ACA RefleXions

American Crystallographic Association
Structure Matters

Number 1

Spring 2016

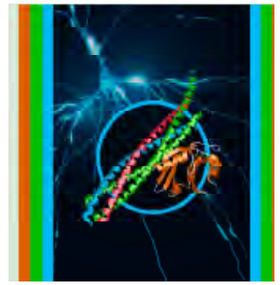
Trueblood Award at Denver ACA Meeting

ACA RefleXions

ACA – Structure Matters
www.AmerCrystalAssn.org

Table of Contents

Tom Terwilliger
ACA President



What's on the Cover
Page 8

Jason Benedict
Etter Early Career Award

Elspeth Garman
Fankuchen Award

To Be Honored in Denver

Benno Schoenborn
Bau Award

Axel Brunger
Trueblood Award

Winnie Wong-Ng

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President's Column

Tom Terwilliger

I hope you are getting ready for the ACA Annual Meeting and are telling your friends about it! The conference will be held in Denver from July 22-26, 2016, and it is going to be a terrific scientific and networking meeting. There will be a wonderful variety of sessions ranging from a *Transactions Symposium* on structural dynamics of chemical, biological, and solid systems, to methods for macromolecular structure determination, new sources and instrumentation, to supramolecular chemistry, and much more! You can see the full ACA meeting schedule on the meeting web site at ***http://www.amercrystalassn.org/2016-meeting-homepage*** and you can follow the meeting on Facebook (***www.facebook.com/AmerCrystalAssn/***) Twitter (***twitter.com/ACAxtal***) and Instagram (***www.instagram.com/acaxtal/***) with the hashtag ***#ACADenver***!

Each day of the ACA meeting will feature a keynote lecture from one of this year's superb award winners. These will include the Etter Early Career Award lecture by Jason Benedict of SUNY Buffalo, the Trueblood lecture by Axel Brunger of Stanford University, the Fankuchen lecture by Elspeth Garman of the University of Oxford, and the Bau lecture by Benno Schoenborn of Los Alamos National Laboratory.

For networking, in the late afternoons there will be poster sessions and concurrent socials alongside the vendor exposition, with many sponsors, vendors and organizations available to present their newest offerings and capabilities. Additionally there will be evening sessions including a networking mixer, a career-development panel, a diversity and inclusion discussion session and the famous *Would You Publish This?* session.

The meeting will continue the tradition of a strong educational component, with workshops on the Friday before the opening ceremony on SHELX, serial crystallography data analysis, small-angle scattering analysis for biological macromolecules, magnetic structure analysis with neutrons, and on the CSD Python API. In addition, sessions throughout the meeting will be including talks designed to introduce complex and emergent research areas.

The ACA is busy with many other activities in addition to the annual meeting in Denver. Here are a few of them!

After much discussion in the macromolecular field, the ACA initiated an effort to provide reviewers of structural papers with the evidence for presence of ligands. This led to agreement among the IUCr, the ACA, the ECA, and the AsCA that this was an important concept. With this uniform support, the PDB took up the issue and held a workshop on ligand validation this past July, followed by a meeting of the PDB X-ray Validation Task Force where this was a major item for discussion. All this should lead to pictures of ligand density in your future PDB Validation reports and better structures in the Protein Data Bank!

The ACA has been very supportive of outreach efforts that bring crystallography to students. Some of the most successful of these are the wonderful crystal-growing contests that have been held. You can see the first Wisconsin crystal growing contest at ***http://amercrystalassn.org/documents//newsletter-highlights-2015/WisconsinCrystal2015.pdf*** and the U.S. crystal growing contest at ***http://amercrystalassn.org/documents//newsletter-highlights-2015/USCrystalGrowing-Contest2015.pdf***

If you haven't already, take a look at the comprehensive History section of the ACA web site (***http://www.amercrystalassn.org/history_home***). It has wonderful memoirs from a variety of ACA members past and present, videos, and ACA beginnings, as well as a section on Nobel Prize winners in crystallography.

I'll be looking forward to seeing you in Denver and hearing from you any time!

All the best,

Tom T

Tom Terwilliger (***terwilliger@lanl.gov***)

News from Canada

Michael James

In this issue of *RefleXions*, I will be highlighting the work of two Canadian crystallographers in research and in education. These two, Jim Britten from McMaster University and Louise Dawe from Wilfrid Laurier University, are very committed people who have advanced not only their research into the structures of small molecules, but also have dedicated their time and energy to advance the teaching of the science of crystallography.

Jim Britten

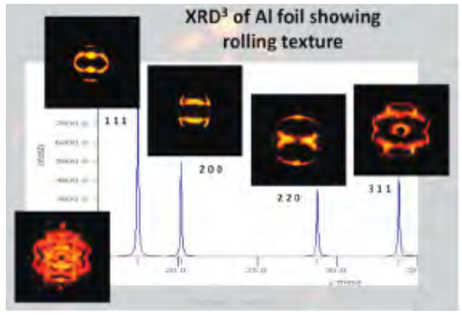
Jim Britten received his B.Sc. in Honours Chemistry from St. Francis Xavier University, Antigonish, Nova Scotia. He then went west to Hamilton, Ontario where he earned a Ph.D. degree in Inorganic Chemistry under the guidance of Colin Lock in the Chemistry Department at McMaster University. Jim's thesis concentrated on the chemistry and crystallography of platinum complexes. He held two postdoctoral positions following the receipt of his Ph.D. The first of these was with Andre Beauchamp at the Université de Montreal and the second was in the Chemistry Department of Dalhousie University, Halifax where Jim worked with Rod Wasylishen. During these postdoctoral years, he became proficient in multinuclear NMR as well as in single crystal X-ray crystallography. Jim's first 'job' was in the Chemistry Department at McGill University where he set up and managed the McGill X-ray Facility. In addition to providing service work for the McGill Chemistry Faculty, he taught the elements of X-ray crystallography as well as working closely with Eric Gabe in the

National Research Council of Canada on software development.

In 1991 Jim moved back to Hamilton to initiate the McMaster X-ray Facility in the Chemistry Department. In addition to providing crystal structures for the McMaster Faculty, this position has a major teaching component for Introductory Crystallography (at the graduate student level). Since 2009, Jim has been Manager and Scientific Director of the McMaster Analytical X-ray (MAX) Diffraction Facility. He has also been a major force behind the design, construction and operation of the Brockhouse Scattering and Diffraction Sector at the Canadian Light Source (CLS) Synchrotron Facility in Saskatoon. The Brockhouse Sector at the CLS is named after McMaster physicist Bertram Brockhouse, who was awarded a Nobel Prize in Physics in 1994 for his work on neutron scattering at the NRU reactor in Chalk River, Ontario.

Jim provides his crystallographic expertise to the academic faculty at McMaster and guides the students and postdoctoral fellows in the Departments of Chemistry, Physics and Chemical Biology. Not only does he assist in the practical aspects of crystal structure determination, but he also assists in the writing of manuscripts that depend largely on the results of the structural work. It is the wide range of topics and materials that makes Jim's work 'fun.' Whether he is examining the diffraction from a quasicrystal or from an incommensurate scatterer or from a protein he is constantly challenged and maintains a high personal interest in the project. Even though he is not the principal investigator, it is his knowledge and understanding of diffraction techniques that get the papers published in high-impact journals such as *Science*. Jim is happy to work closely with his colleagues in MAX and the graduate students who will be primary author on these papers. He knows that many of the publications would not have been possible without his crystallographic input to the research.

'Service' crystallography is not the only area of science in which Jim is a major contributor. Together with his colleague Weiguang Gang, he is developing software (MAX 3D) that will aid in the visualization of diffraction effects from polycrystalline solids and thin films. MAX 3D produces images that aid in the identification of diffuse scattering. Using the software, engineers will be able to employ the X-ray patterns coming from polycrystalline solids and thin films to gain an improved understanding of the texture of materials. An example of 3D spherical sections of a diffraction pattern and the resulting pole figures is shown below.



Jim's contributions to our understanding of materials extend into the realm of biochemistry. Recently he has co-authored two papers describing the effects and the structures of metal chelators of Fe^{2+} and Zn^{2+}. Both studies are associated with the development of transition-metal chelators that are bactericidal via two different mechanisms. The Fe^{2+} chelator disturbs the iron homeostasis in the bacterium and has a direct antibacterial effect, whereas the Zn^{2+} chelator acts to remove the Zn^{2+} ion from the metallo-β-lactamases thereby rendering the carbapenem antibiotics as effective antibacterials. Jim's contribution to these studies was to define precisely the 3D structures of the Fe^{2+} and Zn^{2+} complexes of the spiro-indoline-thiadiazoles that had been discovered by high-throughput screens of large chemical databases by the group headed by Eric Brown at McMaster.

In addition to his research in the many areas of material science, Jim has rendered outstanding service to the crystallographic community of Canada. Jim was President of the Canadian National Committee for Crystallography (CNCC) for more than 10 years. He served as Chair of the International Program Committee for the 2014 IUCr Congress held in August of that year in Montreal, Canada. Anyone who attended this meeting was duly impressed at the organization and the running of the conference. It was excellent. In addition to this public service, Jim is the Founder and Organizer of the Annual Canadian Chemical Crystallography Workshop that runs for 4-5 days and is associated with the annual meeting of the Chemical Society of Canada. These are extremely popular workshops that are pitched at the graduate student and postdoctoral levels to those in chemistry departments who would like to enhance their knowledge of X-ray crystallography. Many are sufficiently excited by these workshops that they are able to carry out their own structure determinations. Jim has also served on many committees and groups within the ACA. He was Program Chair for the ACA meeting in Toronto in August 2009. He served on Council of the ACA from 2008-2010 and as Chair of the Canadian Division of the ACA (2003-2006). It is public-spirited people like Jim that will keep crystallography the prominent science that it is.

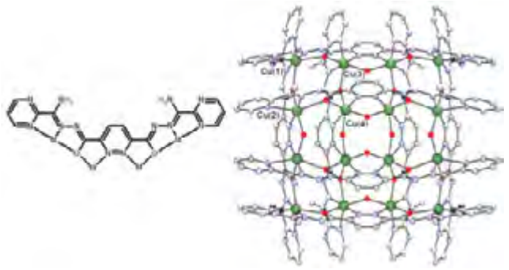
Louise Dawe

The second person whom I would like to highlight in this issue is just as public spirited as Jim; she is Louise Dawe of the Department of Chemistry and Biochemistry, Wilfrid Laurier University, Waterloo, Ontario. Like Jim, Louise hails from the Atlantic provinces of Canada. She studied at Memorial University of Newfoundland in St. John's where she received her Bachelor's Degree in Honours Chemistry and her Doctorate in Chemistry in 2008. Louise also has a Master's Degree in Chemistry from the University of Utah, where she worked in Joel Miller's lab, and she has a Bachelor's Degree in Intermediate and Secondary Education from Memorial University of Newfoundland.

Louise is a small-molecule crystallographer with many interests including metal-organic frameworks (MOFs). She uses

her wide experience in supramolecular chemistry to design and synthesize new organic components for MOFs and then links the organic backbones to metals via specific interactions (covalent or coordination bonds). One of the more exciting applications that these MOFs have in our 'green chemistry world' is the sequestration of CO_2 for storage in the gas and oil industry. Successful carbon storage is still in its infancy in this industry, presenting opportunities for researchers in this field.

Another area that interests Louise is the development of materials for magnetic memory devices. The successful development of magnetic memory devices could have far-ranging applications in enhanced computing capabilities. In a recent review article co-authored by Louise and her former Ph.D. supervisor, Laurence Thompson, and published in *Coordination Chemistry Reviews*, 2015 **289**:13-31, the magnetic properties of several transition metals and lanthanide clusters are modeled and discussed.



As an example, the illustration above shows an organic ligand as well as the structure of the fully metallated Cu_{16} [4 × 4] grid cation $[(L_3)_8Cu_{16}(O)_2(OH)_4(H_2O)_2]^{6+}$ that results from the reaction of the ligand with $Cu(CF_3SO_3)_2$ in MeOH/CH_3CN solution. The cation forms in this reaction, and crystals of the self-assembled complex were grown. The successful solution of the crystal structure revealed the molecular details that allowed the further exploration of the magnetic properties of these compounds. Louise's interests in magnetic [n × n] grids and organic ligands started during her undergraduate days at Memorial University of Newfoundland. She returned for a Ph.D. after teaching high school, where she says students asked her a lot of questions and inspired her to learn more answers!

Louise's dedication to the teaching of crystallography and to the integration of our science into undergraduate curricula is seen in the recent article that she co-authored with Amy Sarjeant, Katherine Kantardjieff, and several other dedicated crystallographers and which was recently published in *Journal of Applied Crystallography*, 2015 **48**: 1964-1975. Section 2 of that article is devoted to the description of crystallographic teaching in the undergraduate chemistry program at Wilfrid Laurier. In the third year course, CH390: 'Chemical Literature and Scientific Communication,' the students selected a topic that involved crystallographic concepts, searched the scientific literature about that topic and then acted as instructors to more junior chemistry undergraduates (CH111: 'Fundamentals of Chemistry II') by presenting posters at a session that involved all students in both courses. The topics were not trivial and covered a wide range of ~40 different topics ranging from: the history of small-molecule crystallography in Canada, to G-protein coupled receptors, to the winners of Nobel Prizes in Chemistry, *e.g.*, Dorothy Hodgkin, to anomalous diffraction and the phase problem. The students from the CH111 course were required to attend the poster session and to write a short summary of one poster that they found interesting and from which they learned about that topic. The whole paper is extremely interesting and I recommend it, not only for the section that Louise contributed, but also for the broad aspects of crystallographic teaching from which we can all benefit.

In addition to her many accomplishments in science and education, Louise also somehow finds time for volunteer administrative responsibilities in the crystallography world. She was the Scientific Program Co-Chair for the 2015 Philadelphia ACA meeting last July; she was a microsymposium co-chair, and the Public Outreach Coordinator for the 2014 Montreal IUCr Congress; since 2012 each year Louise has been a session co-chair and organizer at the summer ACA meetings in Boston, Honolulu, Albuquerque and Philadelphia. Louise has also served as Chair of the Service and Small Molecules SIGs, and the Canadian Division of the ACA. We are indeed extremely fortunate to have people like Louise and Jim to keep the interest in crystallography in Canada at a high level.

2016 Conference Schedule. This year Canada is a hotbed of workshops, schools and meetings. Two of them will be held at the CLS in Saskatoon, Saskatchewan. The first of these meetings is the 6th Annual CLS Macromolecular Crystallography Data Collection School (CLS Mx). It will be a five-day, hands-on synchrotron data collection school held from May 24 to 28, 2016. This year's invited speaker is Jeffrey Lee from the Laboratory of Medicine and Pathobiology at the University of Toronto. Jeff's main research interests are in the application of structural biology to understanding how virus particles gain entry into host cells. He will be guiding attendees in the use of molecular replacement structure determination and the effective use of COOT. Further details can be found at ***http://cmcf.lightsource.ca/school/mxschool***

The second function, also being organized in Saskatoon, is the 4th Annual Meeting on Protein Structure, Function and Malfunction (PSFaM) on June 23 and 24, 2016. This is a very well-attended meeting held in Western Canada and sponsored by the CLS, Proteomics Research in Interactions and Structure of Macromolecules (PRISM), Bruker, and the University of Saskatchewan. In addition to the poster and oral presentations by graduate students and postdoctoral fellows, four keynote speakers are featured this year. They are: Sergio Grinstein from the Hospital for Sick Children, Toronto; Susan Lees-Miller from the University of Calgary; Robert Campbell from the Chemistry Department, University of Alberta; and Srirani Subramanian from the National Cancer Institute in Bethesda, Maryland. More information regarding this meeting can be found at: ***http://cmcf.lightsource.ca/psfam/***

The Canadian Chemical Crystallography Workshop (CCCW) is operated annually and, as mentioned earlier, is associated with

the annual meeting of the Canadian Society of Chemistry. This year the 7th CCCW will be taking place at St. Mary's University in Halifax. The local co-chairs are Jason Masuda and Katherine Robertson, both of St. Mary's University. Jim Britten of McMaster University is the overall organizer of this excellent workshop. It will take place just prior to the 99th CSC meeting and will run from May 30 to June 3, 2016. People are already registering for this CCCW16; registration forms and more information can be found at: ***http://www.canadiancrystallography.ca/cccw16/index.html***

Lastly, the 25th Buffalo-Hamilton-Toronto (BHT) meeting will be a one-day meeting at McMaster University, Hamilton, Ontario held on November 4, 2016. The BHT2016 will be hosted by Alba Guarné from McMaster. The topic for this meeting will be protein structure determination by direct methods; the invited speaker is scheduled to be Isabel Usón from Göttingen, Germany. There were 125 registered attendees at BHT2015 so don't miss this one.

Michael James

YSSIG at the Denver 2016 Meeting

ACA's Young Scientist Scientific Interest Group (YSSIG) has been busy planning a variety of sessions for the Denver 2016 meeting. In collaboration with the Industrial SIG (ISIG), a new session on *Career Development* is being organized this year. This will replace the *Career Odyssey* session that has been held in previous years. The new *Career Development* session will feature members of ISIG, who will assist young scientists, one-on-one, with CV/Resume critiques and practice interviews. With this new emphasis we hope to provide a more active environment to assist young scientists (from undergraduate, graduate, postdoctoral, and early career) in communicating their science to both the public and to professional audiences. The YSSIG will also welcome Joe York from AIP, the American Institute of Physics, to discuss communication of the sciences on a broad level.

No ACA meeting would be complete without the YSSIG mixer; this year we have termed it a 'Networking Mixer sponsored by YSSIG.' Although it is geared to early-career scientists we want to emphasize that the Mixer is open to meeting attendees of all ages. The event is being sponsored by Bruker and will be held in Denver at Marlowe's, shown above, with two drink tickets provided to each attendee and varied hors d'oeuvres. Tickets can be purchased during online registration or at the conference; students and postdocs are granted free admission to the Mixer included with their meeting registration.

We are especially excited for the *Diversity and Inclusion* session. This year's session will feature people of varied backgrounds speaking on a range of subjects including topics concerning people of color, the LGBTQA community, and people with disabilities, all of whom are welcomed by YSSIG and the ACA. This session is particularly important for the success of the crystallographic sciences: to encourage unique perspectives of all audiences to the biological, chemical, physical, and other sciences. As part of the session, Timothy Herman of SMART, Students Modeling A Research Topic, will outline efforts with high-school science teams to discuss protein structure-function relationships, and 3D printing activities to engage high-school audiences.

Finally – in anticipation of the meeting the YSSIG has amped up our use of twitter (follow us at ***@ACAxtal*** and ***@ACA_YSSIG***!) to promote Denver 2016 as well as crystallography and the ACA. We are excited to have a 'publication' voice in real time to update those unable to attend with 140 character snapshots of what will be happening at the meeting this July!

Martin Donakowski

ACA DENVER

July 22 - 26, 2016

Meeting logo designed by John Aspinall

Sheraton Denver Downtown

Special ACA Hotel Rates – Single or Double Occupancy Rooms: $175 + tax
Student and Postdoc Rooms: $141 + tax

Hotel Reservation Deadline: June 28, 2016

for meeting sponsor information, abstracts, on-line registration, and details including room sharing feature see:

http://www.amercrystalassn.org/2016-meeting-homepage

ABSTRACT DEADLINE: MARCH 31, 2016

ADVANCE REGISTRATION DEADLINE: MAY 31, 2016

We are pleased to present the 66th meeting of the ACA in the Mile High City!

Award Symposia

Etter Early Career Award in honor of Jason Benedict
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Bau Award in honor of Benno Schoenborn
Trueblood Award in honor of Axel Brunger

Jason Benedict
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Workshops

The CSD Python API: A Foundation for Innovation
Organizer: Peter Wood

Computational Approaches to the Structural Modelling of Biological Macromolecules using Small Angle Scattering
Organizers: Kushol Gupta, Adam Round

Serial Crystallographic Data Analysis with Cheetah and CrystFEL
Organizers: Tom Grant, Nadia Zatsepin

Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques
Organizers: William Ratliffe, Ovidiu Garlea

SHELX Workshop: Small Molecule & Solid State Chemistry // Macromolecules
Organizer: George Sheldrick

Transactions Symposium

Structural Dynamics
Organizers: Jason Benedict, Arwen Peters

Evening Sessions

Diversity & Inclusion
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ZENOBIA FRAGMENTS

Axel Brunger, Professor of Molecular and Cellular Physiology and Investigator in the Howard Hughes Medical Institute at Stanford University, is to receive the **2016 Trueblood Award** at the Denver ACA meeting in July. In the citation it was noted that 'Axel's contribution to computational crystallography has been invaluable for the development of modern macromolecular crystallography. It was very early in his career (1987), when he was only a postdoctoral fellow, that he developed algorithms based on simulated annealing and molecular dynamics to refine protein structures'. In 1992, to prevent the possibility of overfitting 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. He currently carries out cutting-edge research on the molecular mechanisms of synaptic neurotransmitter release, complementing X-ray crystallography with electron cryo-microscopy and single molecule optical microscopy.

The image shows the crystal structure of the SNARE-synaptotagmin-1 complex (foreground) that triggers synaptic vesicle fusion. In this illustration, the SNARE structure is shown in blue, red, and green, and synaptotagmin-1 is shown in orange. The background image shows electrical signals traveling through neurons.

The crystal structure was determined using diffraction data obtained at the Linac Coherent Light Source (LCLS) X-ray free electron laser at SLAC National Accelerator Laboratory.

Reference: Q. Zhou, Y. Lai, T. Bacaj, M. Zhao, A.Y. Lyubimov, M. Uervirojnangkoorn, O.B. Zeldin, A.S. Brewster, N.K. Sauter, A.E. Cohen, S.M. Soltis, R. Alonso-Mori, M. Chollet, H.T. Lemke, R.A. Pfuetzner, U.B. Choi, W.I. Weis, J. Diao, T.C. Sudhof, A.T. Brunger, Architecture of the Synaptotagmin-SNARE Machinery for Neuronal Exocytosis. *Nature* **525**, (2015) pp. 62-67.

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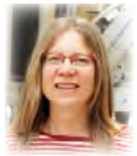

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News & Awards

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Nominations for 2017

ACA Awards: Nominations for the 2017 **Patterson, Etter Early Career**, and **Wood Science Writing** awards, and for the newly established **David G. Ronglie Award** are due by April 1, 2016.

ACA Offices and Committees: In fall 2016 we will elect an ACA Vice President and Canadian Representative to Council, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards & Computing). To suggest a candidate for one of the above positions, please contact a member of the Nominating Committee: **Louise Dawe: ldawe@wlu.ca**, **Ward Smith: smithwar@nigms.nih.gov**, and **Martha Teeter: teeter@ucdavis.edu**. Full details describing the criteria for all ACA awards and offices can be found on the ACA website.

2016 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds.

NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org

Send all award nominations to: marcia@hwi.buffalo.edu

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Anastasiya Vinokur

Net RefleXions

Conferences like ACA are a great way to reconnect with the crystallographic community, to learn new tricks of the trade, and to tap into the greatest minds. But unfortunately such gatherings happen once a year. So how can a young crystallographer connect to our vibrant community for the rest of the year? In this installment of *Net RefleXions*, I would like to highlight two industry-sponsored online crystallographic communities that I use quite frequently to stay in the loop: Bruker User Group and Rigaku X-ray Forum.

Bruker User Group is an online community based on a University of Wisconsin-Madison list server and administrated by Ilia Guzei. All members of the group are frequent users of Bruker instruments, which is a requirement for joining the group. The second rule of Bruker User Group is 'No dollar signs,' as in no discussions of money matters. Sending a message to the User Group's email address reaches the mailboxes of 705 crystallographers in all stages of their career from graduate students like myself to established figures like Ton Spek and George Sheldrick. As a member, you have a choice of how to interact with the group. You can either receive a daily digest, where all the messages of the day have been compiled into one email, or you can receive the messages as they are posted. And you have an option to send a reply privately or publicly. The Group's discussion archive goes back to 2004, and it is available to all group members regardless of when they joined the list serv.

Unsurprisingly, with such a wide range of users, there is a spectrum of topics covered. All aspects of crystallography and Bruker instrumentation are fair game. Keep running into the same checkCIF alert? Strange electron densities? Generator errors? Not sure why commands in SHELXL are called cards? The community will be more than happy to enlighten and to help, and quite often with great humor. In addition, members of the community post about upcoming meetings and job openings. To join the Bruker User Group send a request to Ilia Guzei at ***iguzei@chem.wisc.edu***

The Rigaku X-ray Forum is a more traditional forum community. A quick registration with a creation of username and password gives a member access to topics in Software, General Crystallography, Conferences, and Synchrotron as well as various Off-Topic threads. This forum is administrated by Rigaku's employees, including the software developers, and they frequently answer threads on Rigaku software and hardware inquiries. The forum is a great way to keep up with the latest and greatest from Rigaku, from CrystalisPro updates to new hardware to demos, as well as to find answers to more general questions about solving crystal structures.

An added feature of the Rigaku X-ray Forum is that it sends out a digest of all the most recent threads. This makes it easy to keep up with topics of interest as well as keep track of ongoing discussions. The forum format of this community also allows for an easy search of the previously discussed topics. Personally, I have used this feature of the forum on numerous occasions, and often the answers to my burning questions on importing frames and cell transformations were just a click away. The forum can be reached at ***http://www.rigakuxrayforum.com/index.php***

Hopefully, with these two online communities at your side, you will never find yourself at a loss when confronted by crystallographic issues.

Anastasiya Vinokur

Ned Seeman

ACA Fellow Ned Seeman Is 2016 Recipient of the Benjamin Franklin Medal

ACA Fellow Nadrian C. (Ned) Seeman, the Margaret and Herman Sokol Professor of Chemistry at New York University, has received the prestigious Benjamin Franklin Medal in Chemistry. The award recognizes Ned's founding of DNA nanotechnology, which entails the construction of DNA objects, lattices and machines, and specifically "his conceptualization and demonstration that DNA can be used as a construction material that can spontaneously form sub-microscopic structures of diverse shapes and functions, with potential applications in disease treatment, mechanics, and computation." Ned will receive the award on April 21st, in Philadelphia.

The Franklin Institute was founded in 1824 in Philadelphia, then a flourishing manufacturing center, and was conceived as an outreach institution, as we would call it now. Its aim in fact was to train artisans and mechanics on the basic concepts of science. Through the years, its award program has contributed to raise public awareness on the work of the most notable scientists of the 19th and 20th centuries. Nikola Tesla, Pierre and Marie Curie, Albert Einstein, Max Plank, Frank Lloyd Wright, Jacques Cousteau, Stephen Hawking, Jane Goodall, and Bill Gates are among the Institute's medalists, just to name a few.

With his research on DNA, Seeman has also made history: more than 30 years ago, he was among the founders of the field of nanotechnology, which nowadays is booming with applications in medicine, electronics, and engineering. Using synthetic DNA molecules bearing 'sticky ends' that allow programmed self-assembly, he created for the first time rhombohedral self-assembled 3D DNA crystals.

Ned's studies were initially aimed at understanding the properties of biologically relevant structures, such as the four-arm Holliday junction, which forms during genetic recombination. He was also interested in determining the structural and biophysical characteristics of DNA with specific knotted topologies, as they provide a model system to examine the shape of the DNA under stressed conditions. However, he soon realized that branched molecules could serve as building blocks for the construction of nanostructures and nanomachines. For example, he and his associates employed them to engineer nanomechanical devices and walking nano-robots (nanobots), and they are currently investigating the possibility of using them to create periodic

molecular cages for macromolecular crystallization and biochips for computers.

Ned received a B.S. from the University of Chicago in 1966, and a Ph.D. in crystallography and biochemistry from the University of Pittsburgh in 1970. He then carried out his postdoctoral studies at Columbia University and MIT. His contributions to science have been recognized by an impressive number of awards. Among others: the Sidhu Award in 1974; the Feynman Prize in Nanotechnology in 1995; the Emerging Technology Award from Discover Magazine in 1997; the World Technology Network Award in biotechnology in 2005; the Nichols Medal in 2008; the Kavli Prize in Nanoscience in 2010; a John Simon Guggenheim Fellowship in 2010-11; the Einstein Professorship Award of the Chinese Academy of Sciences in 2012. Besides being an ACA Fellow since 2014, Ned was the founding President of the International Society for Nanoscale Science, Computation, and Engineering, and is a Fellow of the American Association for the Advancement of Science and of the Royal Society of Chemistry.

Chiara Pastore

2012 Charles Supper Award Lecture by Ron Hamlin – An Update

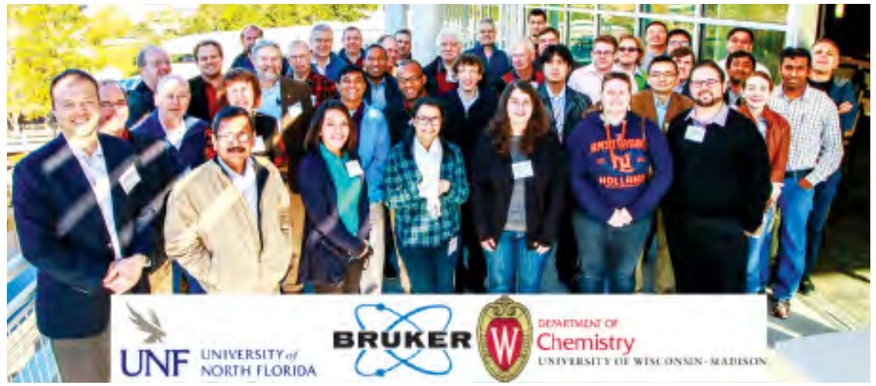
Editor's Note: Following Ron's talk at the 2012 Boston ACA meeting, some questions were asked about the status of the dual-mode pixel array detectors that he had described there. A video of Ron's lecture is available on the ACA History website, and a transcript will be coming there soon. Here's an update from Ron on those detectors.

The 512 by 512 HF-262 k pixel 'proof-of-principle' dual mode HF-262 detector was delivered to Wayne Hendrickson's beamline X4A at NSLS in September of 2013 where, in spite of its relatively small area for protein crystallography, the detector was used to collect good-quality data from crystals of several standard proteins in both the pure pulse-counting mode and in the charge-ramp mode. Remarkably, one data set from crystals of insulin collected at 7 keV with the detector pixels in charge-ramp mode was good enough to yield an *ab initio* structure solution with phasing obtained only from the sulfur anomalous scattering (sulfur-SAD).

The much larger 2 k by 2 k HF-4M (4 million pixel) dual-mode pixel array detector specified in our contract with Wayne Hendrickson was successfully delivered to APS (Chicago) beamline 24ID-E (NECAT) in December of 2015 where it has been used to collect protein crystallographic data for several new protein structures, some using seleno-met phasing. Quite remarkably one data set from crystals of thaumatin collected in December with the HF-4M detector pixels set to the charge-ramp mode was accurate enough to yield an *ab initio* sulfur-SAD structure solution using X-rays of 12.4 keV. At this relatively high X-ray energy the anomalous scattering signal from sulfur is extremely weak and so it requires very accurate spot intensity measurements to get adequate structure factor phasing information from only the sulfur atoms in the structure. This HF-4M detector will be moved to Wayne's new beamline at NSLS II sometime in 2016 when the new beamline is completed.

Ron Hamlin

2016 Bruker Users Meeting Held at University of North Florida



The 2016 Bruker Users Meeting took place on January 17-19, 2016 at the University of North Florida (UNF) in Jacksonville. This year the theme of the meeting was high-pressure crystallography, with two talks by M. Ruf (Bruker AXS) and M. Siqueira (Almax Easy Lab, Inc.) where collection and mounting/handling strategies were discussed, respectively. There was also a hands-on workshop on the Bruker D8 Venture instrument housed in C. Lampropoulos's laboratory at the UNF Chemistry Department on 'High Pressure Crystallography – Finally getting your feet wet!' presented by M. Ruf and M. Siqueira. The meeting included two full days of scientific talks and workshops, a poster session, as well as a tour to the historic city of St. Augustine and an evening welcome reception. One of the workshops included in the program was by G. Sheldrick (U Göttingen) on 'Practical guide to SADABS, TWINABS, XT, etc.' while another was presented by K. Abboud (U Florida (UF)) and B. Noll (Bruker AXS) on 'Crystal structure determinations: the final touches.' J. Reibenspies and N. Bhuvanesh (both from Texas A&M) presented a workshop on 'Comparing predicted powder patterns from SCD with observed PXRD patterns.' Other notable presentations included one by T. Spek (U Utrecht) on 'Updates on validation and SQUEEZE,' one by J. Mague (Tulane U) on 'Rare earth polyoxotungstates: some cautionary tales,' and by B. Burrow (Federal U Santa Maria (Brazil)) on 'Easy access to the Bruker APEX2/APEX3 PostSQL database.' Several talks by Bruker representatives portrayed the latest and greatest on single-crystal X-ray crystallography technologies, including the latest APEX3 software. I. Guzei (U Wisconsin – Madison) gave an inspiring talk about how to organize a crystal growing contest, titled: 'Crystal growing contests: a legacy of the international year of crystallography 2014.' The poster session included 10 posters by graduate students, postdocs, and young investigators, while the program also included chemistry and materials talks showcasing the work by different research groups in Florida. One of those was by T. Albert-Schmitt (Florida State U (FSU)) about crystal structures of transuranium elements, titled: 'Taking the Berkelium leap.' The second talk from Florida was by W. Gao (U South Florida) who talked about the 'Challenges in structural analysis of metal-organic frameworks (MOFs).' The local host, C. Lampropoulos (UNF) talked about 'The great dependence of cluster chemistry on X-ray crystallography,' where several recent results from undergraduate researchers at UNF were presented. The State of Florida was also represented in the poster session, with posters from Florida International U, FSU, and UF, while a number of UNF undergraduates also attended the talks. There were 52 registered participants from North and South America, Europe, the Middle East, and Southeast Asia. The diverse program was organized by I. Guzei, and the local host was C. Lampropoulos (UNF); the Bruker organizers were S. Byram and D. Frankel.

An Almax Easy Lab diamond anvil cell (DAC) suitable for x-ray diffraction mounted on the Kappa goniometer of the Bruker D8 Venture instrument at UNF

For additional information including the complete meeting program, see ***http://brukerusermeeting.chem.wisc.edu*** The UNF X-ray crystallography laboratory was established with support from an NSF-MRI grant (DMR-1429428).

Christos Lampropoulos

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Guest Editors: George N. Phillips, Jr. and José Onuchic

Now Publishing – Selected Papers from the 3rd International Conference on Ultrafast Structural Dynamics. A collection of papers discussing 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.

Guest Editor: Steve Johnson

Now Publishing – The Hamburg Conference on Femtochemistry (FEMTO12)

Ultrafast vibrational dynamics of the DNA backbone at different hydration levels mapped by two-dimensional infrared spectroscopy. Biswajit Guchhait, Yingliang Liu, Torsten Siebert and Thomas Elsaesser, ***Struct. Dyn. 3, 043202 (2016)***

FEMTO12 will bring together scientists from all over the world to present and discuss the most recent advances in femtosciences, including reaction dynamics, coherent control, structural dynamics, solvation phenomena, liquids and interfaces, fast processes in biological systems, strong field processes, attosecond electron dynamics and aggregates, surfaces and solids with contributions from both theory and experiment.

Guest Editor: Jochen Küpper

Open for Submissions – Soft X-rays in Energy and Time (SXET). This issue will have reports on the 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). It will feature technical and methodological developments for high energy and time resolution addressing new scientific questions for solid, liquids, gases and interfaces.

Guest Editor: Emad Flear Aziz

ACA Transactions – Structural Dynamics – Summer 2016

The ACA *Transactions* symposium will focus on the rapidly growing area of structural dynamics of both chemical and biological systems, in addition to solid materials. This resurgence has been driven both by developments in X-ray sources as well as by new approaches for sample delivery, data collection and processing.

The speakers will present recent work on both equilibrium and non-equilibrium dynamics involving time-scales from seconds to femtoseconds. As well as scientific highlights, the symposium will also include case studies and cutting edge advances in methodology.

Guest Editors: Arwen Pearson and Jason Benedict

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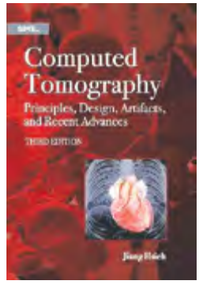
Book Reviews



Computed Tomography: Principles, Design, Artifacts and Recent Advances, Third Edition: Jiang Hsieh, SPIE Press, Bellingham, WA, 2015, 666 pp., ISBN-13: 978-1628418255

You might wonder why I chose this book for review. Recently, I have been doing some work in X-ray microcomputed tomography and have not found a satisfactory text on the topic. In October I received a list of new publications from the Society of Photo-Optical Instrumentation Engineers (SPIE) and saw this text. I thought this might be a good substitute since many of the principles associated with medical CT are the same.

The author is the Chief Scientist at GE Healthcare and so there is a slight bias to GE solutions, but where appropriate other solutions are described. As shown in the title, this is the third edition. I checked the first edition at Amazon and saw that it had only 338 pages. At 666 pages, one can see a lot of material has been added since 2003. The book is laid out as a textbook with problems at the end of each chapter. It is very well referenced, up to and including 2015.

The book starts with an introduction to conventional tomography, and then describes computed tomography and its history. The former method builds the volume of interest by blurring all but one plane. Multiple planes are imaged and an overall volume is generated – not a very low-dose method.

The second chapter is devoted to the mathematical and physical principles that are necessary to understanding image collection, processing and reconstruction. A few pages cover the topic of the sinogram, a reordering of the projection data to detect errors or anomalies before further processing. The next chapter covers the reconstruction of an object from projection data: the Fourier slice method, filtered back projection, fan-beam reconstruction and iterative reconstruction. Chapter 4 covers the display of the reconstructed volume, including such modern methods as 3D printing.

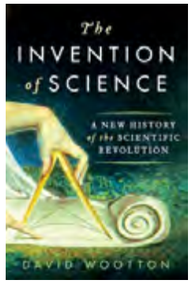
The next two chapters cover the topic of instrumentation, first looking at performance issues and then the components of CT scanners.

I found chapter 7 to be particularly enlightening as it provides a clear description of a number of artifacts that can arise in the CT experiment and how to resolve them either by the correct experimental setup or by specialized algorithms. Here one has to keep in mind that medical CT generally concerns two or perhaps three major components: soft tissue, bone and occasionally a piece of metal. The types of samples measured in non-medical CT have a much broader range of densities and so the algorithms described will not be as effective. Chapter 8 describes the use of computer simulations to understand system performance.

Chapters 9 and 10 cover helical scan CT, multislice CT and cone-beam CT. The advantages and disadvantages of these methods are considered, as are the changes in the measurement relative to simpler CT methods. Chapter 11 covers dose-reduction methods. Chapter 12 describes a number of specialized CT techniques including gating imaging and dual-energy CT.

Someone new to material science would be well served by this text since it provides clear explanations and solutions to problems that will be encountered in analyzing a variety of samples.

Joseph Ferrara



The Invention of Science: A New History of the Scientific Revolution: David Wootton, HarperCollins Publishers, New York, 2015, 785 pp., ISBN-13: 978-0061759529

We often think of invention as the product of scientific inquiry, but it doesn't seem as intuitively obvious to think of science itself as something that was invented. Yet that is exactly how David Wootton presents the history of the Scientific Revolution in his new book, *The Invention of Science: A New History of the Scientific Revolution*.

Although it certainly isn't light reading, Wootton's newest work is jam-packed with information. It reads like a high-energy history textbook. Wootton sets out to provide "A New History of the Scientific Revolution," and certainly does so. He has found a way to reinvigorate this well-trodden tract of scientific history.

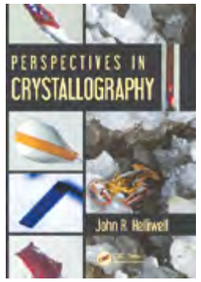
He opens with the claim "modern science was invented between 1572, when Tycho Brahe saw a nova, or new star, and 1704, when Newton published his *Opticks*, which demonstrated that white light is made up of light of all the colors of the rainbow." But despite this claim, Wootton, like any good historian, does not start at this proposed beginning, Brahe's observation of a nova, but rather with the first tool-making humans – 2 million years ago. He gives a brief overview of the initial development of what might broadly be considered scientific progress in the early days of human civilization – nothing revolutionary, other than that it laid the groundwork for future innovations.

He then delves immediately into the Scientific Revolution of the 1600s – the revolution that he claims started with Brahe. It's important to keep in mind that when Wootton refers to science, he is not referring broadly to the many manifestations of human ingenuity, but rather the method of science, which he refers to as "the research programme" and "the experimental method." That is, science as a series of steps, starting with a hypothesis, developing an experiment to test it, doing the experiment, recording and analyzing the results, and repeating the process. The most important part of scientific discovery is reproducibility. If your results can't be reproduced, the theory or development you are proposing lacks the ability to be proven.

One of the statements I found most compelling in Wootton's book came in the last chapter: "science offers reliable knowledge (that is, reliable prediction and control), not truth." This is

something we often forget about science, that it doesn't always offer us immovable truths about the world (and the universe) we live in, but it helps us understand it.

Jeanette Ferrara



Perspectives in Crystallography: John R. Helliwell, CRC Press, Boca Raton, FL, 2016, 171 pp., ISBN: 978-1-4987-3210-9

Helliwell's *Perspectives* is a collection of articles and lectures by the author celebrating the 100th anniversary of the first crystal structures (1912) and the 2014 UNESCO International Year of Crystallography. The book covers a broad range of topics in crystallography from the author's perspective, hence the title. Some of the chapters have already been published in *Crystallography Reviews*.

Section I consists of a single chapter in which the author attempts to answer the question for the general public, "What is crystal structure analysis?" Helliwell describes how the question was answered at several venues including his home institution, the University of Manchester, and the Prisoners' Education Trust.

I found the next section very interesting. Chapter 2 succinctly describes the first diffraction experiments by the Braggs before and during WWI while Chapter 3 provides retrospectives by W. H. Bragg, W. L. Bragg, P. P. Ewald and D. C. Phillips on the work described in Chapter 2.

Section III is titled "Aspects of Crystallography Research" and consists of four chapters. Chapter 4 is a transcript of the author's Lonsdale Lecture at the 2011 annual meeting of the British Crystallographic Association. I found the short biography of Kathleen Lonsdale at the beginning enlightening. I knew of her importance with respect to the early crystal structures of organics and the creation of the original *International Tables for Crystallography*, but I did not know the details of her life story. The lecture then describes the history of the use of synchrotron radiation by the crystallographic community.

The next two chapters cover more specific topics: a comparison of several programs for predicting protonation versus X-ray diffraction results, and the structural of crustacyanin. The last chapter in this section is a short prospective on the future of crystallography.

The last section and chapter looks at how crystallography has been a part, and will continue be a part, of the eight Millennium Development Goals set forth in 2000 by the United Nations. One of the goals is to promote gender equality and empower women. The author points out that compared to other sciences, crystallography has more gender balance. Many of the goals are related to the alleviation of human pain and suffering – clearly crystallography excels here through improving our understanding of the world around us.

Joseph Ferrara

Photo Courtesy of Patricia Craven

Remembrances of Bob Stewart (1936 - 2015)

It's hard to imagine the crystallographic world without Bob Stewart. Bob was a role model and friend for all of us who were part of the Pittsburgh crystallographic community. During my years in Pittsburgh (1967-1970) he was, along with Bryan Craven, arguably the most dynamic character on the local scene. All the rest of us were working on structure determination, but Bob was trying to use 'the X-ray diffraction experiment' (a term he used frequently) to see the features of the electron density we had all learned about in our undergraduate chemistry courses: bonding electrons, lone pairs, and the like, which were ignored in the work the rest of us did. What he was doing was a hell of a lot neater than the spherical atoms we used in the standard crystallographic representation.

That was cool, but this description fails to present Bob as he was. I remember him especially as the founder of the 'Friday afternoon seminar' that he hosted at the Craig Street Inn. Over beer and his Camels and my Gauloises cigarettes, he would hold forth on topics that ranged from Science, to his graduate school days at Caltech with Norman Davidson (when he drove around LA in his MGA, Reginald), to his postdoc back home in Seattle at the University of Washington. It was under Bob's tutelage at the Craig Street Inn that I learned to combine beer and Science, a combination that wound up working very well for me in later life.

At the Craig Street Inn, Bob sometimes talked about his undergraduate summer studentship at Los Alamos: He told the story of having a meal with a guy who worked on developing nuclear weapons. Bob asked him how he could work on these horrible things; the response was, "Well, Bob, I've got a philosophy." "Really?" Bob asked, "What is it?" "People are just no damn good!"

It was fascinating to listen to Bob talk about his early life, particularly his birth to a whore on the Seattle waterfront and his adoption by a wealthy man. He described going back to the orphanage as an adult and the official there said, "I remember you. You crawled up on my lap, looked up at me with those big blue eyes, and said, 'That goddamn sonovabitch Roosevelt'." Bob had been parroting his mother, because FDR was supposed to be helping poor people, but his mother felt she had not received the help that she deserved. Bob talked about how shortly after Pearl Harbor he had been on a boat in Puget Sound with his adoptive father, and had passed a Japanese gardener, whom he had started to cuss out. His father admonished him that Pearl Harbor had not been the gardener's fault, giving him the impression that his father was not a racist. He was wrong, which he learned the hard way when he was disowned for joining SNCC.

Bob took a sabbatical with Ted Maslen in Perth in 1971-1972. I didn't see Bob during that year, and didn't recognize him when

I ran into him at the Kyoto IUCr (IX) in 1972. He had joined Ted's running group, and after a year of that kind of exercise he had temporarily lost a huge amount of weight. I attended his talk at the meeting and was impressed but not surprised when Berthaut got up afterwards and said that Bob had laid out a route that would define the area for years to come.

Of course, Bob worked out the hydrogen atom scattering factor, including the fact that the electron is partly to be found in the bond to another atom; this was just after the then-current edition of the *International Tables* had gone to press, so he was cited in every crystal structure that was reported until the next edition of the *Tables* was published many years later; in its era, that paper was the most cited paper in the chemical literature.

There is a syndrome to which Bob unfortunately succumbed in later life. This was not recognizing when good was good enough. He simply stopped publishing (often taking his name off papers) at the required rate, because he was unsatisfied with the results. It was ironic that even then, when I went to Pittsburgh Diffraction Conferences held in Pittsburgh, I'd go up to Bob's office and couldn't get in to chat with him: He was always too busy holding forth to an audience of wall-to-wall bodies on his thoughts about accurate electron densities. Bob was still the guru, even when he was not publishing or being funded.

At Caltech, Bob was with Davidson as he was switching from physical chemistry to molecular biology. I think Bob was the last physical chemist that Davidson produced. I was fortunate that one of Bob's lab-mates, a molecular biologist, became my dean during my highly vulnerable assistant professorship, certainly not harming my shot at tenure. Between that time and my Pittsburgh era, Bob wrote huge numbers of letters for me, resulting in postdocs, fellowships, and a chance at an independent position.

Bob was *sui generis*. He was a great scientist who was an authentic personality. There are far too few people like Bob in Science, particularly now, when we need more individuals like him. His loss impoverishes the entire enterprise.

Ned Seeman

Bob Stewart (second from left), during a 1996 visit to the author's farm in Denmark. L–R: Syd Hall, Bob, the author, Don Glusker, and Jenny Glusker.

Robert F. Stewart in Memoriam

Bob Stewart's name is intimately linked to the development of charge-density analysis, and it was due to my interest in learning more about this exciting and rapidly developing field that I got to know Bob in 1977. I attended the two-week long Batsheva de Rothschild Seminar organized by Philip Coppens and Fred Hirshfeld and held at the Weizmann Institute, Israel. Bob's lecture 'Total X-ray Scattering and Two-electron Density Functions' was not the easiest to understand, because it required a good knowledge of both physics and mathematics. The lecture notes from the seminar were published the same year in the special issue 'Electron-density Mapping of Molecular Crystals' of the *Israel Journal of Chemistry* that long served as my reference text for the field. Bob and I met again the following year in Arles, at a NATO Advanced Study Institute on charge-density studies organized by Pierre Becker. Charge-density analysis was a rapidly expanding field and Bob and I met regularly at meetings during the following decade, in which Bob also visited Copenhagen several times. At these occasions I noticed how he enjoyed interacting with the students in the group; he showed great interest in their projects and could always contribute with some clever comments.

I was therefore more than delighted when Bob aired the possibility of spending a sabbatical at University of Copenhagen the first half of 1991. Denmark is a small country, so not only my group but also the whole Danish crystallographic community was happy to have Bob Stewart with us for half a year. I succeeded in getting the necessary financial support to appoint him as a visiting professor with a large apartment in Nyhavn, an exclusive address in central Copenhagen, in an old house owned by the Danish National Bank – a historic house where the Danish author Hans Christian Andersen had lived. Bob arrived in January 1991; it was cold and there was snow in the streets. In Nyhavn we were met by the caretaker of the house, who with great pride showed Bob this fancy apartment with three big bedrooms and fully furnished with the best of Danish design. Bob looked more and more tired, and I could see that he just wanted a bed to relax in and getting a chance to look at the TV to follow the news of the Gulf War. Though Bob enjoyed the apartment and its setting in central Copenhagen, I am not sure that he really felt at home there.

Bob started by giving the prestigious Bjerrum-Brønsted-Lang lecture on February 8, 1991. The lecture is named after three well-known Danish chemists and was instituted by the founder of crystallography in Denmark, Axel Tovborg Jensen. The title of Bob's talk was 'How a Chemist Gets a Charge out of Crystallography'. The title shows Bob's great sense of humor, and it marked well the focus of the new area of research that Bob was initiating, namely implementing Richard F. W. Bader's theory Atoms in Molecules (AIM), developed for theoretical electron densities, for experimental electron densities derived from X-ray diffraction data. In his talk Bob presented the first results from his collaboration with Wolfgang Jauch from Berlin on MnF_2. It was clear that AIM had great potential to quantify all the interatomic interactions that make a crystal, and we were keen to use Bader's AIM theory on molecular and hydrogen-bonded systems. VALRAY was the program system that Bob used for the calculations; it originated in Jim Stewart's XRAY System and had been developed in collaboration with Mark Spackman when Mark was a postdoc in Pittsburgh. Claus Flensburg was a master's student in my group when Bob came for his sabbatical; Claus had the responsibility of maintaining the computer systems of the group and served as our computational expert. Claus and Bob hit it off immediately. They discussed mathematics, physics, chemistry, programming, history, philosophy, etc., and Claus soon

played an important role in the new developments of VALRAY. Bob enjoyed his sabbatical in Copenhagen in 1991, and when he left it was clear that he had to come back next summer for a couple of months, though it was obvious that it could be difficult to arrange a similar accommodation for him. Bob's sabbatical in Copenhagen was the start of a very fruitful and productive collaboration that was maintained through his yearly visits each summer for more than 10 years; our group knew – come summer, come Bob. In 1993 I was fortunate to obtain a Center of Excellence grant to develop structural biology, at the same time as our developments of AIM on experimental densities had reached a very promising and useful stage, so for the next ten years we maintained the program of charge-density studies parallel to the development of our structural biology program on carbohydrate active enzymes and enzymes in nucleotide metabolism. It is my impression that Bob enjoyed this mixed bag of activities, in which he always participated very actively.

Bob often said that he would have liked to study history, and it was only due to his poor language capabilities that he did not continue in this direction. He knew the history of the major countries in Europe well before he came to Copenhagen, and during his many visits he became an expert in Danish history. He enjoyed the Danish national historical museums at Frederiksborg castle and could spend hours watching the exhibitions. The Danish astronomer Tycho Brahe fascinated Bob; Tycho Brahe had his observatory at Ven, a small island between Denmark and Sweden that now belongs to Sweden. Bob visited the island several times and knew all about Tycho Brahe's life and therefore was a bit disappointed about the limited information at Ven.

During Bob's sabbatical we started the study of a compound with a very short symmetric hydrogen bond, methylammonium hydrogen succinate monohydrate, in which we used AIM to investigate the nature of this intriguing interaction. It was a long process that also involved detailed analysis of atomic displacement parameters, and employing neutron diffraction to verify that the hydrogen bond is truly symmetric. I think that Bob was happy with this first result from our collaboration when it was published in 1995. Claus did very well in his master's studies and was granted support from the Faculty of Science for his Ph.D. study, naturally with Bob as a co-supervisor. Claus visited and stayed with Bob and his wife Janet in Pittsburgh in the summers of 1992 and 1995. Just before he completed his Ph.D. degree Claus visited again in January 1998 having joint birthday celebrations with Bob. Henning Osholm Sørensen and Anders Østergaard Madsen followed in the tracks of Claus Flensburg by having Bob as co-supervisor in their Ph.D. studies. Their research took other directions towards the analysis of anharmonic thermal vibrations and the modelling of hydrogen atoms in charge-density studies. Both enjoyed and learned a lot from working with Bob and visited him in Pittsburgh, Henning in 2002 and Anders in 2009.

Bob was known as a heavy smoker, but when he encountered severe health problems he quit smoking without any problems. However he was not happy with a situation, where he had to look after himself and his medication. I noted that it affected his usual scientific enthusiasm to some degree when he visited me in Grenoble in 2005. As Director of research for life science I had looked forward to share my excitement of the applications of synchrotron radiation in fields like art and archeology with him, but Bob was not turned on by the large facilities and was not too happy with traveling anymore.

Writing e-mails and letters was not Bob's forte, so it was difficult to communicate during the last years of his life. The last time Bob and I met was in 2010 at the ACA meeting in Chicago. He and Janet had travelled from Pittsburgh by train, as they did not like flying anymore. We had a great lunch together refreshing our good memories on collaboration and friendship from the past three decades, and talked about the three great young men Claus, Henning and Anders.

Everyone who met Bob realized that he was a great scientist who took crystallography to his heart and contributed significantly to the development of this field. He also stood out as a scientist of the old school who only wanted to publish things that he felt were done in the 'right' way. Bob was never tempted to follow the hot topics to attract research funding, and only worked on research he found really interesting.

For those of us who had the pleasure to get close to him, Bob became a dear friend, not only for me, but for all members of my family. He participated in all family events that took place during each summer, and my family and I are grateful for the good times we spent with Bob. He is missed not only as an inspiring and enthusiastic colleague but also as a dear friend.

Sine Larsen

2015 U.S. Crystal Growing Competition

"It's almost non-stop now!" – *David Adamson from Montessori Magnet School in Hartford, CT commenting on the frequency of kids asking to grow crystals and bringing him rocks to inspect for crystals.*

USCGC participants Abigayle Liendecker and Christina Platt from South Lewis Central School located in Turin, NY. Photo: Anne Huntress

Ready for round two!!! The second annual U.S. Crystal Growing Competition (USCGC, ***http://www.uscrystalgrowingcompetition.org/***), organized by Jason Benedict of the University at Buffalo (UB) wrapped up earlier this year. The nationwide contest, based upon a similar contest developed in Canada, challenged America's youth in grades K-12 to grow the largest, highest-quality crystal of potassium aluminum sulfate possible over a five-week period. USCGC was designed to be an important scientific outreach activity that provides students and teachers with a fun, hands-on STEM activity as well as an exciting competition. Sponsored in part by ACA, the USCGC brings the science of crystals into America's classrooms.

In its second iteration, the USCGC has seen exciting growth

in all areas of the contest. Over 90 classrooms and households requested crystallization materials, up from approximately 30 in the first year. And clearly word of the contest is spreading. The contest received submissions from nearly 30 states, up from eight states in 2014. To help keep things running smoothly and to help the contest continue to grow, the USCGC welcomed two professors as new regional coordinators: Fernando Uribe-Romo (University of Central Florida) and Karah Knope (George Washington University).

We had many new winners this year! Anna Maria Tippner and Jayla Walker from Montessori Magnet School in Hartford, CT won the 'Best Overall Crystal' category for K-8. The 9-12 division was won by a team represented by John Thurmond from the Illinois Mathematics and Science Academy in Aurora, IL. Both teams took home $200!

Winners of the 'Best Quality Crystal' (a category that only ranks the quality and not the size of crystal) also received a $200 prize and included Cameron Kelly from the Birch Wathen Lenox School in New York, NY for the K-8 division and Torrey Black's students from the Charter School for Applied Technology in Buffalo, NY for grades 9-12.

A check for $100 for the 'Best Teacher Crystal' was awarded to Jessica Weedon from the Bronx High School of Science in Bronx, NY.

Once again, the contest used social media to advertise and provide contest updates, including a live image of the contest judging! The winners were announced via the contest Twitter account, ***@USCrystalComp*** Many participants sent in pictures of their progress, which were also shared with the world via social media.

The contest, which began during National Chemistry Week in mid-October and concluded in early December, was judged by a number of UB professors from Chemistry and Physics: Alexey Akimov, Timothy Cook, Philip Coppens, and Luis Velarde (Chemistry), and Andrea Markelz (Physics). Regional Coordinator Fernando Uribe-Romo even made a trip to Buffalo and assisted with the judging!

For many participants, teachers and students alike, this was their first opportunity to perform experiments in crystal growth. Many remarked that they found the instructional 'How to grow a single crystal' video series posted on the Benedict Research Lab's YouTube channel (***https://www.youtube.com/channel/UC73kcJKC3BxY2r3k5iSaSdw***) to be instrumental in their success!

The author, National Coordinator of USCGC, holding a crystal of potassium aluminum sulfate. Photo: Douglas Levere

The USCGC gratefully acknowledges the contributions of the Benedict Research Group graduate students, our new regional coordinators, and the support of our sponsors: ACA, Ward's Scientific, Bruker AXS, Krackeler Scientific, the American Chemical Society Western New York Section, the National Science Foundation, and the UB Department of Chemistry. Please consider helping with the 2016 contest! For more information, please visit the USCGC website or e-mail Jason Benedict at ***jbb6@buffalo.edu***

Jason Benedict

From the Editor's Desk

ACA is pleased to announce a new award to honor the memory of David Rognlie. Dave, owner of Blake Industries and a constant presence for many years at ACA meetings, was a much-loved member of the crystallographic community who sadly passed away in 2014. The Award is intended to embody Dave's values and personality: his generosity of spirit, optimism, selflessness and unstinting desire to help others to succeed in their endeavors. Dave played a particular role in the X-ray synchrotron community but had broad and wide-ranging interests in the science and the people doing it across all spectra. The **ACA David G. Rognlie Award** will be given triennially to recognize, "an exceptional discovery or technical development of particularly high impact in any area of structural science, to be awarded at any stage of a scientist's career without prejudice based on age, gender, ethnicity or race." The first Award will be made in 2017 at the ACA meeting in New Orleans, LA. A call for nominations is found on p. 10.

ICDD has announced the 2016 recipients of the Ludo Frevel Crystallography Scholarship. The Frevel Scholarship winners include Anna Gres, a graduate student at the University of Missouri – Columbia and a 2015 ACA Travel Award recipient as well as a Pauling Poster Prize winner for her presentation on 'Crystal Structures of Native and Mutant HIV-1 Capsid Proteins'. For more on the Frevel Scholarship, see ***http://www.icdd.com/resources/awards/frevelwinner.htm***

ACA's open-access journal, *Structural Dynamics*, published jointly with AIP Publishing, continues to grow and thrive under the leadership of our Editor-in-Chief Majed Chergui. For additional information on *Structural Dynamics*, see pp. 18-19. If you're not familiar with the journal, I encourage you to take a look at some of the outstanding papers appearing there for yourself.

Besides all of our regular *RefleXions* features, see pp. 30-34 of this issue for a fascinating *ACA Living History* memoir by Winnie Wong-Ng . Watch for the unabridged version of Winnie's memoir tracing her inspiring life story, *coming soon to the ACA History Website*.

This issue includes moving tributes to Bob Stewart by Ned Seeman and Sine Larsen, on pp. 22-24. In addition to being a great scientist, Bob was one of the crystallographic community's most beloved characters. Bob will be sorely missed by all of us who knew him.

Finally, IUCr has announced with great sadness that former IUCr President and Editor of *International Tables for Crystallography* Theo Hahn passed away on February 12, 2016 (see ***http://www.iucr.org/news/notices/announcements/theo-hahn***) Over his distinguished career Hahn made, "profound contributions … to theoretical crystallography and symmetry theory," while serving the crystallographic community selflessly for many years.

Tom Koetzle

Chris Cahill

Dispatch from 2015-16 AIP State Department Science Fellow

It is indeed a pleasure to pen a few words regarding the experience I have had over the past six months as the American Institute of Physics State Department Science Fellow. The ACA actually has a significant presence at the U.S. State Department at the moment as fellow member Matthew McGrath held this distinction last year, and has re-upped for a second year. We all enjoyed Matthew's updates last year in *RefleXions*! As for me, the opportunities afforded by this program have been amazing and I am looking forward to the remainder of the Fellowship prior to returning to George Washington in August 2016.

Briefly, and in case this is your first time hearing about this program, AIP has a number of Government Science Fellowships that aim to provide professional development opportunities for scientists at various stages of their careers. Take a look at their website for more details: ***https://www.aip.org/policy/fellowships/overview***

Fellows can be placed in Congress, or in my case, at the State Department. Motivations from both sides are many – scientists are afforded opportunities to learn how policy is made, and our government hosts benefit from the technical/analytical skill sets we bring to the table. As a mid-career scientist, I embarked on this trajectory to learn more about the intersection of science and technology policy: what are the drivers for research and innovation from an international policy perspective, and conversely, what kind of policy responses are prompted from technical innovations?

Looking more broadly however, I have been motivated by a desire to be a more well-rounded mentor. I have maintained a research group at GW for 16 years and am very proud of our output and the trajectories of my students. That said, I am admittedly a bit of a 'one-trick pony' in that I tend to groom people for either academic or national lab positions. Clearly there are other opportunities for scientists out there and in order to advise effectively, I felt I needed to go have the experiences myself. Moreover, the employment climate for Ph.D. scientists is very different than it was even 10 years ago. And, our current political climate has never needed the analytical contributions from scientists like it does right now. So, I am eager to develop a comprehensive mentoring approach that promotes critical thinking and effective communication (good skills for any career!) recognizing that many students may pursue 'alternative' career paths. Side note: 'alternative' is in quotes somewhat cheekily as here it means 'non-academic' or 'not a bench scientist'. Statistically, the term 'alternative' is out of whack as more and more Ph.D. scientists are not landing in the traditional positions.

With some of these motivations in mind, as well as an emerging interest in nuclear science issues (policy and otherwise), I landed on the Nuclear Forensics Team inside the Office of Weapons of Mass Destruction Terrorism, which is within the Bureau of International Security and Nonproliferation – for those in the know, ISN/WMDT-NF. I work with a team of dedicated colleagues who are committed to keeping the world safe from the illegal use or possession of nuclear materials outside of regulatory control. We use nuclear forensics – the technical means by which one characterizes nuclear materials as to age, provenance, production history, etc. – as a means to engage with other countries and build capacity to detect, deter, defeat and respond to nuclear incidents. The United States of course has considerable technical expertise in this arena, yet the role of the State Department becomes apparent when one wishes to engage globally. Accordingly, our team provides diplomatic top cover for U.S. nuclear forensics activities abroad from a variety of government agencies. Nuclear security is a complex entity with a broad range of stakeholders and authorities across the departments of Energy, Defense, Justice, State and the intelligence community. Our office engages across the interagency to leverage our domestic capacity for international engagement. It is fascinating, to say the least.

As to what I am doing specifically, well, I am going to save that for upcoming issues. A teaser is that I am working with a short-list of countries to take stock of their current nuclear forensics capabilities and consider what the United States would want them to be capable of. In the meantime, however, let me encourage readers interested in science/technology policy fellowships to explore the AIP website listed above, as well as that from the American Association for the Advancement of Science (AAAS): ***http://www.aaas.org/program/science-technology-policy-fellowships*** Further, I welcome any questions/comments you might have to either ***cahill@gwu.edu*** or ***CahillCL@state.gov*** Thanks for reading.

Chris Cahill

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 cash prize, a trophy and a certificate. The Award in 2013 went to Ana Cuesta (Spain). Matteo Bianchini (France) received the 2014 Award for his combined solid-state electrochemistry and diffraction structural study of multiple phases in the ε-VPO_4O-$LiVPO_4O$-Li_2VPO_4O system.

The winner of the 2015 Award will be decided in spring 2016 by a selection committee that includes established research scientists unaffiliated to PANalytical. Submissions for the 2016 Award will be possible from March 10, 2016 with a deadline of **December 1, 2016** (see: ***www.panalytical.com/award***). Applicants must publish a paper during the period January 1, 2015 – December 1, 2016 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***

Daniel Rabinovich

Louis de Broglie's Big Brother

Most introductory chemistry and physics textbooks include a couple of paragraphs explaining the dual nature of electromagnetic radiation, which under certain conditions can exhibit particle qualities or display wavelike properties. This was first suggested in 1924 by the French physicist Louis de Broglie (1892-1987), who made seminal contributions to quantum theory and received the 1929 Nobel Prize in Physics "for his discovery of the wave nature of electrons." His iconic formula relating the wavelength of a particle behaving as a wave and its momentum (*i.e.*, the product of its mass and velocity) appears on the 1994 French stamp illustrated in this note.

Despite his fame and fortune later in life, Louis de Broglie was not particularly interested in science growing up in an aristocratic family that included several military officers, religious leaders, and two former Prime Ministers. His first degree (1910) was in history and it was only a few years later that he took a keen interest in mathematics and physics, influenced by his much older brother Maurice (1875-1960) who was an accomplished experimental physicist in his own right.

Maurice de Broglie studied physics at the renowned Collège de France under Paul Langevin, who had been a doctoral student with Pierre Curie. He was among the first to investigate the behavior of charged particles in an electrical field, and he conducted pioneering experiments in X-ray diffraction and X-ray spectroscopy including the first detection of absorption bands for silver and bromine in a photographic emulsion. He also carried out observations on cosmic radiation using a Wilson cloud chamber, made a variety of contributions to nuclear physics, and became a member of the French Academy in 1934 and the Royal Society of London in 1940.

Daniel Rabinovich

Join Us in July in Denver!

Meeting logo designed by John Aspinall

Winnie Wong-Ng

Living History–My Journey through Crystallography and Related Science

In her memoir Winnie recalls her odyssey from China and Hong Kong to Baton Rouge, Toronto, Swarthmore, PA and finally to the National Institute of Standards and Technology (NIST) in Gaithersburg, MD, where the broad scope of her research illustrates the wide variety of questions that can be answered by X-ray diffraction. Winnie's honors include being named Fellow of ACA and of ICDD.

Pre-USA Period. When I was a child, I aspired to be a scientist due to the influence of my father, Dr. Wong Shek Hung, who obtained Chinese government support to study in France and Germany at the end of World War I, in 1919 (during the China 'Diligent Work-Frugal Study Movement'). Among those who went to study abroad in France at that time were future Chinese leaders Zhou Enlai, Deng Xiaoping, and others who went on to prominent roles in China. After obtaining his doctorate degree in chemical engineering, my father taught at the Berlin Institute of Science and Technology, then came back to China and taught at Zhongshan University in Southern China. He subsequently served in a relatively high position in the prewar Chinese government, but remained uninfluenced by 'power'. He taught his children to be hard working, kind and generous. After WWII, our family moved to Hong Kong. When I was a child growing up there, my family was quite poor, jobs were difficult to come by, and my father found a job in Thailand. When he died there, I was in the beginning of junior high school, and we were in a desperate situation. My older sister and brother were in China. My mother never had an opportunity to go to school, so she couldn't work. In her generation it was uncommon for Chinese women to have an education. We couldn't really afford schooling for both my younger brother and me. I overheard relatives advising my mother that I should work in a factory to support the family. Unlike in the United States, most schools in Hong Kong were private then. I loved schooling and I worked hard to obtain top grades. I remembered crying myself to sleep and praying for the opportunity to continue my education. I worked my hardest to get after-school work and summer jobs, including tutoring young students and various manual jobs, such as assembling mass-produced plastic goods. Later my high-school administrator Mrs. Lee (Pooi-To Girls School) gave me a partial scholarship and student work during lunch and after school hours. She also gave me used textbooks and used school uniforms. I was thankful to be able to finish my high-school education.

After high school, I passed the Chinese University of Hong Kong entrance examination and received a government scholarship. (At the time there were only two formal universities in Hong Kong. It was a tough competition to obtain a slot to study science.) With continuing after-school and summer jobs, I was able to help my family. I studied chemistry/physics, although my first choice was mathematics. Today, looking back, I am glad that I studied chemistry, which provided more opportunities in later years. I also learned that, given time, one could learn to love subjects that you were not initially fond of. I had good scientific training at the University, and I am proud that one of the professors, Sir Charles K. Kao, became a Nobel Laureate in Physics in 2009 for his fiber optics communications research.

I was quite ambitious even as a child. I wanted to have as high an education as I could, even though my family could not afford it. It eventually took a number of 'miracles' and sponsorships from friends and a stranger to fulfill my dream. For example, U.S. university alumni formed a new club called 'The American University Club of Hong Kong' during my college graduation year, and they wanted to give out travel scholarships to selected students. This was a perfect opportunity for me, as I had been accepted by Louisiana State University but without financial help. Fortunately I was selected, and along with three other winners; we had our 15 minutes of fame,with interviews on radio, in the newspaper, and on television. I was able to borrow money for the first semester's tuition from a classmate's mother (Mrs. Tam). A total stranger was willing to lend me a large sum of money to deposit in the bank (a prerequisite for visa application to the U.S.). I will never forget my experience at the U.S. Embassy. First, according to my fellow students in the waiting room for the interviews, I was assigned the most difficult interviewer, who routinely turned down applicants. But I found her to be strict but kind. Even though she knew the bank deposit must have been borrowed, based on my academic record she was willing to let me go. But I had to promise her that I would try to do my utmost best in my studies, and that I must help others whenever I could. I was really touched. At that moment, I believed that God answered my prayers and that 'the stars were all aligned' for me.

Winnie receiving the scholarship from the American University Club of Hong Kong in 1969

Hong Kong to LSU. After I arrived at LSU, I met the graduate studies director Professor Clyde Day. I told him I borrowed money for one semester, but I knew that with diligence I would be able to find financial help for the next semester. He thought I had great confidence. After I took the Ph.D. qualifying examinations, he told me I did extraordinarily well, particularly in inorganic chemistry. He wanted to know what inorganic chemistry textbooks we used at the Chinese University. After I told him the names and authors of the two books we used, he said he was 'stunned' and informed me that he was one of authors, along with Joel Selbin (I had been unaware that he was a well-known author). I got a teaching assistantship, so I was able to repay my debt and continued to help my family.

Since high school I have appreciated symmetry and what it brings to the beauty of the world. At first I had no concept of what crystallography is. I first heard of the word crystallography from my 'future' graduate advisor Professor Steve Watkins.

Steve Watkins with a Weissenberg camera at LSU in the early 1970's

I thought it was sort of a crossover discipline between arts and science that needed some mathematics skill. So it seemed to me the best field to pursue. I was also glad that Professor Watkins introduced me to the beautiful art of the great M.C. Escher. In addition to learning the rudiments of crystallography and experimental skills, I also learned how to apply molecular orbital (MO) calculations to interpret crystal structures and to understand bonding characteristics and other properties of a compound. The MO technique helped me in later years in a number of projects.

Professor Watkins is an excellent mathematician, adviser, and teacher. In 2002 he received the PAESMEM Award (for outstanding mentorship), presented by President George W. Bush. His hard-working discipline also set a great example for his students. We had a fantastic group that became a second family to me.

Watkins's partial group photo in 1974

We had great fun learning, and playing pranks on one another as we did so. I had a memorable five years, with a teaching assistantship/fellowship that provided the needed support. In 2011, Professor Watkins retired and we had a party for him back at LSU (organized by Frank Fronczek and Julia Chan (2003 ACA Early Career Awardee)). After all these years, we still 'recognized' our fellow LSU graduate students. We visited the well-equipped X-ray facility. Frank Fronczek (an LSU graduate and a Ph.D. graduate from Caltech) has been at LSU for almost 40 years as the departmental crystallographer. We were all impressed by the facility. At the party, most of us gave talks about our ventures in life after LSU. Professor Watkins's own graduate advisor Professor Larry Dahl (University of Wisconsin – Madison) was also there.

Professor Watkins's retirement photo from 2011 with his former students and coworkers (L–R: Madeleine Crozat-Williams, Winnie Wong-Ng, Michael Witt, Jerome May, Larry Dahl, Steve Watkins, Khalil Abboud, Andrea Greene, and Frank Fronczek)

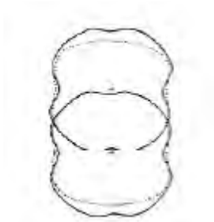
We were indeed very proud that we are the direct academic descendants of Linus Pauling (Watkins —> Dahl —> Rundle —> Pauling).

University of Toronto. After my LSU training, I worked at the Chemistry Department of the University of Toronto, Canada (UT), as a research associate and part-time lecturer. I spent six fruitful years with Professor Stanley Nyburg, learning a great deal. My work included research in areas of theoretical and experimental crystallography.

Stan Nyburg in his office (1960's)

Winnie in Stan Nyburg's lab at UT (1976)

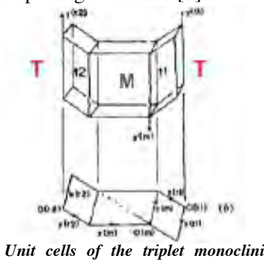
Two particular projects stood out at UT. By applying knowledge of MO calculations, we were able to explain the crystal structure of dichlorine by invoking the principle of zero net crystal force. A spherical atom-atom 6:12 potential does not predict the observed



Shape of the effective atom-atom potential in solid chlorine; broken line: effective shape of the atoms in the crystal

Cmca space group, even including point quadrupole interactions. When one uses difference-electron density and replaces a spherical atom-atom potential by one that is flattened at the poles, the structure is correctly predicted and it is free from internal crystal forces. Our results reflect the non-spherical nature of the dispersion-repulsion forces in structures that have polarizable atoms (the effective shape of these atoms in the crystal is flattened at the top). This is an important concept for interpreting structures [1].

Another work that I am proud of is that of the structure solution of a triplet crystal (a monoclinic form sandwiched by two triclinic forms) of a complex natural product (quasi-racemates of (-)-podopetaline and (-)-ormosanine; both crystal forms have 92 independent atoms per unit cell) [2].



Unit cells of the triplet monoclinic and co-crystallizing triclinic polymorphs of the quasi-racemates of (-)-podopetaline and (-)-ormosanine

Back in the late seventies, we had to use the Weissenberg and precession cameras and a semi-automatic Picker diffractometer to attack this complex problem (I almost gave up a few times). We also found that the triclinic and monoclinic components, while quasi-racemates, like those of many genuine racemates, cannot be resolved by crystallization.

Stan helped me a great deal in areas outside of science. We encouraged each other to receive our piano training at the Toronto Conservatory of Music. We had much fun. Stan is an excellent player and is at a much higher level than I. I miss his piano playing. My daughter Connie was born when I was at UT. In the baby's first six months, I took her to work and Stan even helped out baby-sitting. The 'baby' is now a cardiologist teaching at the University of Colorado. Time indeed flies.

After Stan's UT retirement, he still remained active for many years at the Kings College, and University College London. In 2010, to celebrate his 85th birthday, Stan's former graduate students and postdocs (led by Vlad Kochman) gathered at the UT Chemistry Department. The chemistry building has changed quite a bit, with a new wing added. Some of us met each other for the first time. Our ACA treasurer Sue Byram of Bruker and I studied under Stan at different times.

Stan Nyburg's 85th Birthday reunion at UT (2010)

Winnie Wong-Ng reminiscing with Stan Nyburg at his 85th birthday party

We reminisced about our past and had a great time. Stan still looked the same, always with a great sense of humor. We even talked about possibly working together in the future.

JCPDS/ICDD. In the late seventies, it was difficult for me to get a faculty job or full-time research position in Canada, so I decided to come back to the States. But without a landed-immigrant status it was rather difficult. Around the end of 1981, I had an opportunity to work for a non-profit organization called the Joint Committee on Power Diffraction Standards (JCPDS), which later became the International Centre for Diffraction Data (ICDD), as an X-ray Crystallographer/Critical Review Scientist. It was there that I began my next crystallographic venture, into powder diffraction and database development. ICDD is a scientific organization (with about 300 international members) and a publishing house. It publishes the Powder Diffraction File (PDF) and other database-derived products for materials characterization.

I spent two years at the JCPDS headquarters in Swarthmore, PA. My two-year contract was to critically review 40,000 diffraction patterns, conduct software development, and create a computerized database [3]. I really enjoyed the challenge, because back then I didn't have experience in powder diffraction. The early eighties were known to be the time of the 'renaissance of powder diffraction'. Advances in powder diffraction instrumentation and the availability of advanced software for data collection, reduction and determining/refining structures from powder patterns all contributed to the renaissance.

My review/editorial work couldn't have been successful without the editorial program (AIDS*83) that had become available at the time (co-authored by Cam Hubbard, Alan Mighell and Judy Stalick) [4]. This made it possible to modernize the powder diffraction data by converting it from paper to electronic form. At JCPDS headquarters in those years, I was grateful to Frank McClune (then Editor-in-Chief), Jesse Caum and Julian Messick (general managers) for their guidance. Unfortunately they have all passed away in recent years.

ICDD had an associateship group at the National Bureau of Standards (NBS), in Washington DC to prepare high-quality experimental diffraction patterns to be included in the PDF as phase characterization references. The associateship program was a long-standing (over 35 years), successful industry-government cooperation. After my project was on the way to completion, I requested and received an ICDD associateship at NBS. When I arrived at the beautiful NBS campus in Gaithersburg, MD, I was amazed at the potential opportunities.

Before I became a U.S. citizen in 1988, I couldn't be hired

directly by NBS, and I was a research associate through Jim Stewart at the University of Maryland. (Jim was the 2001 ACA Fankuchen awardee; his memoir was the first in the ACA Living History series and is available online at the ACA History website.) Jim's knowledge of computer software was legendary. I remembered that while I was a graduate student, Steve Watkins had mentioned that Jim was one of his heroes because he had transformed the field of crystallography with his computer skills. As a graduate student, we used Jim's computer software suite XRAY for our structure solutions. (We even enjoyed reading its Ozymandias error messages.) So I was very happy to be associated with Jim on our powder diffraction work (Jim passed away a few years ago in PA). I also learned powder diffraction from Cam Hubbard (liaison of the ICDD research associateship with NBS), Howard McMurdie (leader of the ICDD research associateship; we called him Mac), and other NBS Research Associateship colleagues. Both Cam and Mac were amazing mentors and friends. In 1988 Cam was relocated to ORNL and later became the Director of their High Temperature Lab. Mac was at NIST for more than 75 years, and he passed away at 99½ (not before he revealed his secret of longevity: a bar of chocolate, a shot of whiskey/bourbon plus a glass of red wine per day). The associateship had a number of important publications in those days. In addition to various high-quality reference patterns, we also had papers concerning methods for producing reference patterns [5] and how to use standards for diffractometer calibration [6]. The ICDD/NBS Research Associateship Program was successfully concluded in 1986.

In 1986, the mission of the JCPDS/NBS collaboration was accomplished. The associateship members received a certificate from the NBS Deputy Director Ray Kammer (back row, at left). Winnie is in the front row, at right).

Working in powder diffraction helped me understand the applied side of crystallography. Through ICDD I had opportunities to develop contacts and future research collaborators from industry, universities, and other government labs. Nowadays it is important to perform collaborative research work, and ICDD played an important role in preparing me for my current career.

NBS/NIST. In 1988 I was hired by NBS. President Teddy Roosevelt founded NBS in 1901 with the mission to provide standard weights and measures for international trade purposes, and to serve as the national physical laboratory. In 1988, NBS changed its name to National Institute of Standards and Technology (NIST) to meet new missions including technology development.

In the past 27 years, my work at NIST included largely metrology development, and studies in crystallography, crystal chemistry, phase equilibria, and modeling of technologically important materials (microwave dielectrics, ferroelectrics, superconductors, thermoelectric materials, and carbon dioxide capture materials). The techniques that we use include single-crystal X-ray diffraction, powder X-ray and neutron diffraction. We also use thin film combinatorial methods to conduct high-throughput synthesis and characterization for energy-conversion materials. I was involved in several important projects, including (1) Standard Reference Materials (SRM) development for single-crystal diffractometers (***http://www.nist.gov/srm***) [7], (2) DOE funded (15 year) multidimensional phase diagrams, crystal chemistry and crystal structures for three generations of high T_c superconductor materials [8, 9]; (3) metrology and data for thermoelectric materials [10-13]; (4) carbon mitigation materials and measurements [14]; and (5) environmentally enhanced crack growth [15,16]. I have had many talented collaborators from NIST and outside organizations. It was through all these important collaborations that 800 powder diffraction patterns, 50 phase diagrams for technologically important materials, and more than 300 scientific papers have been produced.

My Involvement with ACA and USNC/Cr. I began involvement with ACA when I was a graduate student, through Steve Watkins. I enjoyed being a member, attending annual meetings, presenting talks, and meeting the 'heroes' of the field. In later years, I organized several symposia/sessions and served on several committees (the Warren Award Committee, Continuing Education Committee, Nominating Committee, and the Data, Standards and Computing Committee).

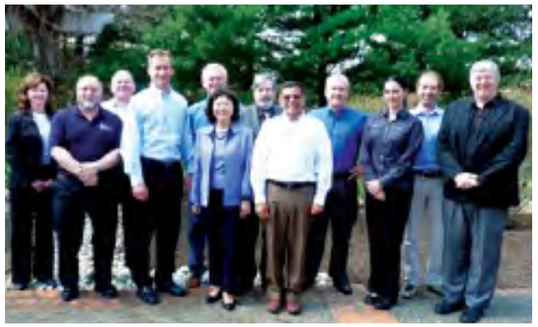
I had the honor of being the local chair of the 1998 annual meeting (under ACA President Penny Codding) held in the Washington, DC area (Crystal City, VA). We worked with program chair Louis Delbaere of University of Saskatchewan, Canada. Together with the hard work of local committee members (Judy Flippen-Anderson, Jeff Deschamps, Charlie Prewitt, Gabrielle Long, Jeff Post, John Barnes, Howard Evans, and others), everything went well - even though we do recall some hair-raising moments. When the meeting hotel (Washington, DC Marriott) pulled out six months prior to the conference due to unforeseen renovation, the committee nearly panicked. But thanks to Judy Flippen-Anderson and ACA treasurer Jane Griffin's ingenious work, not only did we find a nice substitute in Crystal City, but also Marriott compensated ACA financially, which enabled us to have our dinner at the Smithsonian Natural History Museum, as well as providing funding for some other events. During the meeting, we also brought in reporters for a 'meet the press' session to increase our visibility. Together we had a great time organizing and executing the conference. I was very sad that Louis passed away in 2009.

In 2001, NIST celebrated its centennial anniversary. Since NIST has a long history of crystallographic research, a special symposium was co-organized by Alan Mighell and me at the ACA annual meeting in Los Angeles to celebrate this special occasion. Talks included high-pressure, neutron, protein, and synchrotron crystallography, and crystallographic databases. We

also co-edited a special issue of the *J. Res. Nat'l Instit. Stand. Technol.*, entitled 'Crystallography at NIST' [17].

In 1999, Connie Rajnak introduced me to USNC/Cr, first as a member at-large. From 2000-2003 I served as the treasurer and secretary. The involvement with USNC/Cr really opened my eyes. I learned about a number of important issues and policies, as well as the importance of support of national facilities, and the functional relationships between IUCr, ACA and USNC/Cr. During my tenure, the USNC/Cr Chair, Marvin Hackert of UT Austin (current IUCr president) helped me tremendously so that I could fulfill my job as the secretary. I always look back to those days with fond memories.

My Involvement with other Diffraction and Materials Societies. After I left ICDD as a staff member around 1986, I became a member of the ICDD scientific organization and have since been involved with various activities, including serving as chair of several task groups, of the Ceramic Subcommittee, and of the Membership Committee. In 2010, I was elected as an ICDD/Board of Directors (BOD) member-at-large for four years.



ICDD BOD members, ca. 2013 (L–R: Terry Maguire, John Anzelmo, David Taylor, Scott Misture, David Balzar, Winnie Wong-Ng, Jordi Rius, Miguel Delgado, Tom Blanton, Vanessa Peterson, Matteo Leoni, Tim Fawcett)

It was a great experience. The BOD is an important team that works with the Executive Director (currently Tim Fawcett) to manage and guide the organization. We met twice a year to discuss both the business side (financial status, scholarship sponsorship, and the grants-in-aid program for generating quality patterns for the PDF, and others) and the scientific side of the organization. We worked diligently to improve the powder diffraction database and its derived products for scientific applications. ICDD is also involved in organizing and executing the Denver X-ray Conference. We establish scholarships to support graduate students currently working in crystallographic areas. We discuss how to interact/collaborate with other international organizations. Like other scientific organizations, we have to protect and improve our products to benefit the scientific community and maintain the growth of the organization. The job as an ICDD BOD member is always challenging but rewarding.

I have been a member of the American Ceramic Society (ACerS) and the Materials Research Society (MRS), both since 1986. ACerS is divided into 10 divisions. I am a member of the Electronics Division and the Basic Science Division. I became the chair of the Electronics Division in 2006, and have served as a member of the Nominating Committee and Publication Committee, and as an associate editor for the *Journal of the American Ceramic Society*. MRS was founded in 1973, and it is one of the largest materials societies. I have organized a number of conferences and workshops throughout the years involving diffraction science and high T_c superconductors. The annual meetings of both Material Science and Technology (MS&T, of which ACerS is a member) and MRS often have a strong component involving diffraction science. These might be possible venues for ACA to co-organize special symposia.

Afterthoughts. Throughout my career, I have had many opportunities to work in diverse laboratories (industry, university, and government, from basic science to applications). I have worked on crosscutting disciplines involving materials science, chemistry and physics, with materials in different forms (single crystals, powder, bulk materials and thin films). These opportunities gave me different perspectives as a scientist. I have been fortunate to work with many talented collaborators and postdocs/students to develop models, to understand the relationships of fundamental structure and properties, and to develop standard reference materials and reference data. All these years, I did notice that regardless of what material areas I worked on, crystallography has always been at the center of my scientific activities, playing a pivotal role. It has always been the foundation for the understanding of new fields. I believe that we, as crystallographers, are the lucky ones that hold an important position in science. We are the link between different branches of the solid-state sciences. Our association, ACA, therefore is and will always be a key link to other scientific organizations.

Winnie Wong-Ng

References:

[1] *Proc. Royal Soc. London Ser A* **367**, 29 (1979); [2] *Acta Cryst. B* **40**, 151 (1984); [3] *Adv. X-Ray Anal.* **26**, 87 (1982); [4] *NBS Technical Note 1141* (1981); [5] *Powder Diffr.* **1**, 40 (1986); [6] *Powder Diffr.* **2**, 242 (1987); [7] *J. Res. Nat'l Instit. Stand. Technol.* **106**, 1071 (2002); [8] *Physica C* **377**, 107 (2002); [9] *Phys. Rev. B* **41**, 4220 (1990); [10] *Appl. Phys. Lett.* **91**, 132102 (2007); [11] *Solid State Sciences* **48**, 1 (2015); [12] *Chem. Mater.* **23**, 1491 (2011); [13] *J. Mater. Res.* **26**, 1983 (2011); [14] *CrystEngComm.* **15**, 4684 (2013); [15] *J. Am. Ceram. Soc.* **75**, 3097 (1992); [16] *Fracture Mechanics of Ceramics* **12**, 219 (1996); [17] *J. Res. Nat'l Instit. Stand. Technol.*, Crystallography at NIST, **106** (6) (2002).

Index of Advertisers

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 first submitted solutions to the previous ones. As always, I will be pleased to see your solutions (*ffroncz@lsu.edu*) and your ideas for future puzzles.

Frank Fronczek

Crystal Connections #6

What do the answers to these clues have in common?

1) Fossilized tree resin, *electrum* in Latin

2) Felid of genus *Acinonyx*

3) Norman _____, 1066

4) Sound of stepping on very cold snow

5) Solids with long-range order

6) Carbon allotrope, space group 227

7) Element or planet

Previous Crystal Connections – Locations of some synchrotrons in the Americas:

1) "Grassfields" in Portuguese – Campinas, Brazil (*Laboratorio Nacional de Luz Sincrotron*)

2) "POW City" or "City of Bridges" – Saskatoon, Saskatchewan (*Canadian Light Source*)

3) Gave element 97 its name – Berkeley (*Advanced Light Source*)

4) The old state capitol is "pathetic", and should never have been built in this otherwise honorable place, according to Mark Twain in *Life on the Mississippi* – Baton Rouge (*CAMD*)

5) Located far above Cayuga's waters – *Ithaca* (*Cornell High Energy Synchrotron Source, CHESS*)

6) Irving Berlin wrote patriotic songs at Camp Upton here – *Brookhaven* (*National Synchrotron Light Source*)

7) Home of Lemont Quarrymen baseball team is near here – *Argonne* (*Advanced Photon Source*)

The first to provide the correct solution were **Marian Szebenyi** (MacCHESS) and **Frances Bernstein** (retired, Protein Data Bank, Brookhaven National Laboratory). Marian was also the first to solve the DISORDERED puzzle. She points out that the *Stanford Synchrotron Radiation Lightsource* is missing from the list. My apologies for the oversight. Here's a belated clue: 8) "Leland's farm in the tall trees".

Send me those answers and comments!

Frank Fronczek
ffroncz@lsu.edu

DISORDERED

Constructively recombine these scattered words

FERRETINE							
SNORTANE							
CELISTA							
CLAPHRISE							

Answer:

The long-winded lecture on scattering theory was

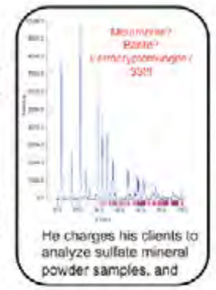
DISORDERED

Correctly index the following words to identify the pattern

TRANYHIDE	A	N	H	Y	D	R	I	T	E
TEDRIVEL									
RUINIGE									
TIMEPOSE									
TETESICLE	C	E	L	E	S	T	I	T	E

Answer:

H E " G Y P S U M "



He charges his clients to analyze sulfate mineral powder samples, and

MAY 2016

27-Jun 5 **49th Erice Course – High-Pressure Crystallography: *Status Artis* and Emerging Opportunities**. Erice, Italy
http://crystalerice.org/2016/

29-Jun 3 **ISC Granada 2016. 5th Granada International School on Crystallization (ISC2016)**. Granada, Spain
www.iscgranada.org

JUNE 2016

26-Jul 1 **7th European Charge Density Meeting**. Warsaw, Poland
http://ecdm7.chem.uw.edu.pl

26-Jul 1 **26th Goldschmidt Conference**. Yokohama, Japan
http://www.geochemsoc.org/programs/goldschmidtconference//

JULY 2016

10-14 **8th American Conference on Neutron Scattering**. Long Beach, CA
http://www.mrs.org/acns-2016/

22-26 **ACA 2016 Annual Meeting**. Denver, CO
Program Chairs: Amy Sarjeant & Edward Snell
www.AmerCrystalAssn.org

AUGUST 2016

7-10 **5th International Symposium on Diffraction Structural Biology**. Knoxville, TN
https://conference.sns.gov/event/2/

28-Sep 1 **30th European Crystallographic Meeting – ECM30**. Basel, Switzerland.
http://ecm30.ecanews.org/ecm2016/home.html

OCTOBER 2016

6-11 **1st Pan African Conference on Crystallography.** Dschang, Cameroon
www.iycr2014.org/__data/assets/pdf_file/0005/113927/FLYER-version-finale.pdf

NOVEMBER 2016

27-Dec 2 **MRS Fall Meeting & Exhibit.** Boston, MA
http://www.mrs.org/fall2016/

DECEMBER 2016

4-7 **14th Conference of the Asian Crystallographic Association. AsCA2016.** Hanoi, Vietnam
http://www.asca2016.org

FEBRUARY 2017

11-15 **Biophysical Society. 61st Annual Meeting.** New Orleans, LA
http://www.biophysics.org/Meetings/AnnualMeeting/FutureAnnualMeetings

MAY 2017

26-30 **ACA 2017 Annual Meeting**. New Orleans, LA
www.AmerCrystalAssn.org

AUGUST 2017

21-28 **24th Congress and General Assembly of the IUCr.** Hyderabad, India
www.iucr2017.org

JULY 2018

20-24 **ACA 2018 Annual Meeting**. Toronto, ON, Canada.
www.AmerCrystalAssn.org

NOTE: New schedule for ACA 2016 Annual Meeting: The meeting will begin on ***Friday, July 22***. The ***workshops*** will be scheduled for all-day on Friday with the ***opening reception*** on Friday evening. The ***exhibit show*** will open Friday evening and end after the Monday poster session.

Poster sessions will run Saturday – Monday, and ***lecture sessions*** will run Saturday – Tuesday. The ***awards banquet*** will take place Tuesday evening, and ***session planning for 2017*** will be on Wednesday morning.

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