diseases.

Elspeth's value as a teacher and as a lecturer is appreciated at large. She is a very popular speaker at workshops all over the world, and her passion and enthusiasm for crystallography have left a long-lasting impression on her students and on her colleagues alike. She has tutored on 75 international courses, given 117 scientific lectures and 41 public lectures on crystallography, and organized 18 workshops. From 2009 to 2012 she was President of the British Crystallographic Association and from 2007-2011 she served as an Auditor of the European Crystallographic Association. The University of Oxford recognized her teaching qualities with the `Major Educator' personal teaching award in 2008; in 2014 she received the Most Acclaimed Lecturer Award for the Medical Sciences Division from the Oxford University Students Union. She is deeply involved in outreach programs aimed at increasing public scientific awareness both in a young and in an adult audience. For many years she has lectured at "Girls into Physics" conferences and she is often invited to give talks in schools all over the UK. She has been a speaker at the Royal Institution multiple times, and last year she delivered a public lecture at the Royal Albert Hall in occasion of the International Year of Crystallography. She is very comfortable with the media and the press: she has participated in over 40 TV and radio programmes and she has been often quoted in the main UK newspapers. In one of her most recent media appearances, an interview for the program "The Life Scientific" broadcasted by BBC4 in October 2014, she spoke at length about crystallography, about her life-long journey into experimental science… and about using her baby's hair to build the first cryo-loops. It is a most enjoyable conversation, which sums up her self-less attitude towards research and her desire to fuel progress in crystallography and in science in general; you can listen to it here: ***www.bbc.co.uk/programmes/b04kbjhg***.

2016 ACA Bau Award to Benno Shoenborn

Benno Shoenborn, from Los Alamos National Laboratory, is the 2016 recipient of the ACA Bau Neutron Diffraction Award for his pioneering work on neutron crystallography and its application to biology. Benno has published over 100 publications on the subject, and has mentored, trained and inspired numerous students, post-docs and early-career researchers, expanding the reach of neutron crystallography to a larger community of scientists and setting the grounds for its further development.

Benno graduated in physics from the University of New South Wales, Australia and completed his post-doctoral research at the University of California in San Francisco. From 1964 to 1966 he was a visiting scientist at the Cavendish Laboratory, at Cambridge University. Those were exciting times in the history of structural biology, and Cambridge was the place to be: John Kendrew and Max Perutz had in fact just received the Nobel Prize for solving for the first time the x-ray structure of two macromolecules, myoglobin and hemoglobin. However, neutron diffraction was still considered an unviable technique for macromolecular structural investigations. Benno was determined to change this view and set up to solving the three-dimensional structure of myoglobin using neutron crystallography. Shortly after leaving Cambridge, he joined the staff at Brookhaven National Laboratory, where he was able to record initial neutron diffraction data. His endeavors gave the long-yearned results in 1969, proving not only that the technique was feasible, but also that it could yield invaluable structural information on the position of hydrogen atoms, which are not visible with x-ray crystallography but are key players for the structural and functional integrity of proteins. Since his first structure, he applied neutron scattering to a large variety of biologically relevant molecules, such as the 30S subunit of the bacterial ribosome, ATPase, gramicidin A, thermolysin, hemoglobin, and the acetylcholine receptor. Being one of the pioneers of the technique, Benno put a lot of effort into optimizing the available instrumentation and neutron scattering facilities in the USA. With Paul Langan, he promoted the creation of the first neutron protein crystallography beamline in North America, the Protein Crystallography Station (PCS) at the pulsed neutron source at Los Alamos Neutron Science Center (LANSCE), a state-of-the-art facility that helps users in every step of a neutron diffraction experiment, from protein production and deuteration, to data collection and analysis.

Chiara Pastore

2016 Etter Early Career Award to Jason Benedict

Jason Benedict, Assistant Professor of Chemistry at the University of Buffalo, is the recipient of the 2016 Margaret C. Etter Early Career Award. Established in 2002, the Etter Award recognizes the outstanding work of scientists who are in the early stages of their independent careers in the field of crystallography.

Jason received his Bachelor of Science in Chemistry in 2001 from Arizona State University, working in the field of fundamental reactions in inorganic chemistry. He completed his doctoral studies in 2007 at the University of Washington under the guidance of Bart Kahr, where he investigated the optical properties of oriented chromophores within technologically important materials. From 2008-2011, he was a postdoctoral fellow at the University of Buffalo in the laboratory of Prof. Philip Coppens. His postdoctoral studies involved time-resolved x-ray diffraction experiments and the synthesis of novel polyoxotitanate clusters for use in solar energy applications. In 2011, Jason began his independent career as an Assistant Professor of Chemistry at the University of Buffalo. His current research efforts are aimed at developing an understanding at the molecular level of the physical processes that occur in stimuli-responsive nanoporous materials with the goal of creating "by design" crystalline materials with tailor-made properties.

During his independent career, Jason has made many outstanding contributions towards the development of new materials and advanced x-ray diffraction methods to characterize their properties. His group recently reported some of the first diarylethene-based photo-responsive metal-organic frameworks that exhibit unusual photoswitching and fatigue properties. Furthermore, he has pioneered new crystallographic methods such as an optical chopper that allows ultrafast x-ray diffraction measurements to be conducted using laboratory sources and an environmental cell that permits examination of the exchange of guest species incorporated within porous materials.

In addition to his stellar research accomplishments, Jason has been consistently recognized as an outstanding mentor to students at all levels. He recently received national attention for launching the US Crystal Growing Competition in 2014, which aims to teach the fundamentals of crystallography to students and educators in the K-12 level across the nation. While at the helm of the Western New York Undergraduate Research Symposium, this event that recognizes undergraduate research has grown to almost 100 participants from over 15 regional institutions. Dr. Benedict has also demonstrated a commitment to advancing diversity in the scientific community as exemplified within his own laboratory.

George Lountos

PANalytical Award Supports Young Scientists

PANalytical is one of the world's leading suppliers of analytical X-ray instrumentation and software. The company seeks to reward early-career scientists who have demonstrated innovative thought to their research when using an X-ray analytical technique with a $5,000 prize. The Award in 2012 went to Thomas Bennett (UK). Ana Cuesta (Spain) received the 2013 Award for her investigation of yeelimite, the most important phase in calcium sulfoaluminate cements.

The winner of the 2014 Award will be decided in early 2015 by a selection committee that includes established research scientists unaffiliated to PANalytical. Submissions for the 2015 Award will be possible from June 1, 2015 with a deadline of **December 1, 2015** (see: ***www.panalytical.com/award***). Applicants must publish a paper during the period January 1, 2014 – December 1, 2015 that demonstrates ground-breaking thinking in a topical field. There are no restrictions on the manufacturer of the X-ray equipment used. Questions can be addressed to ***award@panalytical.com***.

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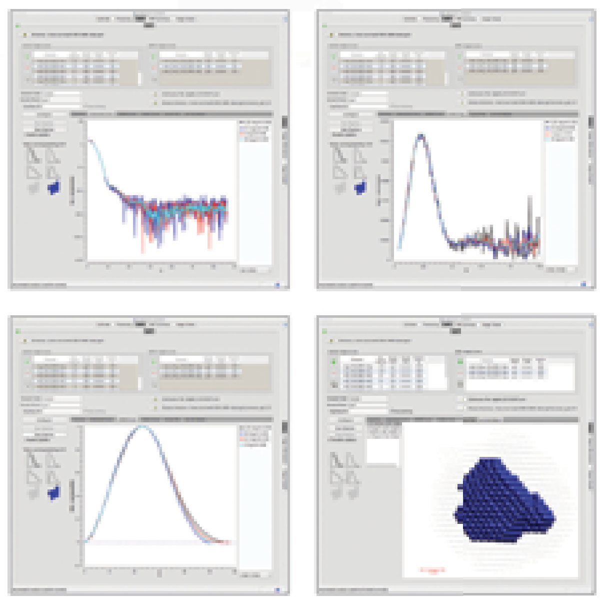

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2015 ACA Fellows

The ACA Fellows program recognizes a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. The Fellows program celebrates the excellence of ACA members, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. ACA Fellows serve as scientific ambassadors to the broader scientific community and the general public to advance science education, research, knowledge, interaction, and collaboration. This program allows the ACA to significantly recognize and honor a broader cross-section of the membership than was previously possible with other, more specific awards.

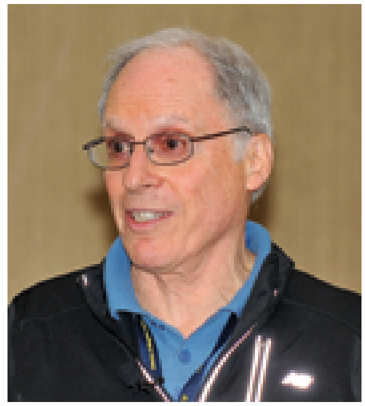
Zbigniew Dauter

Zbigniew (Zbyszek) Dauter promoted single wavelength diffraction (SAD) as an alternative method to selenomethionine labelling in macromolecular structure phasing. In particular, he pioneered the use of "light" heavy atoms such as sulfur and phosphorus (intrinsic components of proteins and nucleic acids) as anomalous scatterers in the phasing procedure. He also developed a method for structure phasing that exploits the anomalous diffraction of halide ions, introduced into the crystals with fast soaking experiments; the method is nowadays one of the most widely used approaches to macromolecular phasing.

He greatly improved data collection and analysis of challenging samples, such as highly twinned crystals or crystals presenting superimposed lattices and pseudosymmetry, contributing to an increase in structure resolution and to obtaining unprecedented molecular details.

Besides being a great scientist, Zbyszek is a sought-after teacher and lecturer; he has organized many workshops and lectured at many crystallography schools. For ten years he has also been co-editor of *Acta Crystallographica Section D, Biological Crystallography*. In 2003 NIH appointed him to a tenured position in the prestigious Senior Biochemical Research Service, which is only granted to few scientists, and in 2010 the Polish Academy of Sciences awarded him its highest honor, the Nicolaus Copernicus Medal.

David Eisenberg



The contributions of David Eisenberg to crystallography are numerous and range from strictly theoretical to biomedical applications. To mention a few, he published some of the most influential papers on amyloid-forming proteins, developed tools for protein structure and function prediction, implemented genome-wide algorithms to predict protein-protein interaction, and deposited a staggering number of structures in the PDB (554!).

His work has provided invaluable insights into the energetics and structural basis of protein folding and protein-protein interaction, both in healthy and diseased states. He introduced the concept of "hydrophobic moment" to measure the distribution of hydrophobicity within a protein, and he was the first to describe the phenomenon of 3D domain swapping, now a widely accepted concept, which he observed in the structure of the diphtheria toxin dimer.

For the past 15 years, his name has been linked to groundbreaking studies on amyloids. He solved the very first structure of an amyloid protein in 2005, publishing his "Structure of a cross-beta spine of amyloid-like fibrils" in *Nature*. Since then he has solved many other fibril structures and has pioneered computational methods for the structure-based design of compounds capable of interfering with fibril formation, making a crucial impact in the field of neurodegenerative diseases.

John Helliwell

John Helliwell, the 2014 recipient of the ACA Patterson Award, has always been at the forefront of macromolecular crystallography, advancing the field with innovative techniques and improving diffraction facilities worldwide. He has championed the use of synchrotron radiation to answer biological questions since the beginning of his career, when, as a PhD student, he was involved in the very first experiments that used synchrotron light in macromolecular structural studies. Since then he has worked hard both on the technical and on the logistic sides to make synchrotron radiation routinely available to crystallographers. He applied novel anomalous scattering techniques to solve the phasing problem and greatly contributed to the development of Laue methods for time-resolved studies. He established the first dedicated synchrotron radiation x-ray source instrument for protein crystallography in Daresbury, UK, set up the first protein crystallography radiation wiggler instrument, and has fostered several international synchrotron and neutron projects. He collaborated extensively with scientists in the USA in many innovative and ground-breaking projects.

Apart from being a prolific scientist, John has served the crystallographic community in many other ways: he is the author of the classic book "*Macromolecular Crystallography with Synchrotron Radiation*"; he founded the *Journal of* Synchrotron *Radiation*; he headed the European Crystallographic Association from 2006 to 2009; he served as Editor-in-Chief of the IUCr journals, launching *Acta Crystallographica Section E* and *Section F*; and more recently he has strongly endorsed ACA's new journal, *Structural Dynamics*, promoting it at conferences and meetings, sitting on the journal's Advisory Board and contributing one of its first articles.

Very recently John has also been awarded the 8th Max Perutz Award by the European Crystallographic Association (ECA). The ECA honored his breakthroughs in crystallography, his determination to apply and to expand the use of synchrotron radiation for structural studies, his constant support to the development of synchrotron and neutron facilities as well as his regular involvement in outreach activities and in the dissemination of crystallography. He will receive the prize during the 29th ECA meeting, which will be held in Rovinj (Croatia) in August of 2015.

Håkon Hope

Cryo-crystallography is Håkon Hope's most notable contribution to the scientific community and one without which we would not have modern day crystallography. Håkon began his work on cryo methods during his graduate and postgraduate studies in Norway. He first conceived a system that enabled him to determine the crystallographic structure of small pyrophoric molecules, extremely unstable compounds that ignite upon exposure to air. He managed to stabilize the crystals in the air-free environment of an oil drop placed at the end of a thin capillary and to record their diffraction pattern under a stream of liquid nitrogen. He then expanded and developed his technique to the study of macromolecules, working to reduce turbulence in the nitrogen stream that caused formation of substantial amount of ice around the crystals. His innovative approach has been immensely valuable to the macromolecular crystallography community in particular, which was struggling to record datasets of delicate biomolecular crystals. In 1987 he succeeded in freezing ribosome crystals for Ada Yonath, giving them, as she wrote enthusiastically in an e-mail to her colleagues, "eternal life", and paving the way to the solution of the ribosome crystal structure (for which Ada won the 2009 Nobel Prize in Chemistry together with Venki Ramakrishnan and Thomas Steitz).

Throughout his career he has been a passionate teacher, a strong advocate of crystallography, and an active participant in ACA and IUCr activities.

Tom Koetzle

Tom pioneered the use of single -crystal neutron diffraction in structural studies, applying the technique to investigate hydrogen bonding in organic molecules and hydrogen location in transition metal hydrides. In 2013 he was the first to receive the Bau Award, named after his frequent collaborator Robert Bau, with whom Tom carried out his studies on metal hydride complexes beginning in the 1970s. Not only did he master neutron diffraction techniques and their structural applications, Tom also extensively promoted them, supporting neutron crystallography over the years at many facilities at Brookhaven, Argonne and Oak Ridge.

His services to the wider scientific community are priceless. In 1973 he became the director of the PDB, when the database was only two years old and the idea of publicly shared structure coordinates was not broadly accepted. Tom, with the support of other scientists from the crystallographic community, was instrumental for the survival of the database; he promoted the PDB in its first years and optimized the procedures for data deposition and remote access. By the end of his mandate in 1994, the PDB contained 2800 structures and had become a well-established repository of crystallographic coordinates and an invaluable resource for scientists all over the word.

Tom has long been involved with the ACA and he served many different roles within the Association. He was president in 2011, and now he is one of the ACA representatives on the American Institute of Physics Publishing Partners Committee (which publishes ACA's own journal, *Structural Dynamics*) as well as one of the editors of our newsletter *RefleXions*.

Paul Langan

Paul Langan started his new role as Associate Laboratory Director for the Neutron Sciences Directorate at the Oak Ridge National Laboratory (ORNL) in January 2015; here he will be responsible for two neutron facilities, the Spallation Neutron Source and the High Flux Isotope Reactor, which nowadays welcome up to 2500 visiting users each year. At ORNL Paul is planning to expand the instrument capabilities and to set up a second target station at the Spallation Neutron Source, with the aim of broadening the impact and accessibility of neutron diffraction techniques to scientists from different realms of science. This ambition has characterized Paul in most of his career; he has greatly contributed to establishing neutron macromolecular crystallography, applying it to the study of several proteins, optimizing the available instrumentation, and developing the relative data analysis software. He led several scientific projects funded by the NIH and the DOE. For example, he has directed research teams involved in the study of cancer and HIV and coordinated efforts for drugs developed against these diseases. He has also carried out extensive research on natural fibers, focusing in particular on the structural aspects of cellulose and on how to efficiently convert its biomass into fuel. The DOE awarded him six formal awards in recognition of his achievements.

He is member of Faculty of 1000, co-editor of *Acta Crystallographica Section D Biological Crystallography*, and guest editor for *Cellulose*, where he also sits on the editorial board. Within the ACA, he has chaired the Neutron Special Interest Group in 2005 and the Fiber Diffraction Special Interest Group in 2009. He currently serves as chair of the IUCr Neutron Scattering Commission.

David Rose

David Rose, Professor and Department Chair in the Department of Biology of the University of Waterloo, has been affiliated with the ACA for almost his entire career. He served twice as the Canadian Representative on the ACA Council, successfully expanding the Canadian involvement in the ACA with several initiatives, including contributing a *News from Canada* column for *RefleXions*. Among others, he introduced the Canadian Pauling Poster Prize; encouraged closer connections between the ACA and the Canadian National Committee; created co-sponsorship of scientific sessions by the Canadian Division; and organized the Canadian nominations for the ACA awards. He is a fiery promoter of crystallography, a keen communicator, a strong supporter of outreach activities and a mentor to young undergraduate students and post-doctoral fellows during social activities at ACA meetings.

At the University of Waterloo his main research focuses on the structural biology and enzymology of mammalian glycoside hydrolases, proteins involved in starch digestion and therefore fundamental in human nutrition and health. David was instrumental in the creation of the Canadian Glycomics Network, GlycoNet, a large initiative dedicated to study the role of carbohydrates in biological processes and in diseases such as obesity and diabetes.

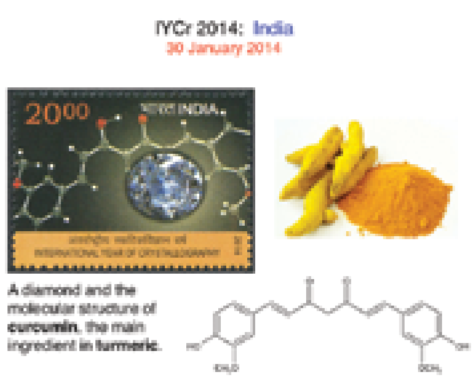
Chiara Pastore

What's New on the ACA History Website

Webmaster Patti Potter has placed interesting articles, photos, and reminiscences about the early days of the ACA on the ACA History Portal. From the ACA History home page ***www.amercrystalassn.org/history_home*** click on the *ACA Beginnings* button at the top of the page. You will see two articles about the creation of the ACA in 1950 from two previous scientific societies. David Sayre's 1974 article on the status of diffraction methods provides a fascinating background for current practices, along with some prescient hints of developments that have turned out to be significant, such as solvent flattening. Finally, there is a plethora of material marking the 50^{th} anniversary of the ACA in 2000, including memoirs written by past Presidents of the ACA and by exhibitors, as well as historical photos.

Elizabeth Wood, David Templeton, Robinson Burbank, and Sidney Abrahams with the ACA 50th birthday cake at the 2000 ACA Annual meeting in St. Louis, MO.

Also newly added is the video of Daniel Rabinovich's talk at the Albuquerque ACA meeting, *The World of Crystallography on Postage Stamps*. Dan's ACA Wood Award presentation gives an entertaining view of crystallographic history featuring colorful stamps from many countries. In addition a selection of talks from recent ACA meetings is now available in video format, including John R. Helliwell's 2014 ACA Patterson Award lecture *Synchrotron radiation macromolecular crystallography: instrumentation, methods and applications*.



Slide from Dan's talk showing stamps that honored IYCr 2014.

Contribute Your Memoir and Photographs: Many of the *Living History* memoirs that you've been reading in *RefleXions* are available online, most recently, Abe Clearfield and Richard Marsh's memoirs. If you would like to write your own memoir please contact Virginia Pett ***(pett@wooster.edu)***. Tell us about your career in government, industry, or academia. We are interested in all aspects of the history of structural science, crystallography, and x-ray diffraction — instrumentation, teaching, research advances, research groups and organizations. And please send historical photographs so that we could add them to the ACA Beginnings page.

Mind the gap(s): The History Committee is looking for volunteers, because there are gaps in our work. We have video recordings of Award presentations that are not yet on the website, for example. If you are interested in helping with the ACA History Project, there are many opportunities for your creativity, such as editing material for *RefleXions* or the website; recording and making videos; archiving materials at the Niels Bohr Library & Archives. Contact Virginia Pett ***(pett@wooster.edu)*** if you would like to help fill the gaps.

Virginia B. Pett

Editors note: *On the ACA balance sheet -no dollar value was listed for the History Fund. Unlike the restricted ACA Award funds, the History Fund spends the money that comes in to help support upkeep and development of the History Portal. If you enjoy the site, please remember to include it when you make your annual donation to support the ACA and its outreach activities - or whenever the mood strikes.*

Edgar Meyer (1936-2015)

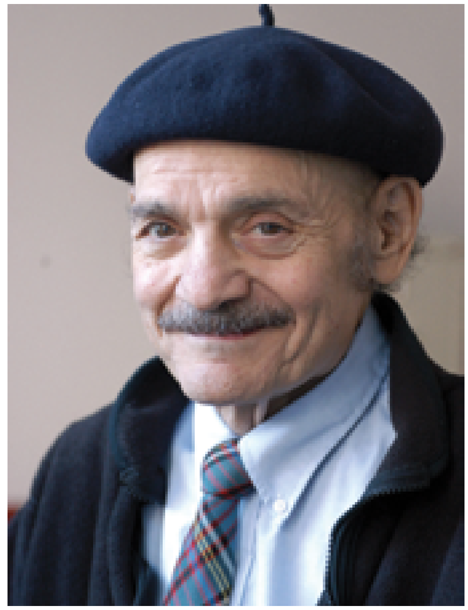
I was very sad to learn that Edgar Meyer had passed away in late April 2015. I first met Edgar at MIT in 1966 when he was a post-doc in Cy Levinthal's laboratory where he was working on visualizing protein structures using what was then a very novel graphics system. Over the next few years we worked together to encourage community interest in setting up the Protein Data Bank. Once the PDB was established in 1971, I visited Brookhaven National Laboratory where Edgar and Walter Hamilton invited me to collaborate on the CRYSNET project. The idea of the project was to enable structural biologists without large computing resources access to the then state of the art computer facilities at BNL and to analyze their results on a home computer with graphics capabilities. Throughout his career, Edgar was devoted to utilizing the newest technologies to understand structure.

When Ed retired from the Department of Biochemistry & Biophysics at Texas A & M where he had been a crystallographer for over 36 years, he moved on to the next phase of his career, as a molecular sculptor. His favorite structure (and sculpture) was co-chaperonin (***cen.xraycrystals.org/edgar-meyers-favorite-structure/***).

When I was asked to write something on Ed's passing for *RefleXions* I remembered that his autobiography had been published in the spring 2014 issue (*pages 38-40*); I quickly realized that I could not tell his story better than Ed did himself. His memoir will also be posted to the ACA history site under the "People" menu item. He will be missed by many of us in the crystallographic community.

Helen Berman

My Time in Alexander Rich's Lab (1972-1977)



Like all laboratories that exist for long periods of time, Alex Rich's lab went through several eras. I was fortunate to be there in the early-middle 1970's, and experienced an irreplaceable period in my scientific development. At the same time it was a transition period: When I got there, large small-molecule structures and the ability to solve them were regarded as important in biological crystallography, but by the time I left, skill at the crystallization of macromolecules was the *sine qua non* in that realm. I came from the first tradition, and have never been really comfortable with the second. Alex was, of course comfortable with any and all approaches to biological structure, and adapted freely as the eras changed. Nevertheless, I was extraordinarily proud when our dinucleoside phosphate crystal structure showing Watson-Crick base pairing between A and U shared the headline of his NYTimes obituary.

When I got to MIT, the lab was in a period of great excitement, because the yeast pheniylalanine tRNA structure was just in the process of being solved. I had nothing to do with tRNA for two years, since it was clear that the credit for that work would not go to a fresh arrival. Having solved a dinucleoside phosphate previously, I jumped instead into projects involving new ones. What took me quite a few years to appreciate was that crystallography was only a part of Alex's lab. There was a large group of molecular biologists working side-by-side with us. Alex's interests in molecular biology, structural or otherwise, were so broad that this group felt quite as much at home as the crystallographers. After a few years of being around the molecular biologists (i.e., drinking with them at the Muddy Charles Pub on campus), I learned how the questions they asked were really quite important. After a few years of Z-DNA crystallography (all after my time), it was clear that in his last years, the biology of Z-DNA was far more central to Alex's interests than the crystallography.

Alex's lab was my second post-doc, and the contrast with my first was like night and day, in that order. Alex largely insisted that his post-docs come on their own fellowships, so he didn't sit around fretting that he was blowing his budget on some of us while we ruminated on things that might lead to ideas. I once heard that he packed us in so tightly that when two people were talking, a third would overhear them and get an idea. Alex often cultivated the image of a buffoon, largely to keep his people from being intimidated; only fools were taken in by the act, he was anything but! I doubt that many of us there at the time actually realized the importance of the things he had done when he was younger: He demonstrated that RNA could form a double helix, and *en passant*, he invented hybridization. He was fond of telling the story that when he mixed poly-A and poly-U to get a double helix, he ran out in the hallway and told the first person coming along what he had done; the person responded, "Without an enzyme? Impossible!" At the time, I didn't realize how important nucleic acid hybridization was, but eventually, I recognized that it was arguably his most important contribution to science.

Alex and I were both nocturnal creatures, so we spent a lot of time shooting the bull during the wee hours. We often got hungry, and would go to get a slice of Hi-Fi Pizza up in Central Square, or maybe, with Bud Suddath and Alex McPherson, we'd go to a deli on Boylston Street, called The Bulkie. However, the happiest I ever saw Alex was when we decided to get a snack at the vending machine row in the basement of the next building. I decided to get an ice-cream cone, and the ratchet failed, so the entire filled circle of cones was available. Alex saw this and sent me upstairs for a box, and we emptied out the machine for the lab to eat ice cream. He was positively beaming as he muttered about "after all the years those bastards have stolen my coins, finally they are paying!."

In another post-midnight discussion, he told me of a conversation he had with some bigwig visiting him at the NIH. Alex told this guy that in the course of the past year he had worked out the fiber structures of three different biopolymers. The guy said to him, "All in one year? You'll never have such a year again in your life." And Alex looked at me and said, "And you know, he was right." I argued with him that the tRNA, ApU and GpC (mini-double helix) crystal structures had all been reported in 1973. His response was, "Sure. But I did that earlier work myself."

Alex made a few mistakes in his career. Who has ever done something significant who hasn't? However, in my interactions with him, he was a very hard-headed scientist. I remember clearly when I tried to convince him that the minor grooves of G-C and C-G base pairs were really the same electrostatically and the implications of that for sequence recognition. He took my drawing of the superimposed base pairs, and drew an extended line from the amino nitrogen atoms, which overlapped, through the two hydrogen atoms, and then onwards for another two Ångstroms in each base pair. It was clear that I was all wet.

There are lots of 'Alex stories'. Probably everybody who spent time in the lab could go on all night telling stories about him. The stories are usually told with good humor, and only rarely with any rancor. In many regards, he was the most direct heir of Linus Pauling's structural approach to biology. Anybody who came to the lab with an open mind learned a lot from Alex. Alex Rich has given all of us a role model to emulate, but none of us will ever replace him.

Ned Seeman

Thoughts of Alexander Rich – His Lab (1070-1974)

I joined Alex's lab as a post doc early in the summer of 1970. I had never encountered Alex before, never seen him in person, had not even seen a picture of him; strictly sight unseen. We met for the first time in the lab and shook hands. He was amiable and jolly, heartily welcomed me into the lab and made me feel at home. Then he looked at me seriously and said solemnly, you know, your name is Alex and my name is Alex, one of us is going to have to change his name. I was thereby re-christened, and since than, I have always been able to recognize friends and acquaintances dating from that time at MIT, including my wife Fran, by their addressing me as "Mac".

At MIT I joined a small band of young innocents that included, among others, Bud Suddath, my best friend, Gary Quigley, JungJa Kim, and later Andy Wang and Ned Seeman. Sung Hou Kim was the straw boss and senior partner. Bud and I were a pair of self described grits-eating crackers from the deep South, Gary was from the sophisticated big city of Buffalo, and JungJa, Sung Hou and Andy were the Far East's best and brightest. Ned of course was *sui generis*. All of us had been trained in crystallography, but none of us had ever played at that level of competition, or for that great and precious a prize, the structure of transfer RNA.

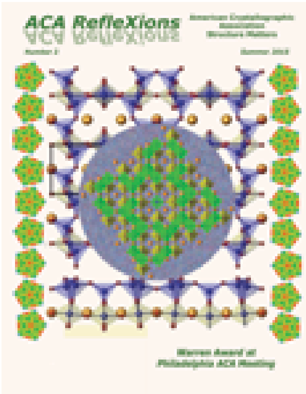
Enthusiasm substituting for experience and energy for insight, we pressed ahead into the fray, one eye on the other aspirants, the other eye, along with both hands and heads, trying to figure out what to do. It would be child's play now, of course, but it wasn't then. Often, we didn't really know what we were doing, but we were all convinced that, somehow, Alex and Sung Hou did. Through mazes of uncertainties, trials and errors, frightening setbacks and uncounted misadventures, along with an occasional advance, some comical relief and a nudge forward, we carried on.

Remarkably, and I sometimes think miraculously, or by the grace of God, we succeeded. We determined the structure of tRNA, and it was magnificent. In the end we emerged triumphant with that great and terrible prize. And we were celebrated; page one of the *New York Times*, editorials in *Nature* and *Science*, the covers of foreign magazines. The glory was manifest and shared among us. We were the champions of the world. It was a time of magic.

About 30 years ago there appeared a widely acclaimed, whimsical little film titled *Stand by Me*. The screenplay was written by Steven King. In the film a band of even younger innocents, about the same in number as our tRNA band at MIT, set off into the depths of a forest seeking to find an extraordinary and frightening prize. In their search they encountered fear and doubt and physical challenge, they experienced setbacks and misadventures, some excruciating, many comical. The youngsters pressed on when wiser souls would have turned back. And, remarkably, they too made their discovery, they found that terrible prize, and in the end they returned triumphant and filled with glory. They were heroes, at least in their own minds.

At the close of the film there was a voice-over, and the voice was that of Steven King, the author. It was evident from his words that, in fact, the film was autobiographical, and that he had been one of those youngsters. He ended by saying *And I have remembered that day all the rest of my life, because it was the most fun I ever had.* And I, like King, have remembered those days of adventure and triumph in your lab because, Alex, that was the most fun I ever had.

Alex "Mac" McPherson



The ***ACA 2015 Bertram E. Warren Award*** will be presented to ***Laurence Marks*** (Northwestern University), during the Philadelphia ACA Meeting. Laurence earned his BA and PhD at the University of Cambridge, UK where he was mentored by Archibald Howie. His PhD thesis was on the structure of silver particles. He has been recognized by a Sloan Foundation fellowship (1987), the Electron Microscopy Society of America's Burton Medal for achievements in electron microscopy by a young researcher (1989), and being named a fellow of the American Physical Society (2002).

Marks studies materials at the nanoscale, analyzing their atomic structures and tweaking their properties with the idea of making them better suited for practical applications. His laboratory uses a wide variety of techniques, including x-ray crystallography, scanning electron microscopy, transmission electron microscopy, atomic force microscopy, and single particle spectroscopy to characterize the surface structure and frictional properties of materials. He uses algorithms developed in house to corroborate the models he has predicted. The images shown on the cover are: in the center of the purple circle, the structure of the $\sqrt{13}$x$\sqrt{13}$ surface of $SrTiO_3$ (001)[1]; surrounding that, the surface structure of the 3 by 1 reconstruction on $SrTiO_3$ (110) and the top bulk layer.[2] where surface TiO_4 tetrahedra are shown in blue, bulk TiO_6 octahedra in yellow, oxygen anions in red and strontium cations in orange. The top four rows show a view perpendicular to the surface with the unit cell outlined in black; the bottom two rows show a view parallel to the surface. The borders are airy stresses in a decahedral multiply twinned particle.

Laurence Marks' research focuses on achieving more efficient catalysis using controlled oxide nanoparticles; improving solid oxide fuel cells in order to produce electricity directly from hydrocarbons; understanding the atomic structure of oxide surfaces, which are still largely uncharacterized, all toward designing 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.

Established in 1970 by students and friends of B.E. Warren when he retired from MIT, the Warren award recognizes an important recent contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques.

1. *Vacant-Site Octahedral Tilings on $SrTiO_3$ (001), the ($\sqrt{13} \times \sqrt{13}$) R33.7° Surface, and Related Structures, D.M. Kienzle, A.E. Becerra-Toledo, and L.D. Marks, Phys Rev Lett, 29th April, 2011, 106, 176102.*

2. A homologous series of structures on the surface of $SrTiO_3$(110), James A. Enterkin, Arun K. Subramanian, Bruce C. Russell, Martin R. Castell, Kenneth R. Poeppelmeier and Laurence D. Marks, Nature Mater. 9, 245 (2010).

3. Elastic Strain Energy Effects in Faceted Decahedral Nanoparticles. S. Patala,, L.D. Marks, and M.O. de la Cruz, J. Phys. Chem. C, 2013, 117, 1485.

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Upcoming Special Topic Issues:

Protein Dynamics. ***Guest Editors: George N. Phillips, Jr. and José Onuchic****: Now open for Submissions*

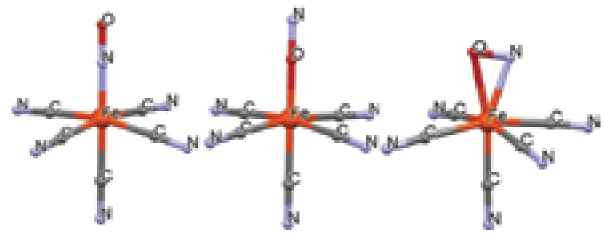
3rd International Conference on Ultrafast Structural Dynamics. Guest Editor: Steve Johnson: Papers will discuss the latest developments aimed at understanding real-time structural changes in materials science, chemistry, and biology using a variety of techniques including: ultrafast electron diffraction, scattering and microscopy; ultrafast x-ray diffraction, scattering and spectroscopy; and ultrafast multidimensional vibrational and electronic spectroscopies. ***http://Icusd2015.ethz.ch/.*** *Publication: November - December 2015*

Soft X-rays in Energy and Time (SXET). Guest Editors: Emad Flear Aziz, Nobuhiro Kosugi, Stephen P. Cramer, and Oliver Gessner: Focused on he current status and new developments in soft x-ray absorption and emission spectroscopy as well as its resonant processes towards the Heisenberg limit (time versus energy limit). Featuring technical and methodological developments for high energy resolution or ultrafast time-resolved approaches addressing new scientific questions for solid, liquids, gases and interfaces. *Publication : Early 2016*

The Hamburg Conference on Femtochemistry –FEMTO 12. Guest Editor Joachen Kupper: Frontiers of ultrafast phenomena in Chemistry, Biology, and Physics. Topics include: the most recent advances in femtosciences, including reaction dynamics, coherent control, structural dynamics, solvation dynamics in liquids and at interfaces, fast processes in biological systems, strong field processes, surfaces and solids, with contributions from both theory and experiment. ***www.femto12.org*** *Publication : Spring 2016*

Recently Published Perspectives

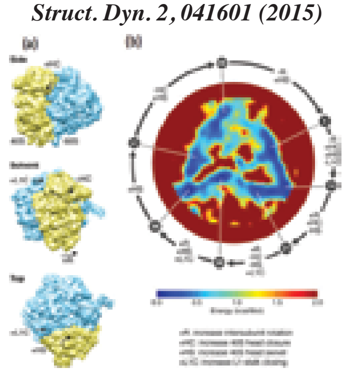
On the relevance of slower-than-femtosecond time scales in chemical structural-dynamics studies by P. Coppens
Struct. Dyn. 2, 020901 (2015).



Abstract: A number of examples illustrate structural-dynamics studies of picosecond and slower photo-induced processes. They include molecular rearrangements and excitations. The information that can be obtained from such studies is discussed. The results are complementary to the information obtained from femtosecond studies. The point is made that all pertinent time scales should be covered to obtain comprehensive insight in dynamic processes of chemical and biological importance.

Single-particle structure determination by X-ray free-electron lasers: Possibilities and challenges by A. Hosseinizadeh, A. Dashti, P. Schwander, R. Fung and A. Ourmazd

Struct. Dyn. 2, 041601 (2015)



Abstract: Single-particle structure recovery without crystals or radiation damage is a revolutionary possibility offered by X-ray free-electron lasers, but it involves formidable experimental and data-analytical challenges. Many of these difficulties were encountered during the development of cryogenic electron microscopy of biological systems. Electron microscopy of biological entities has now reached a spatial resolution of about 0.3 nm, with a rapidly emerging capability to map discrete and continuous conformational changes and the energy landscapes of biomolecular machines. Nonetheless, single-particle imaging by X-ray free-electron lasers remains important for a range of applications, including the study of large "electron-opaque" objects and time-resolved examination of key biological processes at physiological temperatures. After summarizing the state of the art in the study of structure and conformations by cryogenic electron microscopy, we identify the primary opportunities and challenges facing X-ray-based single-particle approaches, and possible means for circumventing them.

Structural Dynamics
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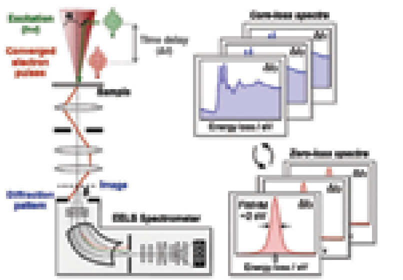
Experimental Methodologies

Ultrafast core-loss spectroscopy in four-dimensional electron microscopyn by R. M. van der Veen, T. J. Penfold, and A. H. Zewail

Struct. Dyn. 2, 024302 (2015)



Abstract: We demonstrate ultrafast core-electron energy-loss spectroscopy in four-dimensional electron microscopy as an element-specific probe of nanoscale dynamics. We apply it to the study of photoexcited graphite with femtosecond and nanosecond resolutions. The transient core-loss spectra, in combination with ab initio molecular dynamics simulations, reveal the elongation of the carbon-carbon bonds, even though the overall behavior is a contraction of the crystal lattice. A prompt energy-gap shrinkage is observed on the picosecond time scale, which is caused by local bond length elongation and the direct renormalization of band energies due to temperature-dependent electron–phonon interactions.

Structural Dynamics Poster Prizes

Poster prizes sponsored by Structural Dynamics are being awarded at a number of meetings this summers: the BCA spring meeting (see below), the ACA meeting in Philadelphia in July, ECM 29 in Croatia August, and AsCA in Kolkata, India in December.

The selection committee at the BCA meeting in York in April (John Helliwell and Semen Gorfman) interviewed 17 candidates for the prize and selected Christoph Zehe (co-authors Joshua Hill, Andrew Goodwin and Jurgen Senker) for his presentation on *The role of dipole moments in bulk structures of 1,3,5-benzenetrisamides*.

Why Publish in Structural Dynamics?

Structural Dynamics is a high impact, gold open access publication - all published articles will be freely available to all readers giving authors the broadest possible distribution of their research and statisying all open access mandates being handed down by various governmental funding agencies.

Metrics: An average time from submission to publication of ~76 days is highly competitive with many of the more established journals, and an average full text download of more than 700 per article in 2014 is a clear indication of both the high quality of the papers and the wide exposure they have had even in the inaugural year of the journal.

Publication Charges & Open Access Fees: Open access is also an "author pays" model. The submission charge was waived for the first 50 papers published in *Structural Dynamics*. Starting in 2015 authors will be assessed an Article Processing Charge of ***USD 2200,*** which covers the cost of publication and allows the author to retain copyright through a Creative Commons Attribution 3.0 Unported License.

ACA members can take advantage of a special discounted Article Processing Charge of USD 1500. The corresponding author must be the ACA member (***membership.amercrystalassn.org/***).

Waivers may be available for certain authors. The ability to pay does not influence whether or not a manuscript is accepted for publication. Please check the journal website for more details: ***scitation.aip.org/content/aca/journal/sdy/info/about***.

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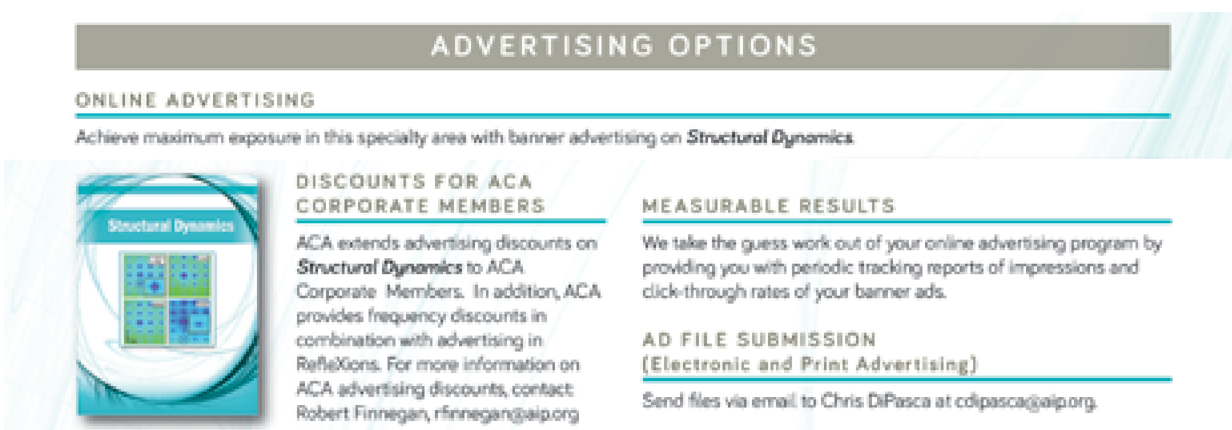


Puzzle Corner

In this issue are the solutions to the previous ***DISORDERED*** and Crystal Connections puzzles, new puzzles of both types, and mention of those who successfully solved the previous ones. As always, I will be pleased to see your solutions ***(ffroncz@lsu.edu)*** and your ideas for future puzzles.

Previous Crystal Connections - All symmetry terms:

1) Used for scrying by Galadriel - ***mirror***

2) The moon's revolution period equals its ***rotation*** period

3) Helical inclined plane -***screw***

4) Tax avoidance by merger with a foreign company - ***inversion***

5) Converting words to a different language - ***translation***

6) In phonetics, the semivowel class of approximants - ***glide***

The answers to this puzzle and to the previous ***DISORDERED*** puzzle were provided by **Amy Sargeant** and **Charlotte Stern**. **Dan Frankel** also gave the correct ***DISORDERED*** solution. Here is the new Crystal Connections:

Crystal Connections #3 - What do the answers to these clues have in common?

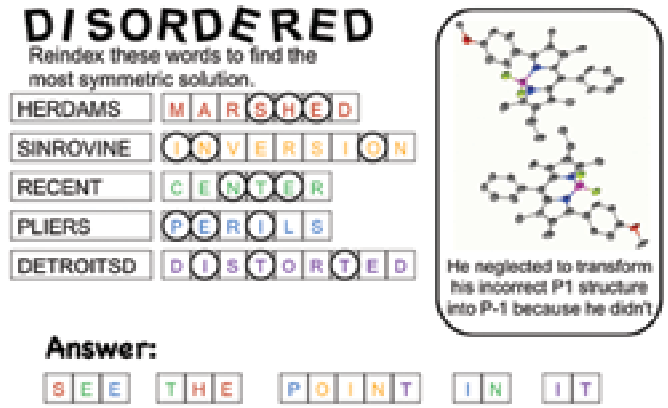
1) First letter of a 2-letter 1982 movie title

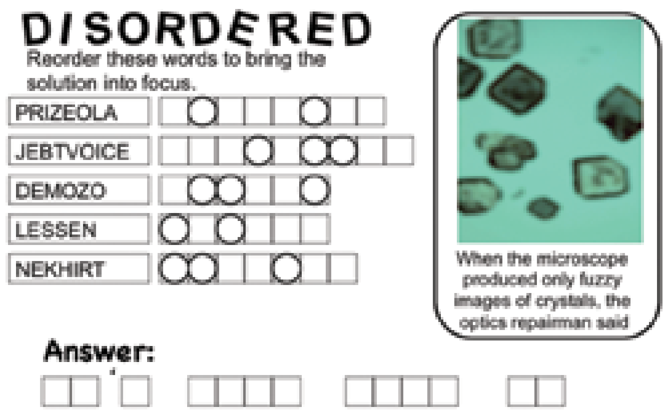
2) Sum of a number and the negative of another

3) Joseph _________, credited with discovery of the greenhouse effect

4) Topographic line of equi-elevation

5) Beth _________, Louisiana Celtic bouzouki musician



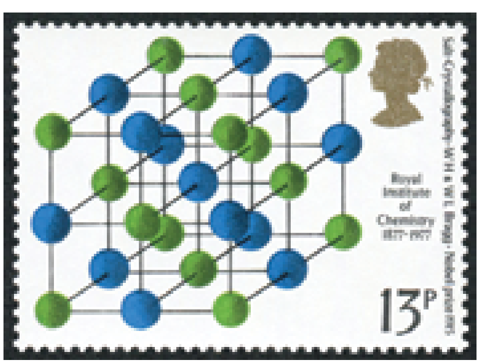


Frank Fronczek - ffroncz@lsu.edu

Spotlight on Stamps: Salt of the Earth

William Henry Bragg (1862-1942) and his son William Lawrence (1890-1971) received the Nobel Prize in Physics 100 years ago "for their services in the analysis of crystal structure by means of x-rays". The recognition bestowed on the Braggs was significant for several reasons, including the fact that it was the first (and to this date the only) father and son team to have jointly received a Nobel Prize. Remarkably, William Lawrence was only 25 years old at the time, which makes him also the youngest Nobel laureate ever in the sciences. The Swedish stamp illustrated below also adorns the cover of the excellent biography of the Braggs written by John Jenkin and published in 2011.

The other stamp highlighted in this note, issued in Great Britain in 1977, features the well-known face-centered cubic structure of sodium chloride, first described by W.L. Bragg in a paper published in the September 1913 issue of the *Proceedings of the Royal Society of London,* a seminal publication that effectively marked the beginning of the science of x-ray crystallography. Today, only a little over a century later, it is noteworthy that the Cambridge Structural Database, the main repository for crystallographic data of organic and organometallic compounds, contains more than 750,000 entries! That's a lot of X-ray structures...



Dan Rabinovich

Most Wanted Particle: The Inside Story of the Hunt for the Higgs, the Heart of the Future of Physics by Jon Butterworth, The Experiment, LLC, New York, 2014. ISBN 978-1-61519-246-5.

Jon Butterworth's book *Most Wanted Particle* is a first-person account (often very funny) of his involvement in the experimental confirmation of the Higgs boson at the Large Hadron Collider (LHC) near Geneva, Switzerland in 2012. Butterworth himself was involved in developing algorithms to analyze the "jets" of particles that are produced in the proton-proton (or other) collisions and how their properties can indirectly detect short-lived and massive bosons. The tale is interwoven with many personal opinions and anecdotes that illustrate the two steps forward, one step back nature of the endeavor. These include the heartbreaking accidental explosion of superconducting magnets in the LHC due to a welding error just after the initial startup that led to a yearlong delay. The author expresses empathy for young excited physics students that had to deal with not taking data for a year. Separate scientific sections explain both the Standard Model of particle physics and the gaping hole that could be filled by proving the existence of the boson predicted by Peter Higgs and his colleagues that imparts mass on all fundamental particles. Not least, Butterworth explains the statistical criteria that had to be painstakingly agreed upon to actually call the data evidence for a "Higgs boson".

The reader will come to appreciate the incredible long range planning, engineering, computing, and infrastructure required to build and maintain a giant instrument to examine matter at it's tiniest and most powerful scale (just thinking of the plumbing and safety and administrative aspects makes one's head hurt). An excellent aspect of the book is how Butterworth had to confront (as a leader and representative for the ATLAS detector at LHC *via* social and other communication media) the constant tension in our culture between funding hugely expensive efforts like the LHC and the inability to say exactly when and how discoveries made there will directly benefit humanity. On that note, Butterworth reminds us that the world-wide-web is a direct result of Tim Berners-Lee figuring out how to instantly share data from large particle accelerator experiments with collaborators across the globe!! As an occasional user of synchrotron light sources, this reviewer is always in awe of what biologists, chemists, and materials scientists have been able to accomplish due to these large physics-based particle accelerators and their spin-off applications. A nice teaching aspect of the book is how Butterworth explains the requirements of wavelength and resolution for probing matter at the level of quarks, gluons, and Higgs bosons in a way that I could relate to as an x-ray crystallographer.

Butterworth's account shows that the Higgs experiment was the result of brilliant theory that makes testable hypotheses (once the energy to test them is accessible), enormous technical and logistical mastery, massive public support (hence funding), teamwork that keeps the "eyes on the prize", and dogged persistence. His enthusiasm and emotional highs and lows are infectious, including funny anecdotes about scientific meetings, chance encounters, and dealing with the public. Sometimes I found the reading to be a bit rambling due to his many digressions. It was not hard to become lost in the nomenclature. I would recommend the book to scientists or nerdy types interested in fundamental discoveries but I am not sure that a non-scientist would enjoy it as much.

Laurie Betts

What Should We Be Worried About: Real Scenarios That Keep Scientists Up at Night (2014, ISBN: 978-0062296238) & , This Idea Must Die: Scientific Theories That Are Blocking Progress (2015, , ISBN: 978-0062374349.), John Brockman, Ed., Harper Perennial, New York, .

The editor of both books is John Brockman, founder of the Edge Foundation, a web based think tank. Each year he asks a large group, many of them members of the Edge Foundation, the question for the year. Each of the books presents a series of short essays that answer the title question from thinkers in many fields. A number of essays are from authors that have been reviewed here including Sean Carroll, Steven Pinker, Charles Seife, Nicholas Nassim Taleb and Sherry Turkle, so some of the answers may be familiar to you. Each essay is accompanied by a short bio of the author and the title, or titles, of some recent book.

The first book came to me as a recommendation from Amazon. I picked up the second book after hearing an interview with Seth Lloyd and Sean Carroll on *Science Friday* last month.

What Should We Be Worried About is one of the most depressing books I have read in a long time, as if I already didn't lie awake thinking about global warming, financial collapse, human population-thinning disease, or stupidity, now I have about 170 other things to worry about it. Only read this book if your glass is half full or you are current on your selective serotonin reuptake inhibitor prescription. There is one vignette that is slightly humorous. It discusses protecting young ears from the seven words the FCC won't let on the air. However, the author suggests making something taboo makes it all the more interesting, and that's the problem.

The second book, *This Idea Must Die*, is based on the tenet of Planck that an existing paradigm will subside when the last proponent is dead. This is much more upbeat in the sense that the essays present solutions to problems as opposed to just listing problems as in the former book. The ideas that "must die" range far and wide: from the idea of the universe, as opposed to the multiverse, to races, anonymous peer review and bad statistics.

I just finished volumes one and two of the epic biography of Lyndon Johnson by Robert A. Caro. When I picked up these books I did not think this subject would hold my attention but both *The Path to Power: The Years of Lyndon Johnson, Vol. I*, (ISBN: 978-0679729457) and *Means of Ascent: The Years of Lyndon Johnson, Vol. II* (ISBN 978-0679733713), Robert A. Caro, Alfred A. Knopf, New York, 1990, I) did just that. The books are not just about Johnson but proide a detailed look into life in the Texas Hill Country in the early 20th century as well Texas and US politics until 1948. I will start *Master of the Senate* this summer.

Joe Ferrara

Robert G. W. Brown selected as the new AIP CEO

On June 1, 2015 Robert G. W. Brown became the new Chief Executive Officer of the American Institute of Physics (AIP), succeeding Fred Dylla, who had served in that capacity for eight years and will be CEO Emeritus.

Brown studied at the University of London and received a BS in Physics in 1973 followed by a PhD in Engineering from the University of Surrey in 1983.

With more than 40 years of experience in the physical sciences in roles that include practicing physicist and engineer, research director, editorial director, chief technology officer and leading sensor scientist, Brown is a passionate advocate for the global impact the physical sciences have in our world today, especially as the basis for most technologies we use every day. He has published over 120 peer-reviewed research papers in the global physical science literature.

Prior to joining AIP, Brown served as chief sensor scientist at the Advanced Technology Center of Rockwell Collins Inc., a US aerospace and defense company. His accomplishments in that role include nano-plasmonic detectors for UV, visible light, all infrared and THz regions; also the invention of a nano-plasmonic ultra-fast computing scheme, in addition to the creation of ultra-high-index nano-plasmonic glass.

Brown has also served on the UK Government's Home Office Science and Technology Advisory Board, in addition to serving on NASA's International Microgravity Advisory Committee, and also as Professor and Director of Nanotechnology for Northern Ireland. He was elected into the European Academy, Academia Europaea in 2002.

His career took off when he became Principal Scientist at the Royal Signals and Radar Establishment within the Ministry of Defense of the UK where he specialized in photon-correlation laser velocimetry and spectroscopy and invented new ways to use laser diodes, single-photon-counting avalanche-photodiodes and single-mode optical-fibers to miniaturize and improve upon previous light-scattering instruments. These technologies have become industry standard today, being used in many scientific instruments and basic physics experiments.

Brown has also served as the International Editorial Director of the United Kingdom's Institute of Physics (IoP), which works to advance physics. There he led the creation of new IoP centers in China and Russia.

Since 2009, in addition to his nanotechnology research activities at Rockwell Collins, Brown has worked concurrently as an Adjunct Full Professor in the Beckman Laser Institute & Medical Clinic of the University of California, Irvine, and in UC Irvine's Department of Computer Science.

Adapted from the announcement at www.aip.org

Index of Advertisers

Candidates for ACA Offices in 2016

The Nominating Committee (Ward Smith, Cheryl Stevens and Victor Young) proposes the following candidates for the 2015 elections for ACA offices in 2016.

Officers:

Vice-President: **Amy Sarjeant & Eddie Snell**

Treasurer: **Lesa Beamer & Sue Byram**

***Committees*:**

Communicatons: **Karena Chapman & Jim Fettinger**

Data, Standards & Computing: **Danielle Gray & Mark Whitener**

Continuing Education: **Joe Ferrara & Allen Orville**

Continuing Education: **Paul Davie (***Appointed to replace Tom Terwilliger)*

To nominate write-in candidates for any office, write to the ACA Secretary: **Diana Tomchick, Dept. of Biophysics, University of Texas, Southwestern Medical Center, Irving, TX 75061 (diana.tomchick@utsouthwestern.edu.** Letters must be received by September 15, 2015 and must be signed by five 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 2015***.

Vice-President - Amy Sarjeant

Currently: Research Assistant Professor, Northwestern University, Evanston IL

Soon-to-be: Outreach and Education Manager, Cambridge Crystallographic Data Centre, Piscataway, NJ

Education: BS Chemistry, The College of William and Mary, Williamsburg VA (1995). PhD Chemistry, Northwestern University, Evanston IL (1999).

Professional Activities: Member: US National Committee for Crystallography since 2011, Continuing Education Committee ACA since 2012; Chair: Small Molecule SIG (2013), Service SIG (2010); Secretary General Interest SIG (2012-2014); ACA Member since 2000. Co-organizer ACA Summer School for Small Molecule Crystallography since 2012.

Research Interests: Single-crystal, small molecule crystallography, crystallographic education, publication trends in crystallography.

Statement: Think back to when you first joined the ACA. Was it last year or seemingly a lifetime ago? Now, as you read my statement and the others of those fortunate enough to be running for Council or Committee positions, take a moment to consider what drew you to the ACA and what has kept you here. For myself, and I suspect for many of us, I came to the ACA searching for a professional home, a place where, as a crystallographer, the trials and tribulations of my work would be understood and where I might find inspiration. Ask any crystallographer what he or she thinks of the ACA and almost universally you will hear what a tight-knit community this is, how helpful other crystallographers are, and what fun it is to be part of such an organization. Where else can a first-year graduate student present her research in the same session as the authors of her textbooks? In what other society might an undergrad feel free to strike up a conversation with his idols over coffee at a poster session? These interactions are what make the ACA such a vibrant and essential organization to our science.

There is much talk these days of dwindling membership and a lack of relevance in the ACA. It is true that we are at a critical period in our existence. How can we attract new members and keep the ones we have? What do we need to do to stay relevant in the ever-changing landscape of crystallography and scientific research in general? These are hard questions to ask and even harder to answer. We must face these challenges head on and continue moving forward in order to provide the same environment to the next generation of crystallographers that drew us into the ACA in the first place.

I firmly believe that one of our biggest responsibilities as a society, and perhaps the best tool we have for staving off these challenges, is to promote crystallographic education. As a co-organizer of the ACA Small Molecule Summer School for the past four years, I have seen first-hand how little crystallography is taught, even in major research institutions. While it is certainly true that solving a crystal structure today is a far easier task than it was 50 years ago, the science of diffraction is anything but routine. However, if we cannot change the way we educate young scientists about our craft, if we cannot impress upon them how useful, changeable and exciting crystallography is, we risk losing the foundation of our society.

The swell of interest in promoting crystallography to the general public that began last year with the IYCr should provide us with the momentum we need to grow and improve the ACA. I have had the pleasure of being involved with organizing a video contest for K-12 students as a way to bring crystallography into the classroom on that level. It was a joy to see how young children responded to the ideas and theories of crystallography and it is clear that we can do more to spark interest in our science at such a young age. At the IUCr Congress in Montreal last August, I orchestrated a mentoring event for young crystallographers. The overwhelming interest in this Young Observers program highlighted the great need for mentoring the newest members of the crystallographic community. As a member of the ACA Council, I would seek to promote our society and our science through mentoring, education and outreach

– both to the general public and through other scientific communities. The road ahead of us is challenging, but I welcome the opportunity to walk it with you.

Vice-President - Edward Snell

Education: BSc Applied Physics (1st), John Moores University, Liverpool, UK (1993); PhD Chemistry, University of Manchester, UK (1996) (advisor John Helliwell); National Research Council fellow, NASA Laboratory for Biophysics at Marshall Space Flight Center, Huntsville, AL, USA (1996-1999).

Professional activities: ACA Communications Committee (2012-2015); Stanford Synchrotron Radiation Light Source Users Executive Committee Chair (current); SSRL representative on Linear Coherent Light Source Executive Committee (current); International Organization for the Crystallization of Biological Macromolecules Council member (current); Co-chair, Gordon Diffraction Methods Conference (July 2014, Chair in 2016); Chair of the ACA Biological Macromoles SIG (2013-2014); Member of the American Institute of Physics News and Media Advisory Committee (2014-2017); Chief Executive Officer of the Hauptman-Woodward Medical Research Institute (2014-).

Research Interests: Methods development for crystallization and x-ray and neutron data collection. Complementary techniques to help reveal the dynamic mechanisms of macromolecules. Information mining and display.

Statement: I have been a member of the ACA since 1996 and have attended every meeting since then. The ACA, as an organization, has helped me grow my career, establish many of the collaborations I have today, and develop a network of friends in the field. It is a broad organization with members of diverse research background and career stages and one that, beyond the annual meeting, strongly promotes continuing education in the community, standards for crystallographic information, and encourages software development and propagation. It is an important organization for crystallography as a whole and fulfills a key role in representing our field on an international stage through the IUCr. My initial experience has been with attending the annual meetings, but over time I have talked with colleagues who have been involved with the ACA at a deeper level and have been encouraged to take a similar plunge. I quickly realized that what makes the ACA strong is that it is a member supported and driven association. Beyond the scientific sessions that take place at the annual meetings, there are also special interest group sessions, and the members meeting. I started attending these (anyone can and I would actively encourage it), all the opinions are heard, from new students to seasoned professors, and through this mechanism, the members help drive the content and direction of the annual meeting and the association. People matter and people make a difference.

The ACA has strongly supported a 'nuts and bolts' education effort with the Young Scientist Special Interest group running blackboard sessions where technical aspects of the crystallographic process are illustrated. Even at this level, there is much new information to take in. These sessions are phenomenally popular and in addition to the content presented, also allow some of those Young Scientists to get their feet wet learning how to organize and run a session – skills that are not normally taught. I would actively support the continuation of these efforts and see one of the ACA's roles as building the field.

The annual ACA meeting is a diverse one with research areas in different fields of science connected by a common theme. That theme used to be crystallography but it has now grown to encompass complementary techniques that supplement crystallographic information and provide structural and mechanistic stories. My own research area uses crystallography for biological studies but I have built this research on a physics background and more recently (from frustration at getting well-diffracting crystals) I have made increasing use of small angle scattering. There are two points to this: firstly, that I speak many of the 'scientific languages' within the ACA and secondly, and more importantly, a statement on the openness and inclusivity of the ACA. Small angle scattering is field that is growing in representation within the ACA; the openness to include this community is an indication of the culture of the association and one I would strive to continue.

I have been involved with the Communications Committee of the ACA and as part of that have served on the News and Media Advisory Committee of the American Institute of Physics (AIP). The AIP produces *Physics Today* magazine that appears in your mailbox every month. That might be the only thing that ACA members are aware of, but the AIP brings other services to its members and has a role in government relations promoting science as a whole and with that the research areas of the ACA members. I would like to see a better awareness of what the AIP offers ACA members and more use of them to support our activities.

The ACA has activities beyond the annual meeting. These are predominately represented by three standing committees: Communications, Continuing Education and Data Standards and Computing. Among other things, the communications committee coordinates publications, press conferences and the recording of key lectures at the annual meeting. The continuing education committee coordinates workshops at the annual meeting, other development opportunities and travel support for students. These are important for the field and should continue and grow. I strongly support the recording and archiving of key research talks and the vibrant workshops associated with the annual meetings. The Data Standards and Computing committee represents the community in driving standards for recording and presenting data and has been a strong voice in the international community as a whole with initiatives such as a common minimum standard on the information necessary to be included with a structural publication. I see their role as maintaining a high scientific bar and acting as a body that helps different computational approaches to seamlessly interface with each other – an important function for the ACA and one that I also strongly support..

In my career in crystallography I have seen the field go from glass capillaries, photographic film, and semi user-friendly synchrotrons (with amazing staff support), to cryogenic approaches, brilliant beams, remote operation and rapid detectors, and now to serial approaches with femtosecond illumination and streams of crystals, many too small to see. The field of crystallography moves fast and with each advance come new methods and best practices. The ACA has a role in making sure that the community effectively makes use of the future. It has an important role in training and educating the community. The mix of capabilities is becoming so broad that it also has a role in bringing collaborations together. Most importantly, it should serve as the incubator for new talent that will make use of many of the rapid developments. I would be honored to help the ACA be part of this future.

Treasurer - Lesa Beamer

Assoc. Professor, Depts. of Biochemistry and Chemistry, University of Missouri

Education: BS Chemistry, Kent State Univ. (1986); PhD Biochemistry, Cellular & Molecular Biology program, Johns Hopkins Univ. School of Medicine (Advisor, C. Pabo, 1991); Postdoctoral research in biophysics, (UCLA, D. Eisenberg, 1991-97)

Professional Activities: Co-editor, *Acta Cryst. F* (2009-); Study section panelist for NSF & American Cancer Society; Contributor to ACA *RefleXions* (2010, 2012); Session Chair & Program Director ACA annual meeting (2004); Chair BIOMAC SIG (2004)

Research Interests: Protein structure and function, x-ray crystallography, HDXMS, SAXS, NMR, computational biology. Current projects include studies of enzymes in the a-D-phosphohexomutase superfamily, including the role of enzyme flexibility in catalysis.

Statement: It is an honor to be nominated for a position on the ACA council as Treasurer. I have been an ACA member for more than 20 years. I believe that professional organizations like the ACA are critical for supporting the training and development of young scientists and maintaining the scholarly standards of the field. During my career, the ACA has been invaluable for connecting with like-minded scientists and learning about new methodological advances.

As treasurer, I would have the opportunity to serve the membership in new ways. Among other duties, the ACA treasurer determines the amounts of travel grants to the annual meeting and reports to both the membership and the ACA council. I will strive to provide accurate information in a clear and effective fashion, and help continue ACA¹s tradition of fiscal responsibility and transparency. If elected, I look forward to serving ACA members in this capacity.

Treasurer - Susan K. Byram

Business Manager of Crystallographic Systems, Bruker AXS, Madison, WI

Education: BSc, Mathematics, Physics & Chemistry (1967) and MSc, x-ray crystallography (1970), University of Toronto, Canada. University of Wisconsin Management Institute and Siemens Management Institute certifications.

Professional Activities: At Bruker AXS, for the past 14 years I was responsible for the USA and Canada crystallography sales force, coordinated global sales activities through the global team, and managed the crystallographic application laboratories and activities of the application scientists for demonstrations, samples, new product testing and application courses. This included setting and meeting the annual budgets for these groups. For 18 years prior, I was product manager variously of single crystal and powder diffraction systems, defining hardware and software functions for new product development. This position was also responsible for the marketing plans and budget for scientific meetings, exhibits, product literature, web and print advertising.

My current career started when I was fortunate to obtain a unique position in software development at our predecessor company, Syntex, reporting to Bob Sparks who became my mentor. We automated single crystal diffractometers and wrote the first commercial minicomputer-based structure solution package. With Bob Sparks and others, I co-founded California Scientific Systems to develop automation systems and advanced software for powder diffraction. I managed this small business for 4 years until its acquisition by Nicolet, learning in my heart that you need reliable income in order to develop and sell products, pay staff and handle expenses. And I learned to fill a vacuum – if nobody else is doing it, then you do it. This has stayed with me throughout. Previously, I was a research officer at the National Research Council of Canada, participating in the early development of the NRC crystallographic software suite. Prior to that, I was a staff member in polymer diffraction at Raychem Corporation, Menlo Park, CA, where I actually built a pole figure camera and conducted XRD experiments on cross-linked polymers for heat shrinkable tubing.

I have taught at the ACA Summer Schools in Pennsylvania, Pittsburgh and Notre Dame, have co-organized and presented at many Bruker user meetings, and enjoy giving technical and instrumentation presentations at crystallographic, chemical, mineralogical and structural biology meetings. During my career, I have attended virtually all ACA and IUCr meetings and many ECM meetings. For the past ten years, I have managed the finances for Soil Net, my husband's small business, including necessary budgets and reports for a major USDA grant. In the non-profit arena, I am the long-time treasurer of a fraternal organization and review financial information as vestry member of our church.

Research Interests: My interests are generally in the areas of x-ray instrumentation and methods. I first learned crystallography as an undergraduate at University of Toronto, and was entranced (as so many of us have been) by its capability to give us definitive knowledge about new materials. I had a natural affinity towards the software side of crystallographic research, and was fortunate to work with some of the great people developing crystallographic software, including Larry Calvert and Eric Gabe at NRC Ottawa, Bob Sparks at Syntex and successor companies, and George Sheldrick as a long-time consultant. It has been really special to work with the people, instrumentation and methods evolving over the past decades. I reviewed some of this in my 2012 ACA talk on *Evolution of Small Molecule Instrumentation in North America*, which can be seen on the ACA history site.

Statement: I love crystallography and the people in crystallography, and I want the ACA to thrive. The ACA Treasurer has specific duties, including working with staff on day-to-day operations, reviewing monthly reports, and presenting the Financial Report annually, as well as coordinating with the AIP and the USNCCr. I expect we should also coordinate with other member societies. I have scaled back to part-time at Bruker and feel I could devote time, expertise and energy to give back to ACA, which has meant so much to me over my entire working career. As a member of ACA Council, the treasurer should seek input from our membership and work with ACA Council to present a stable vision for our future. I have hands-on experience in single crystal, powder and polymer diffraction and would try to engage all our research communities and all our vendors. Further, I believe we need some innovative methods to attract and engage new members from all our geographic groups in Canada, the USA, Latin America and beyond. ACA already does an outstanding job of educating budding crystallographers in our science. I believe scientific societies such as ACA should also be educating our political representatives and funding committees about why our science is necessary and important. I believe the financial basics of maximizing income and controlling expenses to achieve our strategic goals can guide us as we go forward.

James C. Fettinger - Communications

Department of Chemistry, Univerity of California, Davis, Davis, CA.

Education: BS, Chemical Engineering (1982), PhD Inorganic Chemistry (1987), The State University of New York at Buffalo; Postdoc, Northwestern University (1987-1988), Research Associate, CIBA-Geigy (1988-1992) and Postdoc U. Mass Medical Center (1992-1993).

Professional Activities: ACA member since 1990, Service SIG secretary (2003-04; 2011-2013), Poster Judge, ACA New Orleans (2011), and reviewer for several journals.

Research Interests: Small molecule single-crystal x-ray crystallography, variable temperature experiments with phase transitions, non-routine crystallographic experiments, twinning, and the ongoing development and utilization of crystallographic software.

Statement: I wish to thank the committee for nominating me for a position on the Communications Committee. While I have been a member of the ACA now for nearly 25 years I have not served on any committees so this would be a first, should I be elected.

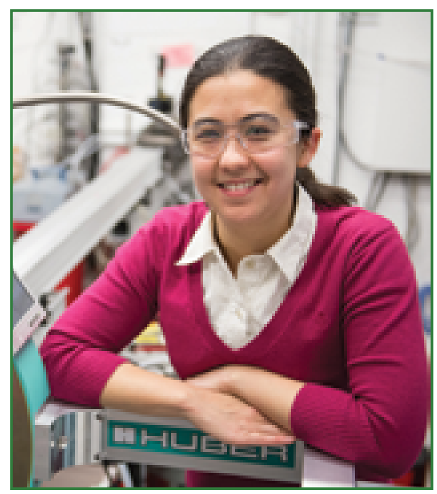
Whenever I have given a talk to the general public at one of our local high schools, junior high's or even at the elementary school level the students are usually awed at what x-ray crystallography is capable of showing them. University talks to graduate chemistry classes are similar. It's as though x-ray crystallography is something new, not over 100 years old, so it's fairly clear that our area of expertise is not well presented to the general public or in general chemistry classes.

It's also apparent that our local school's chemistry classes don't really have any time allotted for learning x-ray crystallography or anything related to structural chemistry so if this is a nationwide problem it may be an area that the Communications Committee may consider for the future now that the International Year of Crystallography has ended.

As an amateur videographer for the past nearly 25 years, I have gained quite a bit of experience videoing a wide range of activities and then editing for content and feel this would be complementary among the tasks assigned this committee.

Helping the committee in their endeavors towards promoting our conferences with the local media and the general public would be quite illuminating.

Karena Chapman - Communications



Chemist, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Illinois

Education: PhD in Chemistry (2005), BSc (2002), University of Sydney, Australia.

Professional Activities: *Journal of Applied Crystallography* co-editor (from 2014). National X-ray & Neutron Scattering School co-organizer (from 2013). Symposium organizer (IUCr 2014, ECM 2013, MRS 2013, ACA 2011. Reviewer for the Advanced Light Source, Spallation Neutron Source, National Synchrotron Light Source.

Research Interests: Broadly speaking, I am a materials chemist interested in developing and applying synchrotron-based crystallographic tools to explore the coupled structure and functionality of energy-relevant materials. In recent years, I have studied battery electrodes and electrolytes, catalysts, and nanoporous framework materials for strategic gas capture, including as part of the NECCES and ICDC Energy Frontier Research Centers and the JCESR hub.

My research career began at the University of Sydney, Australia in the area of small molecules single crystal XRD, and evolved towards synchrotron-based *in-situ* powder diffraction and pair distribution function studies. Following my graduate studies, I made the Advanced Photon Source my in-house diffractometer, joining Argonne as a research fellow, becoming staff in 2009. I am now responsible for the dedicated Pair Distribution Function instrument, 11-ID-B, which provides insight into the atomic and nano-scale structure of crystalline, nano, and amorphous materials that are beyond the limits of Bragg crystallography.

Statement: I would be delighted to serve on the ACA Communications Committee. Conveying impact and insights from our research to our peers, students, public and policy makers is vitally important to our crystallographic community. And the ACA communications committee plays a key role in this.

Beyond the publications of the ACA, press releases, and videotaping of plenary lectures at the Annual Meetings, new media provides exciting opportunities to reach out to members, broaden our audience and amplify our message. For example online videos and webinars can be an on-demand resource and serve as an educational platform to train the next generation of crystallographers. At the APS, I have developed such videos, hosted on YouTube, to help train users to operate our instruments and reduce and analyze data. These videos have more than 18000 views to date, from all around the world. I imagine, that by embracing new media opportunities such as this, the Communications Committee could only enhance ACA member engagement and interactions.

Danielle Gray - Continuing Education

Director of the G.L. Clark X-ray Facility, School of Chemical Sciences, University of Illinois, Urbana, IL

Education: BA (2001), Chemistry, Augustana College; PhD (2006), Inorganic Chemistry, Northwestern University.

Professional Activities: Member: ACA since 2005, ACA's IYCr committee (2014).

Research Interests: Structure elucidation of complex small molecules especially modulated crystal structures via single crystal diffraction.

Statement: It is an honor to be nominated to stand for election to the Continuing Education Committee. Knowledge of the fundamentals of the crystallographic technique seems to be disappearing more and more with each new generation of chemists. Instrumentation with shutterless data collection and auto solve are allowing the rapid collection and analysis of vast numbers of crystal structures with little effort. Because of these and other advances, a casual user can collect and solve a structure with little to no formal training. Consequently, the technique is often relegated to being a 'black box' where little understanding is necessary as long as the desired structure solution is obtained. Unfortunately this also leads to a lack in understanding of the power and limitations of the experiment. Without a grasp on the fundamentals, how are inexperienced practitioners who use crystallography to support their research supposed to diagnose problems in their structures or assess the reliability of the structure solutions?

As chemistry advances so does the complexity of the structure solutions being sought. Now more than ever we need a push for crystallographic education at both the undergraduate and graduate levels. It is essential that a comprehensive crystallographic education be taught to the next generation of crystallographers so that not only can our knowledgebase be maintained, but emerging techniques can be expanded upon to improve research goals. 2014 saw the International Year of Crystallography (IYCr) come and go. During the year many workshops, outreach programs, and educational opportunities highlighted the importance of crystallography to science in the past, present, and future. Let us not halt the educational momentum built up over the past year and continue to not only highlight the importance of crystallography but illuminate the fundamental principles of the technique. Developing and maintaining quality educational programs like the ACA Summer School and continuing to support workshops for both inexperienced and experienced crystallographers will go a long way to improving the overall knowledgebase of current and future crystallographers and scientists. If elected, I will build upon the momentum of the IYCr and work to facilitate educational opportunities for the crystallographic community.

Mark Whitener - Continuing Education

Associate Professor of Chemistry, Department of Chemistry and Biochemistry, Montclair State University, Upper Montclair, NJ

Education: BS Chemistry and BS Mathematics, Southern Methodist Uni-

versity, (1982); PhD Chemistry, Harvard University, (1990); Postdoctoral, Inorganic Chemistry, Northwestern University, with Professor James Ibers, (1990); Postdoctoral, Organic Structural Chemistry, University of Minnesota, with Professor Margaret Etter, (1991-1993).

Professional Activities: Member: ACA since 1991, ACS since 1982. Co-presider, Margaret Etter SIG Lecturer, Chicago ACA meeting (2004).

Research Interests: I am interested in the coordination and structural chemistry of first row transition metals. I have two ongoing research projects. First, my students and I prepare and study hydrogen bonding interactions between metal bound imidazole and carboxylates. Metal imidazole complexes serve as good models for histidine in metal proteins. My second project is to prepare and study the structure of metal based quasi-racemates. A quasi-racemate consists of two molecules of opposite chirality that have slight differences in their structure. These molecules often crystallize about a pseudo center of symmetry. Metals provide a good way of predictably organizing such molecules.

Statement: I am honored to be nominated for membership in the Continuing Education Committee. Since 1990, I have attended nearly all the annual ACA meetings. Through service on this committee, I can repay an organization that has greatly benefited my professional career. The duties of the Continuing Education Committee provide a vital service to the ACA in developing workshops, encouraging student travel, and serving ACA members through other educational and professional activities. I have learned a great deal of relevant information through attendance at several ACA workshops. I was impressed with the density and quality of information disseminated during these meetings. I would enjoy playing a part in this tradition of recommending future excellent workshops as well as fulfilling the additional charges of the committee.

I teach and do research as a faculty member at a primarily undergraduate university. The ACA has some such voices, but needs to hear more from faculty at these types of institutions. Researchers at such colleges and universities face challenges in developing a viable research program. Time, money, information, awareness of opportunities, and availability of resources all tend to be in short supply. The ACA and this committee can play a strong role as advocates, supporters, educational providers, and generators of networks for researchers at undergraduate institutions. Not all news is bad for those at undergraduate schools. For example, benchtop diffractometers with simpler maintenance make it possible for x-ray laboratories to be set up at more locations. Opportunities for grants, collaborations and formation of consortia are all positive developments. In parallel to these research interests, I wish to find ways integrate more crystallography throughout the undergraduate curriculum. For example, the explosive growth in macromolecular structures has been incorporated into biochemistry texts, but not always with an appreciation for the foundations of the methods of x-ray crystallography. I am not solely an advocate for faculty in positions similar to myself. I am excited to have a chance to share my ideas, and discuss the ideas of colleagues on the committee that can advance the professional and educational development of all crystallographers. I thank the nominating committee for considering me.

Joe Ferrara - Data, Standards & Computing

Deputy General Manager, Product Marketing and R&D, Rigaku Oxford Diffraction. Deputy Director, X-ray Research Laboratory, Rigaku Corporation

Education: BS, Case Institute of Technology (1983); PhD in Organometallic Chemistry, Case Western Reserve University (1988) with Wiley J. Youngs.

Professional Activities: Board member, Lone Star College Biotechnology Institute Scientific Advisory Board (2005-present, chair 2011-2012). Reviewer, NSF and DOE proposals. Reviewer, *Acta Cryst. D*. Books editor, *ACA Reflexions* (2009-present).

Research Interests: My research interests cover two main categories: X-ray diffraction and x-ray imaging. In the field of x-ray diffraction I have been either the team leader or a team member for numerous projects that have brought new tools to the diffraction community including microfocus x-ray sources, multilayer optics, CCD and HPA detectors, automation, long wavelength phasing and software tools. In the field of imaging I have been developing tools for x-ray microscopy and I have an ongoing collaboration with groups in the US and UK to develop fast, low dose phase contrast imaging methods for early detection of breast cancer.

Statement: I came to this candidacy in a rather unorthodox manner; I was asked by a colleague to take their place as a nominee. I live for challenges, so I decided to run. I have been a member of the ACA since I joined Molecular Structure Corporation (now Rigaku) in 1988. Over the years I have been an active participant in the development of the hardware and software tools that crystallographers use every day. This experience gives me a unique perspective that will benefit the Data, Standards and Computing Committee. My knowledge base spans all fields of x-ray science and allows me to apply what I learn in one area to another. For example, recent discussions with colleagues suggest the next step in improving the publication and review process is the production of an executive summary of the very comprehensive PDB validation report akin to the IUCr CheckCIF report for small molecule structure validation. An executive summary would highlight the features of the structure that might prevent publication. Such a scheme would make it much easier for non-scientists doing crystallography to submit more polished structures and make it easier for reviewers to catch errors.

Allen M. Orville - Data, Standards and Computing Standing

Biophysicist, Photon Sciences Division Brookhaven National Laboratory, Upton, NY

Education: BS, Biology, University of Minnesota (1983), PhD, Biochemistry, University of Minnesota (1997), postdoctoral fellow Howard Hughes Medical Institute, University of Oregon (1997-2000)

Professional Activities: ACA member since 2003. Co-chair: Structural Enzymology session at ACA 2008, Knoxville, TN; Chair: Structural Enzymology: Mechanistic session at ACA 2010, Chicago, IL; Structural Enzymology I – Spectroscopy & Complementary Methods session at ACA 2011, New Orleans, LA; Instructor and beamline scientist at Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement (RapiData, 2007 – 2013); Organized Removing the mystery from mystery density: A workbench for correlated single-crystal spectroscopy and X-ray crystallography at Brookhaven National Laboratory (2011); Spokesperson for NSLS-II beamline SM3: Single-Crystal Spectroscopy & Macromolecular Crystallography at a Three Pole Wiggler Beamline, (2010 – present); State of Georgia voting board member for the South East Regional Collaborative Access Team (SER-CAT), Advanced Photon Source, Argonne National Laboratory, Argonne, IL (2004 - 2006).

Research Interests: Structural basis of enzyme reaction mechanisms; macromolecular crystallography, especially at synchrotron and free electron laser x-ray sources; spectroscopy; systems biology at the microbe-plant interface, especially symbiotic N2-fixation by rhizobia within root nodules of leguminous plants; serial micro-crystallography; oxygen activation and enzyme reactivity in solution, and in low temperature crystals; methods for poising and promoting enzyme reactions in crystals; single-crystal spectroscopy correlated with x-ray crystallography from the same sample.

Statement: I have extensive experience in characterizing the structure-function relationships for many metalloproteins and flavoproteins. In particular, I developed techniques to collect (polarized) electronic absorption and (polarized) Raman spectroscopic data from single crystals during x-ray diffraction data collection at beamline X26-C of the National Synchrotron Light Source (NSLS). This yields three types of data (two spectroscopic plus x-ray crystallography) from the same sample, experimental conditions, and nearly simultaneously. The electronic absorption data (200 – 1000 nm) is collected from an approximately 18 – 100 μm diameter area of the crystal that is coincident with the x-ray beam. We also take off-resonance and resonance Raman spectroscopic data from the same 18 – 100 μm region of the crystal. Our Raman instrumentation includes 785 nm, 633 nm, 532 nm and 473 nm excitation lasers connected with optical fibers to the microprobe heads and the spectrometer. The capabilities of beamline X26-C are transitioning to NSLS-II in various forms, and include the off-line laser spectroscopy lab.

My research philosophy is to extract as much information as possible from every sample. As suggested above, we obtain a better functional understanding by correlating electronic, vibrational and atomic structures. For example, we and others often collect correlated single crystal spectroscopic data from the crystals that also yield atomic coordinates. To this end, I recently asked the PDB to host/link our spectroscopic data with the atomic coordinates to be released with our most recent paper in J. Am. Chem. Soc. We wanted the community to have access to our orientation-dependent and X-ray dose-depended spectroscopy collected from crystals held at 100 K. Unfortunately, linking spectroscopy with coordinates is not currently possible. Thus, one of my goals for the ACA and the Data, Standards and Computing Standing Committee is to help enrich the PDB archives by hosting and curating correlated datasets.

Paul Davie (Data, Standards and Computing)

Upon assuming ACA Presidency in 2016 Tom Terwiller will step down from the Data, Standards and Computing Committee. The ACA Council has named Paul Davie to complete Tom's term)

General Manager at Cambridge Crystallographic Data Centre Inc., Piscataway NJ.

Education: BA Honours, MA, Chemistry, Oxford University. MBA, Open University, UK. Post-graduate research: Surface Physics Dept, Fritz-Haber-Institut der MPG, West Berlin.

Professional Activities: Thirty years in a variety of roles in molecular modeling companies, including Chemical Design, Oxford Molecular Group. Served as European General Manager Accelrys; COO at InforSense; Founder & CEO at Secerno (database security, now Oracle); CEO at InhibOx.

Interests: Like all at the CCDC, I am passionately committed to helping chemists worldwide gain access to all the small molecule crystallographic data and derived knowledge that they need to develop understanding in their area of research. The Cambridge Structural Database has been a valuable resource for structural chemists for fifty years, and I am dedicated to maintaining universal access to the CSD for the education and research communities, while developing the CCDC's long term successful model for sustainability. Thee CCDC's newly-established operations in New Jersey, co-located with the PDB, gives us a great opportunity to build even closer ties with the crystallography community, through sponsored studentships and collaborations with US academic groups and other data suppliers.

Thank you, again, for the opportunity to serve on the Data, Standards and Computing Standing Committee. I hope to be able to help in some way during my short term.

From firehose drinker to knife juggler.

That's how I would describe my past few months as the junior fellow of the American Institute of Physics at the U.S. Department of State. The information still comes in at a frenzied pace, but my portfolio has solidified somewhat and I know better how to sort the data stream. I see what I need to know, things that I should at least be aware of, and things which I can safely ignore. New items to track certainly still appear, but the firehose has been tamed.

Once you start learning about things, however, the next step is to actually do something with that knowledge. This is what I've been starting to do in the past three months. For the most part, this includes participating in meetings, discussing issues over the phone, and briefing people. The Department of State has both written and oral cultures, the style of which scientists are not traditionally trained for. Meetings are generally not relaxed environments where everyone has a fair chance to speak. Time is limited, and people are trying to convey as much information as possible. This means you have to be ready to confidently interject a succinct message at the appropriate time. I cannot remember scientific meetings of this nature from my time in academia.

One other aspect of life here which I've found somewhat difficult to adapt to is being an "expert." In science, I feel that being an "expert" requires several years of study in the field with some demonstration that you've mastered the subject area: at least one excellent publication (or several good publications) and some conference talks. I'm sure there are people who would even laugh at this definition for being too lax, instead preferring 20 years of experience in the field and elevation to a full professorship. If so, prepare yourself for a shock:

An expert here at the Department of State is someone who sits in one of the functional bureaus.

This definition is somewhat misleading, since it completely depends on the field. If part of your portfolio deals with China, you are not going to be considered a China expert after a couple months. There are people here with 20 years of experience interacting with the Chinese government. In science, however, covering water issues for four months has made me a water expert in the eyes of many. I was introduced that way earlier this week. The surprising thing is, they were not wrong in introducing me in that way.

What is the definition of an expert, really? An expert is someone who can answer questions about a subject. Between the general overview of my portfolio items that I have in my head (and can deliver at meetings and in the corridors) and the list of contacts in other agencies and academia that I am building up, I can provide answers to people both in person (where questions are typically more general) and over email (where I have time to consult my contacts). From the point of view of the person asking the question, I know everything about the topic. Therefore, I am an expert in their eyes.

As mentioned before, once you're considered an expert, people begin to ask you to do things. It starts out with a single thing. You find yourself working on that when another task comes up that you're also asked to do. So now you're alternating attention between the two tasks. Perhaps you finish one, perhaps not, but then a third item comes in. And a fourth. And a fifth. Some tasks are finished, some get dropped and forgotten about. New tasks always come in. Instead of doing a job to your complete satisfaction, you recognize when things are "good enough". Finishing up the last 10% is not always worth delaying completion of half a dozen other things. Eventually you get into a rhythm: the movement of your arms, the flash of objects in front of your eyes, a cadence in your head around which the whole world revolves. Congratulations, you've become a juggler.

The objects you're tossing around are not always benign, however. A lot of my communication is with people outside of my team: people in other bureaus, people in other agencies, and people in other governments. There are sensitivities. There are issues and ways of phrasing things which can make life more difficult, both for you and others. This information is not written down anywhere, and it's not even known by everyone you work with. Even if it was, everyone else is just as busy as you are, so there is not always time to ask if a given phrasing in an email is correct. The objects you're juggling, therefore, are capable of cutting.

Let's be honest, though. As a new fellow, I'm not going to be given an issue which could provoke war if I phrase an email wrong. The Department is not that stupid. However, I could easily sour relations between my office and other organizations/offices/agencies upon which we depend to get projects done. So while the blades are not razor sharp, I still need to be careful with every new item tossed my way. Most are dull, but it only takes one for me to have a really bad day, and I'm never really sure which one that may be because I don't have time to test them all.

The idea of a "knife juggler" may seem overly dramatic to some readers, but I think it captures the essential: a lot of things need to be kept track of, and there is an element of excitement caused by doing a task in which a mistake can have unpleasant consequences. I can't wait to see how things change over the next few months! Hopefully I still have all my fingers.

Disclaimer: The views expressed in this article are those of the author and do not necessarily reflect the views of the U.S. Department of State or the U.S. Government.

Matthew McGrath

Further Adventures on Capitol Hill

The past 3 months have been a flurry of activity in the Senate Energy and Natural Resources (ENR) Committee! As I mentioned in the spring issue, the ENR Committee held budget hearings for the Department of Energy (DOE), Department of the Interior, and United States Forest Service (USFS) in February. It was very impressive to see the heads of these agencies defend their FY16 budget requests, and field a wide variety of questions from Senators whose states each have their own distinct priorities. As an example, Senator Franken took this opportunity to ask Chief Tidwell of the USFS about the possibility of using flammable forest waste to generate heat and electricity in communities that are adjacent to the forests. Such projects would reduce the risk of severe forest fires, while simultaneously establishing a local, reliable, and environmentally responsible source of energy for these communities.

Climate change was another prominent theme throughout the ENR Committee hearings this spring. For example, at the same hearing, I helped Senator Franken pose a question for Chief Tidwell about the impacts of climate change on the forestry industry. This is a particularly important issue for Minnesota, because many of its economically important timber species are projected to vanish from the state by the end of the century due to rising temperatures. In addition, at a later hearing on the Arctic, I helped Senator Franken highlight the feedback between oil and gas development and climate change: burning fossil fuels leads to rising temperatures and, in turn, the melting of permafrost and sea ice. As a result, we are gaining access to more oil and gas reserves in the Arctic which, if developed, will only exacerbate the impacts of climate change. Given the priorities of other members of the ENR Committee, I was pleased and very grateful that Senator Franken vocalized this side of the debate on oil and gas development!

The final major focus of the ENR Committee this spring was a series of legislative hearings, which will serve as the foundation for a broad energy bill that Chair Murkowski is planning to craft and bring to the Senate floor this fall. My role in this process has been to work with stakeholders on brainstorming ideas for legislation that will advance Senator Franken's energy priorities. Learning about the process of drafting and introducing bills has been fascinating, and it is exciting to help shape the debate on how we can best modernize and advance America's energy sectors.

For example, one of the bills I worked on for Senator Franken was S.1053, *Promoting Alternative Fueled Vehicle Fleets and Infrastructure*. The U.S. federal government is one of the largest energy consumers in the world, with vehicles and equipment accounting for over 60 percent of its energy use, and over 70 percent of its energy expenditures. S.1053 would help the federal government reduce its overall energy consumption and expenditures by allowing federal agencies to enter into energy savings performance contracts (ESPCs) for the deployment of alternative vehicle fleets and infrastructure. This financing mechanism would help the federal government avoid the large upfront cost associated with acquiring alternative fueled vehicles, and instead pay for the fleets with their energy savings over the course of many years.

A second bill in which I played a major role was S.1256, the *Advancing Grid Storage Act of 2015*. Senator Franken and I frequently discuss the fact that energy storage is the key to a resilient, efficient, clean, and cost-effective electric grid. However, as in the case of alternative fueled vehicles, one of the major barriers to the deployment of energy storage systems is the high upfront capital costs. Therefore, S.1256 would help drive the deployment of energy storage systems by establishing direct loan, technical assistance, and grant programs for states, tribes, utilities, and universities. Such systems would be designed to improve the security of emergency response infrastructure, integrate renewable energy resources onto the grid, provide ancillary services for grid management, and help meet electricity demanding during peak and nonpeak hours. In turn, such investments would strengthen the reliability and resiliency of energy infrastructure, as well as reduce greenhouse gas emissions and maximize job creation; all top priorities of Senator Franken!

The Advancing Grid Storage Act of 2015 will be considered at the final ENR legislative hearing in early June, along with 2 additional bills that are being led by Senator Franken. I look forward to reporting back in the fall on the progress of these bills, in addition to the status of Chair Murkowski's broad energy bill!

Caitlin Murphy

Contributors to this issue: Lesa Beamer, Helen Berman, Laurie Betts, Sue Byram, Chris Cahill, Karena Chapman, Mirek Cygler, Zbigniew Dauter, Paul Davie, Emil Espes, Joe Ferrara, Jim Fettinger, Frank Fronczek, Danielle Gray, Pawel Grochulski, George Lountos, Alex MacPherson, Matthew McGrath, Krystle McLaughlin, Caitlin Murphy, Allen Orville, Chiara Pastore, Virginia Pett, Dan Rabinovich, Connie Rajnak, Narasinga Rao, John Rose, Amy Sarjeant, Ned Seeman, Eddie Snell, Vivian Stojanoff, Alison Sundermier, Mark Whitener

Cover: Images provided by Laurence Marks; production by Connie Rajnak.

Jennifer Doudna – HHMI Breakthough Prize

Jennifer Doudna, Professor of Chemistry and of Molecular and Cell Biology at the University of California, Berkeley and investigator at the Howard Hughes Medical Institute, shared the 2015 Breakthrough Prize in Life Sciences with her colleague Emmanuelle Charpentier. The prize, created by tech billionaires, honors their ground breaking work on the CRISPR/Cas9 bacterial immune system, which *The New York Times* defined "one of the most monumental discoveries in biology".

CRISPR sequences, for "clustered regularly interspaced short palindromic repeats", are short repeats of DNA sequences that are found in bacterial chromosomes. They were discovered at the beginning of the 1980s, but their role remained elusive until ten years ago, when bioinformaticians recognized them as fragments of viral DNA. This suggested that they were part of a bacterial adaptive immune system, a revolutionary concept in biology. These findings piqued Jennifer's interests, and in 2007 she and her team decided to embark on the study of Cas proteins that are closely associated to CRISPR sequences.

In a groundbreaking publication that appeared in the journal *Science* in 2012 she and her collaborator Emmanuelle Charpentier then at Umeå University, characterized the CRISPR/Cas9 system, an RNA-dependent mechanism that bacteria use to fight viral invasion. When a virus attacks the cell, a small RNA is replicated from a CRISPR sequence produced during a previous invasion. This RNA, in complex with a helper RNA molecule, binds the endonuclease Cas9 and guides it to its complementary sequence on the viral DNA. The protein cuts the DNA, interrupting the viral life cycle. The implications of the CRISPR/Cas system for biomedicine derive from the remarkable fact that the RNA guide can be designed to drive Cas9 to any desired DNA sequence, including eukaryotic DNA, providing an exquisite tool for specific DNA editing. Moreover, the many available flavors of CRISPR/Cas systems offer virtually limitless genome editing possibilities. In the past few years, pharmaceutical companies specializing in CRISPR have mushroomed, racing to optimize the technique and to transform it into a precision instrument for correcting faulty human genes. It is easier and quicker than the genome-editing techniques available nowadays, and once its whole potential has been harnessed, it might be useful to cure diseases, from AIDS to cancer to genetic diseases, with unprecedented consequences for human health and for therapeutics development.

But CRISPR is only one of Jennifer's big achievements in biology. Fascinated by science from an early age, she earned her BA in chemistry from Pomona College. She then moved to Harvard University to pursue a PhD in biochemistry, under the supervision of Nobel laureate Jack W. Szostak. Here she started her journey into the RNA world, looking at small catalytic RNAs called ribozymes. Using a ribozyme as a model, she engineered an RNA that was self-replicating in a test tube, demonstrating that ribozymes could in fact be both templates and catalysts in a self-copying reaction, and thus establishing a tight link between them and appearance of early life on Earth. Eager to see how they worked at the molecular level, she headed to the University of Colorado at Boulder, to carry out her post-doctoral research in the laboratory of another Nobel laureate, Thomas R. Cech. Here she determined the first crystal structure of a ribozyme. In 1994 she started her independent work as an assistant professor at Yale University; in 1997 she became investigator of the Howard Hughes Medical Institute and in 2002 she moved to University of California at Berkeley.

In recognition of her seminal work on the biology of non-coding RNA, Doudna won several prizes: in 2000, the Alan T. Waterman Award for exceptional young researchers from the National Science Foundation; in 2001 the Eli Lilly Award for Biological Chemistry of the American Chemistry Society; in 2002 and 2003 she became fellow of the National Academy of Sciences and of the National Academy of Arts and Sciences; in 2010 she was elected to the Institute of Medicine; in 2014 she received the Lurie Prize in the Biomedical Sciences from the Foundation for the NIH. And in 2015 *TIME* magazine nominated her as one of the 100 most influential people on the planet.

Venki Ramakrishnan – Elected President of the Royal Society

In March 2015 the Council of the Royal Society confirmed Sir Venkatraman (Venki) Ramakrishnan as the new President Elect of the Society, starting on December 1, 2015. The Royal Society is a prestigious organization of the most eminent scientists in the world, and the oldest existing academy of scientists. It started around 1640 as a weekly meeting of philosophers who exchanged their ideas of the natural world as perceived through observations and experiments. The Society, however, was properly founded in 1660 by a group of twelve people who gathered at Gresham College to listen to a lecture by the Astronomy Professor Christopher Wren and who created "a College for the Promoting of Physico-Mathematicall Experimental Learning" (more information here https://royalsociety.org/about-us/history/)

Sir Venki Ramakrishnan is currently the director of the MRC Laboratory for Molecular Biology (LMB) in Cambridge, UK, and member of the Trinity College. In 2009 he shared the Nobel Prize in Chemistry with Ada Yonath and Tom Steitz, for his structural studies on the ribosome and on the mechanisms of protein translation. He started his career as a physics undergraduate, receiving a BSc from Maharaja Sayajirao University of Baroda, in Vadodara, India, and a PhD at Ohio University. However he was partially unsatisfied with his degree of choice, and felt a stronger pull towards biology. So much so that, shortly after his graduation in physics, he embarked in a second PhD course in biology, at the University of California, San Diego. After only 2 years he moved to Yale University, as a post-doctoral fellow, working with Peter Moore on ribosomes. Subsequently, he became a tenure-track researcher at Brookhaven Laboratories before becoming professor of Biochemistry at the University of Utah. In 1999 he moved to the LMB at Cambridge, where he succeeded in determining the crystal structure of the 30S ribosomal subunit of *T. Thermophilus*, an achievement that led to his Nobel award.

Chiara Pastore

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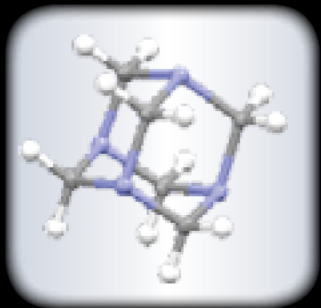

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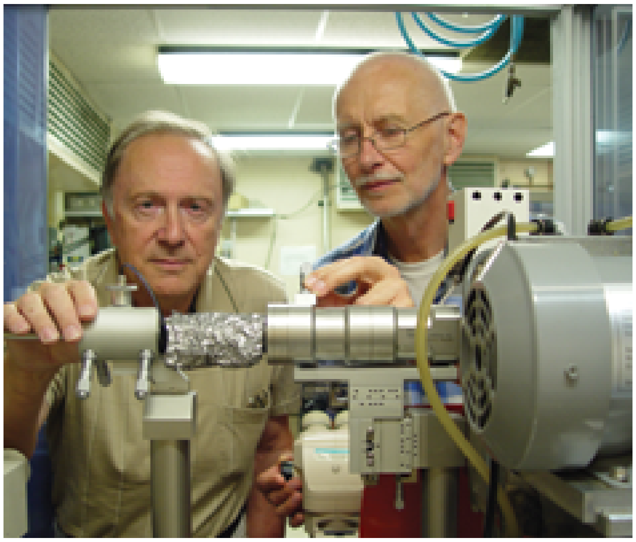
The Poland – US Science Award to Jaskolski and Wlodawer



The newly established, prestigious award established jointly by the Foundation for Polish Science (FNP) and the American Association for the Advancement of Science (AAAS) honors pairs of collaborating scientists from these two countries. The first such award went to two macromolecular crystallographers for their studies on important proteins of medical relevance, which contributed to the development of therapies combating, among others, AIDS and leukemia. The recipients, selected from more than 50 nominations, are Mariusz Jaskolski from the Adam Mickiewicz University and the Institute of Bioorganic Chemistry in Poznan, Poland and Alexander Wlodawer (seen on the left) from the National Cancer Institute, USA. Both of them are very well known in the world-wide community of structural biologists for their high-impact publications, services on various scientific bodies, and presentations at many conferences and meetings.

Their collaboration began almost 30 years ago, when Jaskolski joined the laboratory of Wlodawer at the National Cancer Institute in Frederick, Maryland and made an important contribution to the solution of crystal structures of retroviral proteases from the avian Rous sarcoma virus and from the human HIV-1 virus. This work paved the way for development of successful drugs against AIDS by several pharmaceutical companies, after only 7 years of effort. As a result, AIDS is not any more a terminal disease.

After returning to Poland Jaskolski established the first macromolecular crystallography laboratory in Central Europe, and his collaboration with Wlodawer continues to this day. Among a number of collaborative accomplishments, of note is the structure solution of asparaginase, a target in the therapy of acute lymphoblastic leukemia.

Wlodawer and Jaskolski not only collaborated on a variety of research projects, but also published jointly a number of educational and instructive papers on crystallographic methods and techniques. Together, they co-authored 37 publications which to date received more than 2,500 citations. The first FNP/AAAS prize for collaborative USA-Polish research accomplishments emphasized the importance of biocrystallography to human society. It went to a pair of highly deserving recipients.

Zbigniew Dauter

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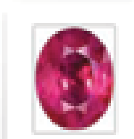

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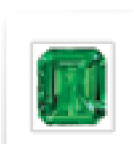

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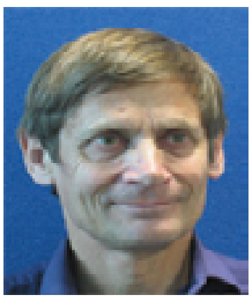
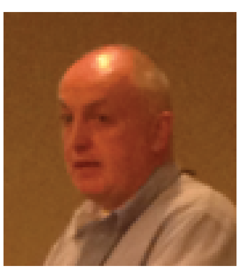
The Future of Synchrotron Based Structural Biology - Canadian Light Source - May 6, 2015.

This year the Canadian Light Source Users Meeting was dedicated to innovations in synchrotron-based science. The workshop *The future of synchrotron-based structural biology* organized by Albert Berghuis (McGill University), Pawel Grochulski (CLS) and Mirek Cygler (University of Saskatchewan) was devoted to exploring the trends in instrumentation and applications of synchrotron light in this field. Invited speakers included Colin Nave (Diamond Light Source Ltd., UK), Sean McSweeney (Brookhaven National Laboratory), Andrzej Joachimiak (Biosciences, Argonne National Laboratory, Argonne, USA), Greg L Hura (Lawrence Berkeley National Laboratory, USA), Marius Schmidt (UW-Milwaukee, Physics Department, Milwaukee, USA) and So Iwata (Riken Spring-8 Center, Graduate School of Medicine, Kyoto University).

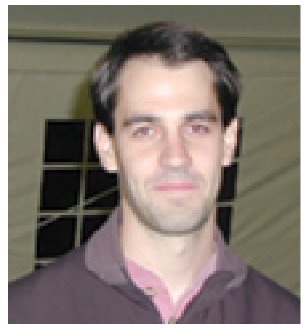


Colin Nave delivered a lecture entitled "Will Coherent Beams from a Storage Ring be Useful for Macromolecular Crystallography?" Recent proposals for decreasing the emittance of present storage rings by incorporating multi-bend achromats as well as for diffraction limited storage rings are partly based on the potential uses of coherent radiation. Crystallography requires some degree of coherence to resolve diffraction spots. Is there an advantage to using radiation which is coherent across the entire sample? The presentation described potential benefits together with initial results from recording coherent diffraction at cryo-temperatures, from polyhedral crystals of approximately 2 microns in size. Measurements provided information about crystal imperfections at the sub-micron level, and changes due to radiation damage.



Sean McSweeney presented the lecture "New light at NSLS-II: New opportunities for structural biology". He described the status and beamlines dedicated to macromolecular crystallography (MX). The FMX beamline – Frontier MX – is optimized to addressing microbeam applications. A second, called AMX – Highly Automated MX – is optimized for highly automated throughput. A third beamline for life science X-ray scattering applications, called LIX – High Brightness X-Ray Scattering for Life Sciences – will offer multiple modes of study. Once fully operational these beamlines will deliver unsurpassed flux densities.

Andrzej Joachimiak presented a lecture entitled "Targeting Inosine 5'-Monophosphate Dehydrogenase for Novel Antimicrobials". He described the application of third generation MX beamlines and Structural Genomics efforts to address rising antibiotic resistance and the urgent need for developing effective new drugs. He reported on their efforts to develop potent and specific inhibitors of inosine 5'-monophosphate dehydrogenase (IMPDH), which controls the guanosine monophosphate pool. Their structural studies showed that the new inhibitors of bacterial IMPDHs bind in a pocket that is absent in eukaryotic IMPDHs and which is part of the NAD+ cofactor binding site and which differs from NAD+ binding to eukaryotic IMPDHs and other dehydrogenases. This new NAD+ binding site involves the same pocket that is utilized by the inhibitors.



Greg L Hura presented a lecture entitled "Combining SAXS and Crystallography to build intuition in interaction networks and macromolecular engineering". He described how a fully automated SAXS beamline helps in probing the solution state under many conditions and provides information at resolutions sufficient to distinguish conformational states. Combining this information with high resolution structures significantly enhances our understanding of biological networks beyond what either a high resolution structure or informatics analysis can yield.

Marius Schmidt presented a lecture entitled "Time-Resolved Crystallography at the Synchrotron and at the X-ray FEL". Time-resolved crystallography allows extracting reaction kinetic parameters from diffraction data alone. A molecular movie of difference maps allows extracting the molecular structures of reaction intermediates as well as the temporal evolution of the associated concentrations. Powerful synchrotron beamlines such as BioCARS (APS) and XFEL make this possible. He described time-series data for the Photoactive Yellow Protein (PYP) and discussed the advantages time-resolved serial femtosecond crystallography (TR-SFX) at the XFEL. He also presented the first difference maps determined from TR-SFX at beamline CXI at the LCLS.

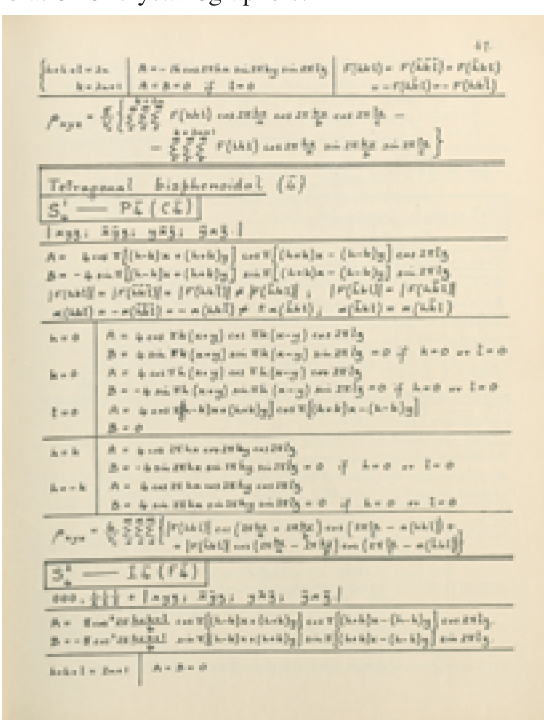
So Iwata presented a lecture entitled "Serial femtosecond crystallography at SACLA" and described recent technological advances at the Japanese XFEL facility, SACLA. Very high dose rates delivered by FEL intense femtosecond pulses allow the collection of diffraction patterns from very small crystals ("diffraction before destruction" paradigm). Single shot diffraction patterns are collected from a very large number of small crystals and combined into a complete dataset without any serious radiation damage, a data collection system is being developed focusing on membrane proteins and flexible multi-modular proteins. The system is composed of a diffraction chamber with an injector for crystals and a fast readout multiport CCD (mpCCD) detector. The sample injector is optimized for data collection from crystals in the lipidic cubic phase, used commonly for crystallization of membrane proteins. The injector handles other crystals obtained from solution by increasing viscosity with additives including gels and grease. With the use of nanometer size crystals, as little as 100 micrograms of proteins can be sufficient to collect a complete dataset. The system can dramatically accelerate the structure determination of membrane proteins.

The discussion following the presentations concentrated on the future developments at CLS. High on the priority list was the improvement of the existing beamlines and source to allow experiments with sub-micron crystals and S-SAD data collection, automatic adjustment of the beam size, high capacity and high-speed automounters. Building a dedicated fully automated SAXS beamline with remote access was also high on the list. In the longer term, a new, high brilliance source will be required to employ techniques such as room temperature data collection in a collection mode fast enough to outrun radiation damage on crystals, as well as time resolved and serial crystallography, and coherent imaging of crystals.

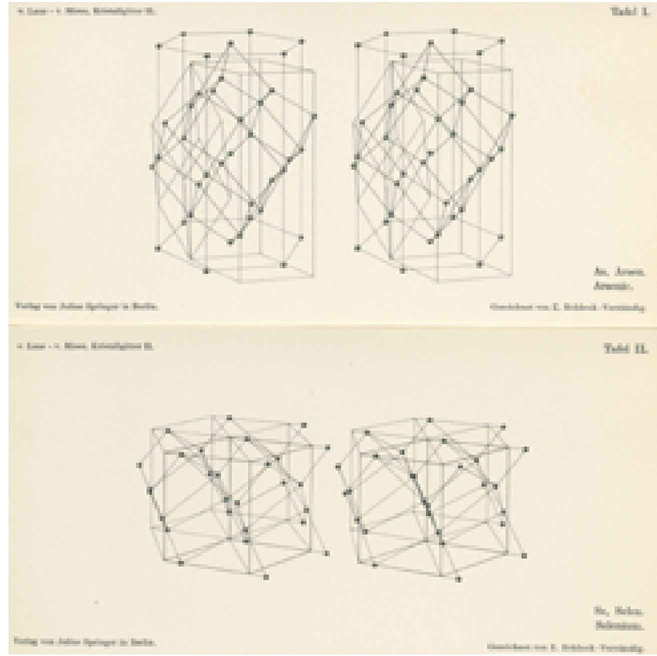
Pawel Grochulski and Mirek Cygler

Donation from the Ewald Family Expands the American Institute of Physics' Crystallography Library

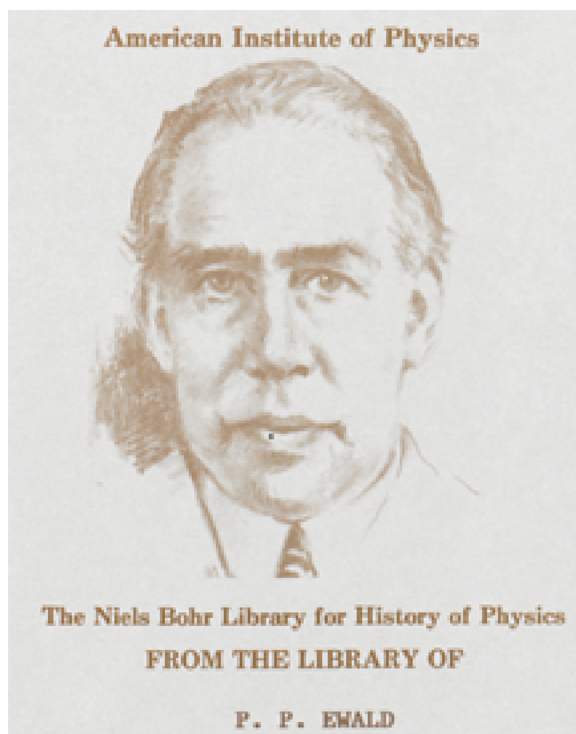
Monica Bethe is donating 47 titles from the library of her grandfather, pioneer crystallographer Paul P. Ewald, to AIP's Niels Bohr Library & Archives (***www.aip.org/history-programs/niels-bohr-library***). These titles are a substantial addition to the family's earlier book donations which are comprised of publications by Ewald himself and his contemporaries. The [first] illustration shows a page from one of the books, Kathleen Lonsdale's "*Simplified Structure Factor and Electron Density Formulae for the 230 Space Groups of Mathematical Crystallography*," published in 1936. Written entirely by hand to avoid printer's errors, the book was a standard reference for more than a generation of crystallographers.



The second is an image of stereo-cards from "*Stereoskopbilder von kristallgittern*," edited by Max von Laue, 1926-36.



We are very pleased to add these new titles to our core crystallography collection, and we welcome donations from others to build our holdings. We are interested in both historical and recent books. For information on donations, contact us at ***nbl@aip.org*** or 301 209-3177, or go to ***www.aip.org/history-programs/news/seeking-your-book-donations***.



AIP is a 501 (c) (3) organization. Donations are tax deductible, and each book receives a book plate recognizing the donor. The Niels Bohr Library & Archives is located in AIP's headquarters in College Park, MD and is open to the public Monday through Friday, 8:30 to 5:00 except for federal holidays

Joe Anderson

5th Winter School on Soft X-rays in Macromolecular Crystallography - March 1 - 5, 2015

This location was selected on the premise that the school would experience sunny days and warm nights instead of a good place to ski. The weather did not cooperate until the end of the second day which turned into a glorious winter day for Georgia.

We started with a welcome by B.C. Wang and UGA Provost Pamela Whitten. Manfred Weiss (Helmholtz-Berlin) chaired the first session and provided some historical background to the use of softer radiation in macromolecular crystallography. B.C Wang provided the theoretical basis for single wavelength anomalous diffraction (SAD) and solvent flattening as well refreshed our collective knowledge about some early SAD structures. Martha Teeter (UC Davis) told us about how she came to find crambin, and how she and Wayne Hendrickson (Columbia) solved its structure, the very first sulfur SAD structure, in 1981.

After the first coffee break James Liu (iHuman Institute) discussed the structure of obelin, the second *de novo* sulfur SAD structure, solved nearly two decades after crambin. Next Roger Durst (Bruker) talked about the Excillum liquid metal jet source and applications in crystallography. Joe Ferrara (Rigaku) presented the chromium SAD work of Cheng Yang and the iodide quick soak work of Jim Pflugrath. To close out the morning James Holton (LBNL) talked about a particularly interesting noise problem in hybrid pixel array detectors, which turns out to be due diffraction by the sensors themselves.

Meitian Wang (SLS) chaired the second session. Manfred Weiss started off with a discussion about some of the problems and solutions related to longer wavelength data collection. Armin Wager (DLS) explained how their new beamline fitted with a Pilatus 12M, cylindrical detector operating in a vacuum, was being commissioned. Naohiro Matsugaki (Photon Factory) talked about how they resolved the air absorption problem by building a helium cryostat and recirculating the helium in the enclosure with recovery of the helium for future use. The last talk was given by George Sheldrick (Göttingen) who explained about how the suite of SHELXC, SHELXD and SHELXE could be used to solve SAD structures. George also ran a workshop on the third day, described below.

After a dinner of southern treats including roast beef and hush-puppies we returned to the lecture hall for a session on detectors chaired by John Rose. Roger Durst introduced the audience to charge sharing. Joe Ferrara presented the details of a new hybrid pixel array detector from Rigaku. Clemens Schulze-Briese (Dectris) updated the audience on the latest in Swiss detector technology, EIGER. To close out the session Zhongmi Jin (SER-CAT) showed some results he had from the new Rayonix High Speed CCD detector recently installed at SER-CAT.

The second day started with James Liu chairing a session that included a talk by Meitan Wang. We learned they had fine-tuned their data strategy for low dose and high redundancy to extract the weak anomalous signal from marginal cases. John Rose followed up with a survey of SAD structures over the years from the Univ. of Pittsburgh, the University of Georgia and SER-CAT. Joe Bauman (Rutgers) told us about a magic bullet molecule with bromine or iodine that can bind to many sites to provide enhanced phasing. The morning closed with short presentations from the poster prize winners, Yen-Ting Lai (Arizona State), Joseph LaMattina (Univ. of Georgia), Charles Packianthan (Florida International Univ.) and Ryan Grumpper (Georgia State University).

Armin Wagner chaired the final session in which Wayne Hendrickson presented his latest technique: multi-crystal averaging with appropriate rejection of outlier crystals. Kamel El Omari (Wellcome Trust) provided two examples using multi-crystal averaging. B.C Wang closed the session and the technical side of the conference with a view to the future of long wavelength SAD phasing and other opportunities.

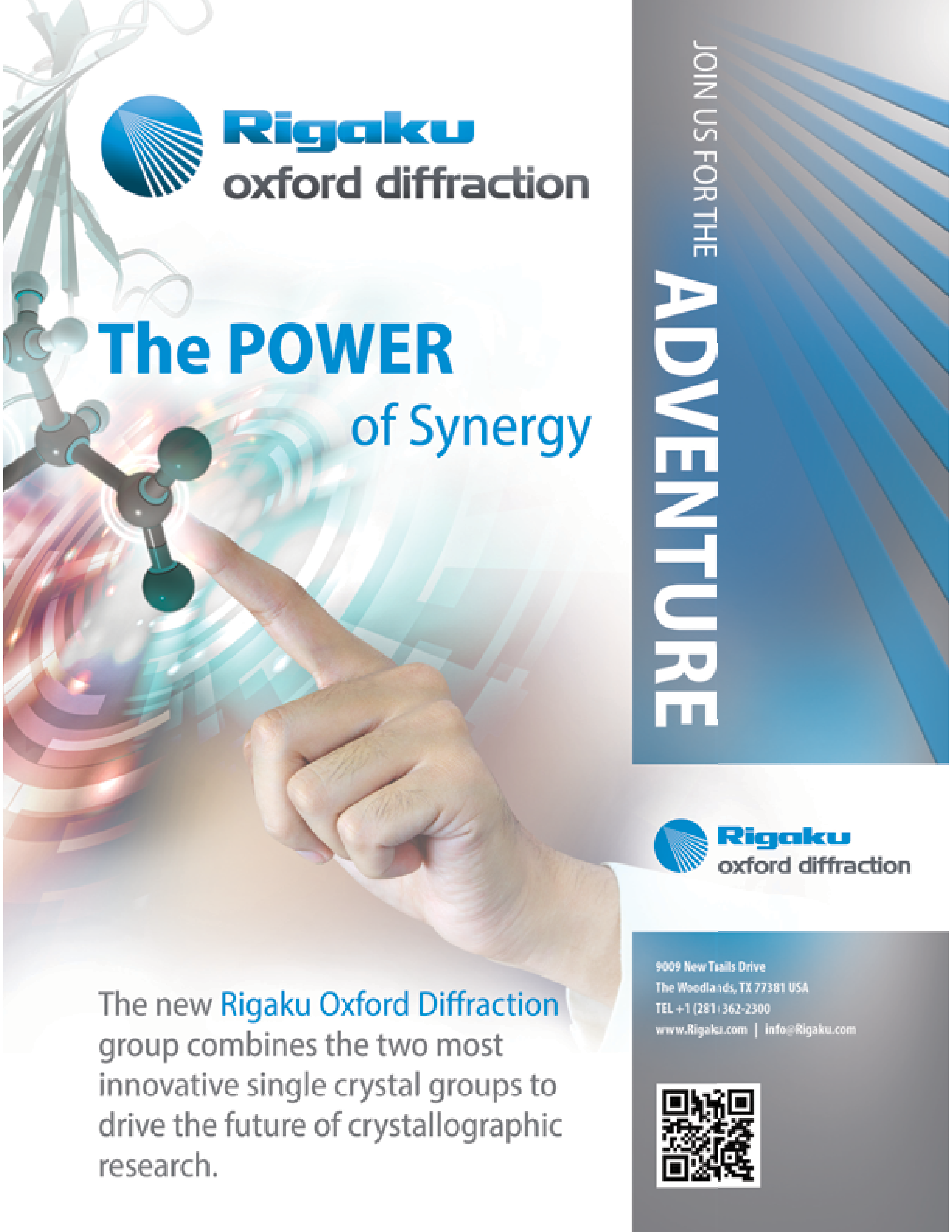
The meeting closed with dinner of southern Bar-B-Que at State Botanical Gardens of Georgia, a beautiful preserve just a few miles from UGA. Wilf Nicholls, Botanical Garden Director, gave an interesting presentation on the Gardens today and plans for future development.

Wednesday activities included a round table discussion on native-SAD and what the community can do to make it a first choice phasing method. Zhi-Jie (James) Liu then volunteered to host the 6th Winter School in Shanghai in 2018. The session ended with participants either electing to take a guided tour of Atlanta ending with a Chinese banquet or attending a series of workshops on Optimal Data Collection (John Rose), Data Reduction (Zheng-Qing (Albert) Fu) and the SHELX CDE (George Sheldrick).

The SHELX workshop was well attended. The finer points of remote crystal screening and data collection at SER-CAT were demonstrated along with data reduction techniques and strategies. After lunch George gave an outstanding demonstration/tutorial on how to use SHELX CDE to generate a starting polyalanine model and importantly how to interpret the program output.

The Winter School organizers would like to thank the following sponsors for their generous support: The Office of the Provost, University of Georgia, the IUCr, the Pittsburgh Diffraction Society, the USNCCr, Bruker AXS, Rayonix, Rigaku, Dectris, TTPlabtec and MiTgGen.

Joseph Ferrara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The 72nd Annual Pittsburgh Diffraction Conference, University of Georgia, October 26-27, 2014

The Conference began with a Sunday workshop given by **Robert B. Von Dreele** and **Brian Toby** *(*X-ray Science Division, Advanced Photon Source, Argonne National Laboratory) on *Powder Diffraction Structure Solution with GSAS-II***.** The workshop was well attended and attracted scientists from across the country. Sunday's activities concluded with an Opening Reception held in the Hill Atrium.

After opening remarks by **Bi-Cheng Wang** and **John Rose**, the Conference began with a session entitled *100 years of X-ray Diffraction* Chaired by John Rose (University of Georgia), which featured a keynote address by **Brian Matthews** (University of Oregon) entitled *From Bragg's Hometown to the MRC, Cambridge: Early Experiences in Protein Crystallography* where he gave an overview of the early days of protein crystallography and crystallography in general including many anecdotes and personal experiences. **Charles Campana** (Bruker AXS Inc) gave an overview of the technical revolution in Chemical Crystallography from 1964 to today that took the field from the hands of a few crystallographic experts to a routine tool used by chemists. **David Blum** (University of Georgia) presented a historical perspective on protein production from the days of tissue extraction to modern protein expression with synthetic cDNA constructs. **Aina E. Cohen** (Stanford Synchrotron Radiation Lightsource) brought us up to date with a report on femtosecond crystallography at the LCLS using a new goiniometer based system developed at SSRL that will improve LCLS data collection. The session concluded with a talk by **B.C. Wang** (University of Georgia) about a Pilot study he is carrying out at APS that is exploring the use of wavelength-dependent diffraction data collected at points spanning a metal's absorption edge to provide site-specific information about metal valence.

The after noon session *Structure Elucidation, Refinement and Interpretation through Powder Diffraction Crystallography* was Chaired by **Charles Lake** (Indiana University of Pennsylvania). **Brian H. Toby** (Advanced Photon Source, Argonne National Laboratory) began the session with a talk entitled *Plan B: 98 Years of Powder Diffraction Crystallography*, which presented an overview of the field and its future potential. **Robert B. Von Dreele**, (APS, Argonne National Laboratory) gave an interesting talk on the 25-year history and development of the GSAS-II package for structure solution from single crystal and powder diffraction data. **Ashfia Huq,** (Oak Ridge National Laboratory) described the use of neutron powder diffraction and the POWGEN diffractometer at the Spallation Neutron Source to study energy storage materials. **Angus P. Wilkinson** (Georgia Institute of Technology) reported on his recent studies on how pressure effects both the properties and phase transitions in NTE (Negative Thermal Expansion) materials. **Clarina R. Dela Cruz** (Oak Ridge National Laboratory) presented her powder diffraction studies on magnetism in correlated electron systems using the ORNL neutron scattering diffractometer. The session concluded with **Scott Speakmann** (PANalytical, Inc.) presenting several examples about what information can be learned from in-situ diffraction experiments together with the challenges and limitations of the technique.

The afternoon session was followed by a Poster Session in the Hill Atrium. Posters were presented by **Cassandra Hanley, Brett A. Duell** and **Charles McLouth Culbertson** (Indiana University of Pennsylvania), **Marta A. Witek, Eric Hoffer, Marc A. Schureck, Jack A. Dunkle** (Emory University), **Thomas Hartmann** (Stoe & Cie GmbH), **Joshua T. Greenfield** (University of California, Davis), **Joseph W. LaMattina**, **David L. Blum, Michelle K. Deaton** (University of Georgia), **Leighanne C. Gallington** (Georgia Institute of Technology), **John Chrzas, Zhongmin Jin** *(SER-CAT, University of Georgia)*.

Winners of the Pittsburgh Diffraction Society's Chung-Soo Yoo Award for Best Student Poster were: Undergraduate - all at Indiana University of Pennsylvania) **Cassandra Hanley**, *Using Multiple Wavelength Synchrotron Data to Identify the* Cd^{2+} *Site in* Ag_2CdGeS_4, and **Brett A. Duell,** *X-ray Diffraction Investigation of* $Na_2(Zn,Co)GeO_4$ *and* **Charles McLouth Culbertson** *Synthesis and Characterization of (Zn,Co)Te* and *Graduate -* **Joshua T. Greenfield** *(University of California, Davis) Achieving Superconductivity In Solution-Produced βFeSe* and **Marc A. Schureck** *(Emory University) Mechanism of HigB-Mediated Ribosome-Dependent mRNA Degradation*.

Tuesday's activities began with a session on *Crystallographic Education* Chaired by **Joseph Ng** (University of Alabama in Huntsville). **Cora Lind-Kovacs** (University of Toledo) presented an overview of ACA outreach activities associated with the International Year of Crystallography, which marked the 100th anniversary of the Nobel Prizes to Max von Laue (1914) and Sir William Henry and William Lawrence Bragg (1915). **Ng** also described a program he developed to engage students and teachers in learning about crystallography by preparing crystallization experiments for the International Space Station. **William L. Duax** (Hauptman Woodward Medical Research Institute) presented a program for high school students at HWMRI he designed in

Structural Bioinformatics. To date the program has trained over 200 students from 25 local schools. The session concluded

with a talk by **Claudia J. Rawn** (University of Tennessee) who described the ACA and USNNCr sponsored CWOW (Crystallography World of Wonders) workshops for science teachers aimed at encouraging them to in include crystallographic content in their lessons. A CWOW workshop kit has been developed and is available to the community.

Following the Pittsburgh Diffraction Society Business Meeting the afternoon session on *Advances in Neutron Crystallography* Chaired by **Paul Langan** (Oakridge National Laboratory) began. **Irene T. Weber** (Georgia State University) explained how she employs neutron crystallography in conjunction with atomic resolution X-ray crystallography to analyze the hydrogen atoms and their interactions in hydrogenated and perdeuterated HIV PR-inhibitor complexes. **Donald Ronning,** (University of Toledo) presented a combined x-ray/neutron diffraction study of 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase, the causative agent of stomach ulcers, which may also play a role in gastric cancer. **Alison J. Edwards** *(Australian Nuclear Science and Technology Organization)* gave an informative talk on the power of single crystal neutron diffraction with the caveat that "Critical Thinking Provides The Key To Valid Application." **Andrey Kovalevsky** *(Oak Ridge National Laboratory)* described how he uses X-ray and neutron diffraction data coupled with high-performance computing (QM and QM/MM calculations, and MD simulations) to investigate enzymes and their mechanisms important to renewable energy and chemical synthesis. **Daniel Unruh** (Texas Tech University) reported on his work related to hydrogen bonding studies of nanoconfined water in a uranyl based nanotubular materials by x-ray and neutron diffraction using the SNS TOPAZ beamline. The Conference concluded with a talk from **Mayank Aggarwal** (Oak Ridge National Laboratory) about his work using neutron diffraction to develop novel acetazolamide-based carbonic anhydrase inhibitors having fewer side effects than that of current generation inhibitors.

The conference organizers would like to thank the sponsors of the 72[nd] Pittsburgh diffraction Conference: Agilent Technologies, Art Robbins Instruments, Bruker AXS, Molecular Dimensions, Mosaic Distribution LLC, Rayonix, Rigaku and ß

NSLS: first light of its kind!

The year was 1982. Brookhaven National Laboratory (BNL) in Upton, New York was celebrating a milestone at its newest facility: the National Synchrotron Light Source (NSLS) had achieved its first light. It might sound insignificant, like a baby's first sneeze or the first time a pair of newlyweds bought a couch together. But this was a moment that scientists had been building toward for over four years. Batches of electrons rushed through the accelerator at almost the speed of light. Gigantic magnets bent the path of these electrons into a circle, forcing them to lose energy in the form of x rays. Beam lines directed these x-rays into a detector, towards a brighter future with more science and stuff. Bottles popped, confetti rippled, crowds roared.

Remembering the NSLS, on its last day of operation September 30, 2014, J. Hastings (LCLS, former NSLS R&D group leader, far right) and the "golden boys". The support provided by A. Lenhard, R. Greene, G. Nintzel, M. Caruso and D. Carlson (absent S. Cheung) through the years to the researcher community has been invaluable.

"It was a whole different world back then," said Richard Greene, a technician who helped to build some of the first beam lines at the NSLS. "We always cracked a bottle of champagne for every beam line."

Before the development of dedicated synchrotron light sources in the '60s, synchrotron radiation was seen as a nuisance in the scientific community. At that time particle accelerators were primarily used to study collisions between certain particles, and synchrotron radiation caused an undesired loss of energy. When scientists realized that they could use this radiation to do different experiments, they began extracting the radiation and using it to study problems in biology, chemistry, material and environment sciences you name it!

"The principle of a synchrotron is that when electrons go around a bend, they lose energy in the form of synchrotron light, which is basically high-powered x rays," said Robert Rainer, who started as a floor coordinator at NSLS and moved on to be one of the lead operators at the NSLS-II. "Those are the x rays that people came here to use at the NSLS, and that they will be using early this summer at NSLS II."

There are three main types of experiments performed at synchrotron light sources: diffraction, microscopy and spectroscopy. Topics ranging from the proteins in your body, to the soil you walk on, to the batteries in your phone and the chips in your computer are being explored at these facilities.

A key feature of synchrotron storage rings like the NSLS is a special periodic arrangement of magnets called a Chasman-Green Lattice. Proposed by BNL physicists, Renate Chasman and George Kenneth Green, in the mid '70's, - the Chasman-Green lattice (CG) was fundamental to the development of dedicated synchrotron sources. Designed specifically to enable dedicated synchrotron light sources, the CG lattice is meant to bend and focus an electron beam in the storage ring. Because of its design electrons circulate in this lattice with very low emittance, and the synchrotron light produced is incredibly bright.

"The one thing that always occurs to me immediately with respect to the significance of NSLS at the beginning is the story of Renate Chasman" said Bruce Ravel, a National Institute of Standards and Technology (NIST) physicist. "If we only judged work on its significance, Renate would be completely amazing - the Chasman-Green lattice remained the standard until very recently and NSLS-II in itself is a CG lattice. Of course we live in the real world and in the real world, there just weren't many female accelerator physicists in the late 70s. For me, that puts her in a category that includes mid-century scientists like Rosalind Franklin - a real ground-breaker."

Both Chasman and Green died shortly before their lattice was put to use, for the very first time, in the NSLS. Their work was continued by Samuel Krinsky, who had joined the group in 1976. Sam lead the NSLS accelerator physics group and served on several occasions as interim chair of the Facility. Sadly, Sam, who had been managing the accelerator physics group within the Photon Sciences Directorate since 2008, died shortly before his team achieved a stored current of 50 mA at NSLS II, with a newly installed superconducting radio-frequency cavity in July 2014.

Since its early days it was clear that the NSLS was a game changer. Peter Stefan, a physicist who started working at the facility in 1984 recalls:

"When I first arrived at NSLS, commissioning of the x-ray ring was underway," Stefan said. "We quickly learned something significant about the beam: it carries some real power."

Stefan, who currently works at the SLAC National Accelerator Laboratory, Linac Coherent Light Source (LCLS), explained that many significant technological developments were made at the NSLS in its lifetime. Among these developments, there were small-gap and in-vacuum undulators, which made their appearance in the special X-Ray Ring straight sections. These upgrades, Stefan said, brought about the realization that a missteered electron beam could have the SR beam burn through the storage-ring chamber in milliseconds, and so scientists developed high-speed logarithmic amplifiers on electron beam position monitors so that the orbit could be known over the full range of beam current. They also developed fast radio frequency (RF) trip systems, which enabled a sudden bad orbit to dump the beam before damage could occur.

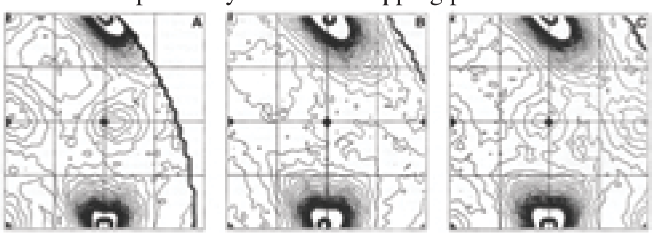
"Such protection systems have been implemented everywhere since then," Stefan said.

Gene Ice (Oak Ridge National Laboratory, ORNL) explained that, "Electron beams of unprecedented low emittance, and consequently much better brilliance than previous sources, together with the outstanding beam stability and specially-built first-of-their-kind beam lines of the NSLS allowed for crystallography that had previously been possible at only a proof-of-principle level or totally impractical on earlier synchrotron radiation sources." Examples included, anomalous diffraction, surface diffraction, and microbeam diffraction. A great example of early surface diffraction experiments was the studies on X15, which helped pioneer truncation rod scattering.

Ice, a former member of the X14A PRT, one of the very first beam lines on the NSLS experimental floor, remembers that they brought the beamline pre-assembled on rails on the back of a truck.

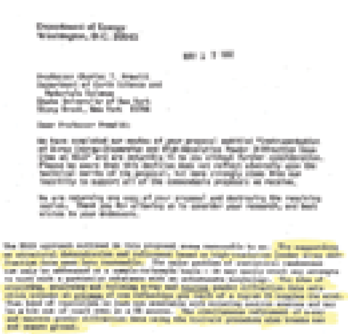
"We arrived (from Oak Ridge) on a Friday but did not get fully unloaded ... The riggers left the forklifts behind so we finished unloading (the truck) and assembled it (the beam line) over the weekend," Ice said.

Together with X14, the X13 beam lines constituted the first core beam lines dedicated to crystallography. Designed with very revolutionary dynamically-bent sagittal-crystal focusing optics, X14 was specially built for diffuse anomalous diffraction experiments and served to explore a number of new scientific directions such as anomalous powder diffraction, tomographic imaging, quasi crystals, x-ray fluorescence holography ... X14 evolved into a workhorse beam line for studies of battery materials, transportation alloys and other materials where anomalous diffraction, high-resolution diffraction and/or high-intensity could be used to help identify minor overlapping phases.

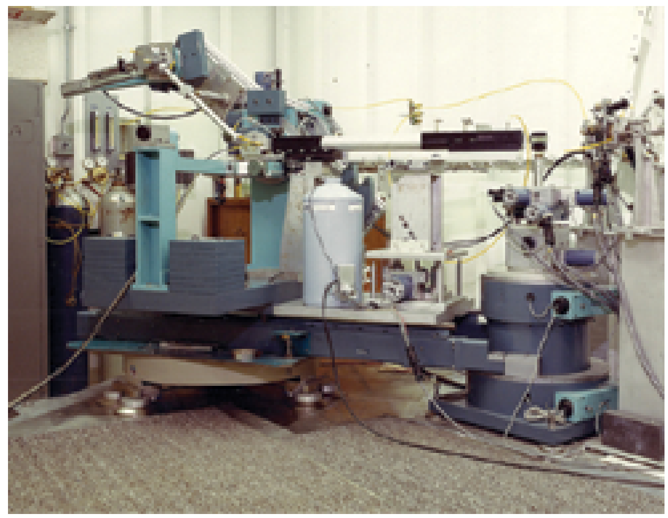


One of the first diffuse scattering maps from a single crystals of a nickel-80, iron-20 alloy from X14, the Oak Ridge National Laboratory (ORNL). ***www.iaea.org/inis/collection/NCLCollectionStore/_Public/19/036/19036488.pdf***

The X13 beam lines were dedicated to structural crystallography and were later moved to X7 station. X13 A was specifically designed for powder diffraction, and X13 B was dedicated to single-crystal diffraction. The team proposing X13A was a typical PRT formed by members from the University community and BNL (T. Egami, University of Pittsburgh, and C. T. Prewitt, SUNY Stony Brook, and with David Cox, BNL Physics, as spokesperson). They proposed to the Department of Energy (DOE) a powder diffraction beam line that used energy-dispersive solid-state detectors, along with high resolution, energy-dispersive crystal analyzers and high-resolution, angle-dispersive monochromators, to study the structure of disordered materials, phase transformations, kinetics and structure at high pressure and the crystal structure of inorganic solids. David Cox remembers that the initial proposal



was returned without being considered for funding since most of the project was considered of high risk. However members of the PRT persisted (D. Cox, J. Hastings and W. Thomlinson) performing a series of experiments at CHESS (Cox, Hastings, Thomlinson and Prewitt (NIM, 1983); Hastings, Thomlinson and Cox, J. Appl. Cryst. 1984) to demonstrate the feasibility of the techniques. Subsequently, a high-resolution powder diffraction beam line was commissioned on the X13A port in 1984. This pioneering initiative attracted several companies such as DuPont, Geophysical Lab, CIW, Union Carbide Allied Chemical and later Mobil. The rest is history.



X13B was developed by the BNL Chemistry Department for crystallographic research and started operation in May 1985 with Åcke Kvick (Maxlab Lund, Sweden) as spokesperson. In the early '90's Åcke moved to the European Synchrotron Radiation Facility (ESRF, Grenoble, France). The experimental station included a 6-circle diffractometer and an oscillation camera for data collection on film. The optical components included a double-crystal Si monochromator and Rh coated horizontal focusing mirror. Early protein crystallography experiments with unfocused radiation included the collection of partial oscillation data for the proteins metallothionein, aconitase and ferredoxin in collaboration with Drs. C. D. Stout and A. Robbins (University of Pittsburgh) and W. Dytrych (University of Chicago). In fact the first complete data collection on a protein crystal at the NSLS was performed on the b2 component of the iron containing protein ribonucleotide reductase out to a resolution of 3 A in collaboration with P. Nordlund and his group from the Agricultural University of Sweden (***www.iaea.org/inis/collection/NCLCollectionStore/_Public/17/065/17065212.pdf,*** p 228). The group published the structure later in Nature (*Nature* 345, 593 - 598 (14 June 1990); doi:10.1038/345593a0) to 2.8 Å resolution. However, the first reference in the RCSB to a structure determined at the NSLS was that of the regulatory domain of scallop myosin at 2.8 Å resolution by Cohen's Group on X12C (*Nature* 368, 306-312 (24 March 1994); PubMed: 8127365; DOI: 10.1038/368306a0; PDB 1SCM). In addition to the protein crystallography experiments, X13 B was used for a broad range of chemical crystllogrphy investigations as well.

The X12 B and C beam lines of the former BNL Biology Department were initially commissioned by Benno Schoenberg

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(now at Los Alamos National Laboratory), to the NSLS, where J. Hastings (now at SLAC Linac Coherent Light Source, LCLS) and W. Thomlinson (now at Canadian Light Source, CLS) designed and commissioned the optics. R. Sweet built and commissioned the end-station with an Arndt-Wonacott Rotation Camera (Apple-IIc), that he brought from UCLA. For several years the only way to collect data was on film. Always supporting the use of electronic detectors, the X12 Biology Department beam lines, through Sweet, became a natural place for prototype testing or to be one of the first beam lines to own a newly developed detector. The addition of an electronic detector to X12 C and later a cryogenic system to cool the crystals was a real boost to the structural biology program at the NSLS. The small-angle scattering program, on X12 B, was developed by Malcom Capel (now at APS-NECAT), who had joined the biology group in 1985; however by the late '90's the high demand for single-crystal macromolecular crystallography had taken over most of the beam time available on X12 B.

"The X4 beam lines started rather late" recalls Wayne Hendrickson (Columbia University), spokesperson for the Howard Hughes Medical Institute (HHMI) PRT. "The program rose HHMI decided to invest in the work we were doing at Columbia University and I proposed at that time they were talking to me that what we really should do is to build a beam line at a synchrotron to take advantage of the advances that were happening. ... The program really took off when Craig Ogata (now at APS) joined us and with a lot of help from Howard Hughes people. Together we celebrated our first successful experiments in 1992."

The X4 beam lines were specially designed for multiple anomalous diffraction (MAD) experiments. X4A was designed to cover a very broad energy range … "essentially from the Uranium M edge to the Uranium K edge" explained Hendrickson. Using a sagittal focusing monochromator and toroidal mirror this was the beam line for MAD phasing!

Macromolecular Crystallography (MX) exploded at the NSLS in the late '90's. With the advent of reliable cryosystems and better detectors, and further supported by increased funding, the number of PRTs and structural biology beam lines increased to a total of 10 beam lines at the NSLS. Cold Spring Harbor, Los Alamos and NCI partnered with the recently created Protein Crystallography Research Resource (PXRR) to manage several beam lines dedicated to MX. The development of a macromolecular program on insertion-device beam lines by Lonny Berman, Robert Sweet (NSLS II) and the late Paul Sigler (Yale University) on X25 enabled research programs such as those pursued by Mackinnon's group and the groups of Ramakrishnan and Steitz. Anomalous sulfur signal was explored by Z. Dauter (NCI) on the X9 beam line and more recently by Q. Liu on X4. Two new crystallography beam lines were built in the early 2000's: one, X6A on a bending magnet, was built solely by the NSLS with support from the NIGMS, while the second, X29, was built as a partnership between the PXRR, NSLS and Case Western Reserve. This investment contributed to roughly to 1/3 of the user population and approximately 1/3 of the publications.

"Many people, students, post-doctoral and visiting researchers, of various cultural backgrounds, came to the NSLS attracted by the intellectual environment ...," said Chi-Chang Kao (SLAC). He himself joined the NSLS as a post-doctoral fellow in 1988 attracted by the vibrant scientific community.

According to Barry Karlin (NIST), who arrived at the NSLS in 1983 , " ... many graduate students came to be famous scientists ..."

Several courses and workshops promoted at the NSLS took on their own identities and were adopted, modified and perfected at other facilities ... like the "Rapid Data" workshop initiated by Robert Sweet (NSLS II). Others dedicated to several subjects relevant to special interest groups were organized and highly attended by the community, like the Absorption Spectroscopy workshops organized by Bruce Ravel, Anatoly Frenekel, Simon Bare and Syed Khalid or the Crystallization focus on: ... by Vivian Stojanoff. These courses brought large numbers of graduate students, post-doctoral fellows and scientists together: for many it was their first visit to the NSLS. Smaller workshops like the X6A workbench targeting smaller groups provided a more basic view on MX data collection, along with molecular structure determination, and were further extended to other methods such as with the X9 Small Angle Scattering workshop.

The NSLS had a very dynamic user community and will always have a special place in the memory of those who did their first synchrotron experiments there. The Friday lunch seminars established by Dennis McWhan (NSLS chair 1990-1995; Associate BNL Director 1995-2000) brought the community together. He used to tour the experimental floor on Thursday nights asking users about their experiments and inviting two groups to present their latest results hot of the press! It was a great way to exchange ideas and initiate multidisciplinary research … but the highlight were the cookies and cakes provided by Carolyn McWhan, Denis wife.

But synchrotron science entered a new era and BNL began phasing out the NSLS in the late 2000's, for a bigger and brighter facility: the NSLS-II. The NSLS-II, which celebrated its own first light in October 2014, is currently considered one of the world's most advanced synchrotrons, producing x rays up to 10,000 times brighter than the NSLS. The new facility is almost half a mile in circumference–nearly five times the circumference of the NSLS. And while the concept of synchrotrons–bunches of electrons propelled by magnets traveling around and around in giant circles–might seem abstract, the consequences of the research done at these sorts of facilities is monumental, affecting everything from technology to human health.

According to Timur Shaftan, an accelerator physicist at NSLS-II, in the early 2000s scientists came to the realization that the NSLS was becoming too old—other machines were providing brighter and more intense x-rays to enable more exciting experiments. So scientists decided to construct a new light source, the NSLS-II, which would support beamlines equipped in a much better way.

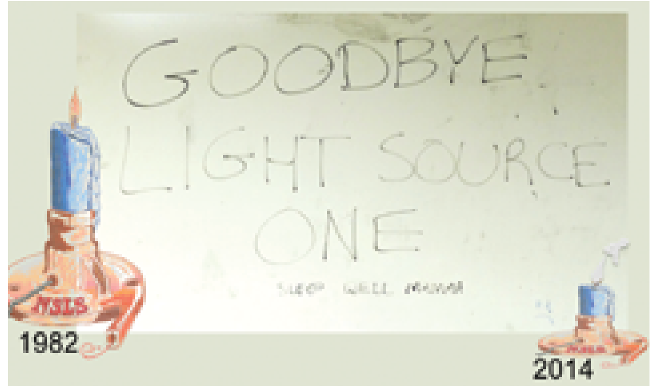
"It's a different level of science now," Shaftan said. "Once you have a better source of light you can see much clearer, you can see many more details and have a look at those phenomena that nature hid for us."

Peter Siddons (NSLS-II) has been working at the NSLS since 1985. He was involved in many of the "firsts" devising new

experiments and new detectors. One of the detectors developed by his group, the Maia x ray fluorescence microprobe detector, allows for very fast elemental mapping. High-resolution elemental maps obtained with this detector provided conclusive evidence (*Journal of Physics: Conference Series,* 499, 012001 (2014) (doi:10.1088/1742-6596/499/1/012001*)* that the painting known as "Old Man with a Beard" was by Rembrandt. Siddons explained that the new synchrotron makes a lot of new things possible. One of these is the spatial resolution ... "At the NSLS, scientists could focus the x-ray beam into a 10 micrometer spot. At the NSLS-II, scientists are hoping to focus it down to one nanometer".

"The job of this group is to come up with bigger and better detectors to suit the increased capability of the NSLS-II," he said. This will allow scientists to study a broader range of samples like minerals, rocks, machinery, biological samples and disease tissues.

The NSLS will always keep its place in history as a landmark in synchrotron radiation. It has been 32 years of successful science and technology. It was a pioneering accelerator that produced world-class science, contributing to two Nobel prizes and had many illustrious visitors, including Rembrandt. It contributed significantly to workforce training and technology development having attracted a number of industries. From whatever angle one may choose to look at the NSLS, its contributions to science, technology and educationare undeniable. Historians one day will refer to the NSLS as the accelerator where everything began, shepherded by an enthusiastic team of scientists and engineers who set out to explore new possibilities.



"One thing that really stands out in my mind is the astonishing number of methods that were pioneered in part or completely at NSLS," Ravel said. "Coherent scattering, non-resonant inelastic scattering, infrared spectroscopy, ... Virtually everything we do today at synchrotrons anywhere-including a huge number of things we associate with 3rd generation source-can be traced back to the NSLS."

Alison Sundermier and Vivian Stojanoff

Acknowledgement : We wish to thank all those who contributed to this note and especially D. Cox, R. Greene, W. Hendrickson, G. Ice, C-. C. Kao, C. Ogata, R. Rainer, B. Ravel, T. Shaftan, P. Siddons, P. Stefan, and R. Sweet for sharing their thoughts and notes with us.

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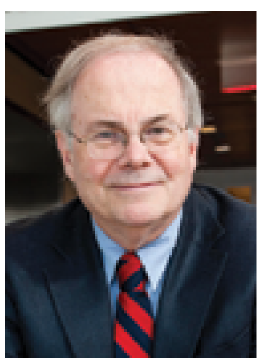
Buerger Award in honor of Greg Petsko
Etter Early Career Award in honor of Jan (Jessie) Zhang

Laurence Marks
Warren Award



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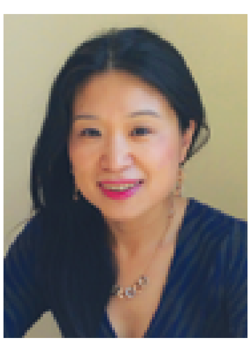
Buerger Award



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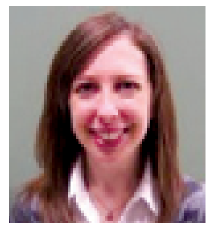

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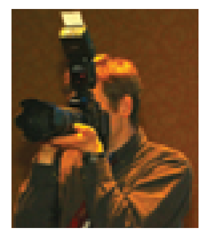

Poster Chair
Ilia Guzei
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Photographer
Peter Müller
pmueller@mit.edu

Workshops

Intro to Modeling High-Pressure Single-Crystal Diffraction Data
Organizers: Elinor Spencer, Nancy Ross, Carla Slebodnick

Serial Crystallographic Data Analysis with Cheetah & CrystFEL
Organizers: Nadia Zatsepin, Tom Grant, Eddie Snell, Cornelius Gati

Rietveld Refinement Analysis
Organizers: Clarina Dela Cruz, Oliver Gourdon

SAS: Structural Biology & Soft Matter
Organizer: Richard Gillian

Transactions Symposium

Crystallography for Sustainability
Organizers: Cora Lind-Kovacs & Robin Rogers

Evening Sessions

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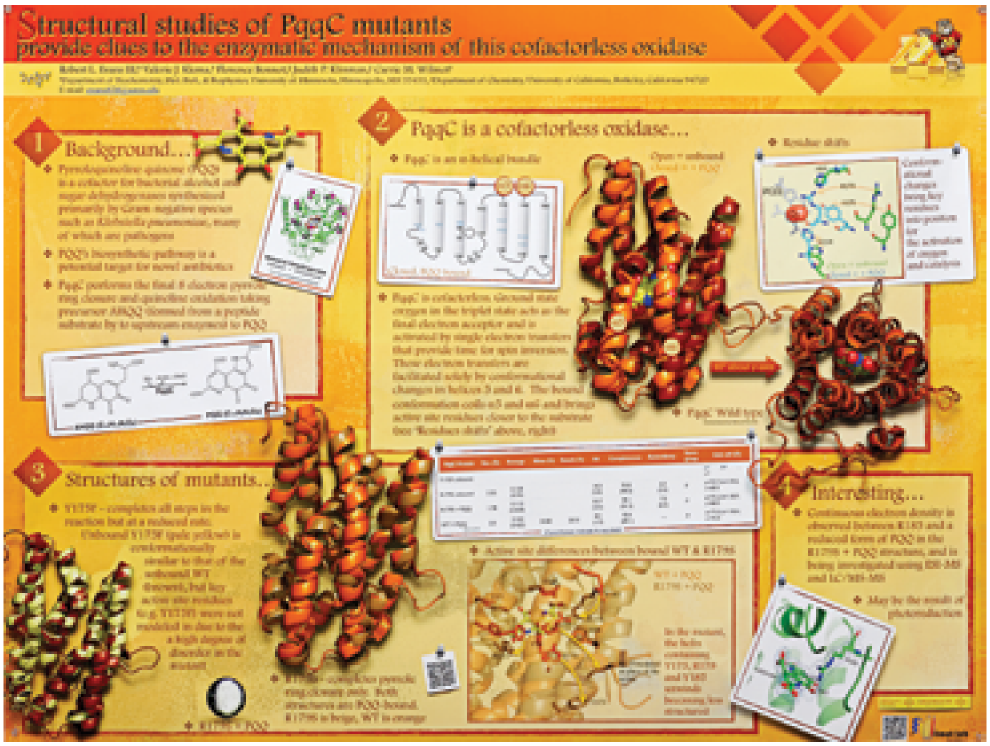
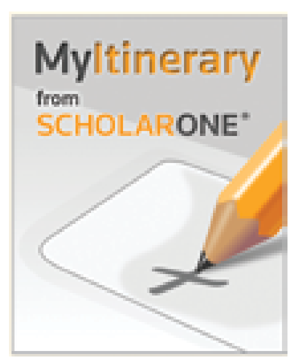


Poster by Robert Evans, receipent of 2014 IUCr Poster Prize
Albuquerque, New Mexico ACA meeting

Planning your Schedule



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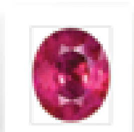

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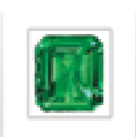

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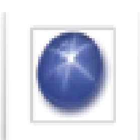

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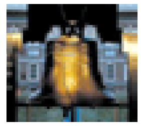

25-29 **ACA 2015 Annual Meeting**. Philadelphia, PA, Sheraton Philadelphia Downtown. Program Chairs: Kraig Wheeler & Louise Dawe. ***www.AmerCrystalAssn.org***

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3-7 **64th Annual Denver X-Ray Conference (DXC2015)**, Westminster, CO. ***www.dxcidd.com***

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4-18 **XLIV Congress of the Italian Crystallographic Association.** Vercelli, Italy. ***www.cristallografia.org/congresso2015***

6-18 **14th Oxford School on Neutron Scattering,** Oxford, UK. ***www.coxfordneutronschool.org***

7-9 **Design and Engineering of Neutron Instruments.** Budapet, Hungary. ***www.bnc.hu/denim2015***

7-10 **VI International Conference on Synchrotron Radiation in Polymer Science.** Madrid, Spain. ***www.srps6.com***

14-18 **23rd International Congress on X-ray Optics and Microanalysis (ICXOm23).** BNL, Upton, NY. ***www.bnl.gov/icxom23***

23-28 **FEL 2015 - 37th International Free Electron Laser Conference.** Daejeon, Korea. ***fel2015.tjlink.co.kr/ab-844***

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DECEMBER 2015

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

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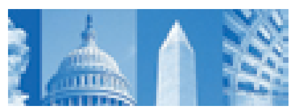

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