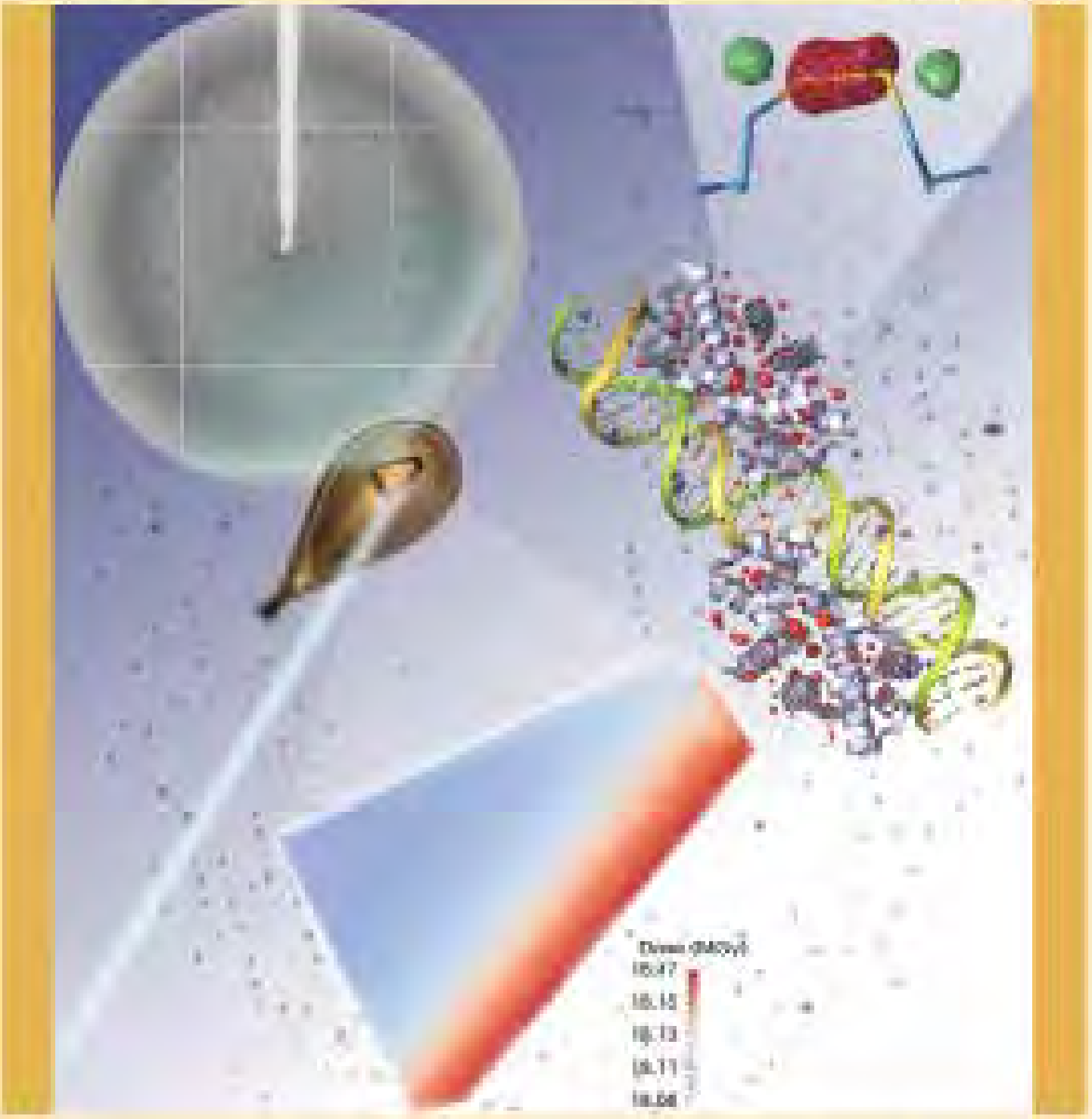
ACA RefleXions

American Crystallographic Association Structure Matters

Number 2

Summer 2016



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ACA RefleXions

Summer 2016

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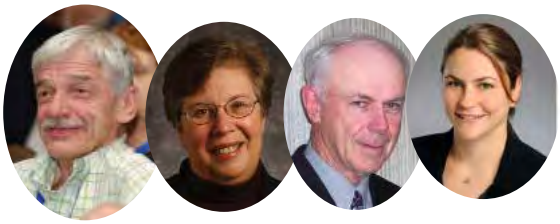

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Hi ACA Members!

You'll probably be reading this just around the time of our terrific 2016 ACA annual meeting in Denver, Colorado! Our 2016 Program chairs, Amy Sarjeant (CCDC) and Eddie Snell (HWI) and their session chairs have put together an exciting meeting with something for every kind of structural scientist including sessions on methods, education, mineralogy, hot structural results, and hot new techniques such as cryo-electron microscopy and femtosecond laser serial crystallography. Additionally, I am excited to report that the presentations in the *Transactions Symposium* on *Structural Dynamics* will be published as a special topic issue in *Structural Dynamics*, our own ACA journal.

Did you ever wonder who decides what sessions there should be at the ACA meetings? Well, the answer is…you! Or at least you can!

Here is how it works. The ACA has 12 Scientific Interest Groups (SIGs), and each one of these SIGs gets to sponsor one or more sessions. The 2016 SIGs (and their chairs) include: Biological Macromolecules, Barry Finzel (University of Minnesota); Fiber Diffraction, Joseph Orgel (Illinois Institute of Technology); General Interest, Graciela Diaz de Delgado (University of the Andes in Venezuela); Industrial. Eugene Cheug (Amgen); Light Sources, Allen Orville (Brookhaven National Laboratory);Materials Science, James Neilson (Colorado State University); Neutron Scattering, William Ratcliff (NIST): Powder Diffraction, Tiffany Kinnibrugh (Argonne National Laboratory); Service Crystallography, Victor Young (University of Minnesota); Small Angle Scattering, Alex Hexemer (Lawrence Berkeley National Laboratory); Small Molecules, Yulia Sevryugina, (Texas Christian University), and Young Scientists, Martin Donakowski (Naval Research Laboratory). You can learn more about the SIGs at ***www.amercrystalassn.org/content/pages/main-special-interest-groups***.

You can join one or more SIG when you pay your dues and you can use that connection to help choose what goes into the next annual meeting!

Each year, during the meeting, all SIGs meet to plan sessions in their subject area. Any ACA member (and particularly any one who has joined a SIG) can come to the planning session where ideas for sessions are proposed. Often, more than one SIG will work together on planning a joint session.

The morning after the meeting ends, the program chairs meet with the SIG chairs to plan the overall schedule for the next meeting. There are usually more sessions proposed than there are slots available, so the SIG chairs propose sessions they would most like to have. What follows is a lively, give and take, discussion that results in a diverse and exciting set of scientific sessions for the next meeting. To fill things out session chairs/organizers are proposed for each session.

An important aspect of the meeting planning is ensuring that the sessions adequately represent both the breath of research interests and overall diversity found within our membership. The ACA has formally adopted a speaker policy (***www.amercrystalassn.org***/speaker-policy) that emphasizes the importance of ensuring this diversity. The ACA also enhances the opportunity for giving an oral presentation by ensuring that 40% of the talks are selected from submitted abstracts.

The program chairs then invite an ACA member to chair each session. The chairs are responsible for inviting some of the speakers in their session and for advertising the session to encourage others to submit abstracts. Once all abstracts are in hand, the session chairs choose their final set of speakers, and chair the session at the meeting itself.

Now that you know how the sessions at the ACA meeting are organized, be sure to take part in the process in Denver and suggest some great sessions for 2017 in New Orleans!

I hope to see you all there – all the best,

Tom Terwilliger

Highlights from 2015 Fall ACA Council Meeting

The 2015 fall council meeting was held at the ACA office in Buffalo, NY on October 20th. Several important issues addressed during this meeting included efforts to increase membership and a succession plan for ACA headquarters.

The ACA is a member organization of the American Institute of Physics (AIP), which most members recognize as the publisher of *Physics Today*. Many members may not be aware that the AIP has the potential to provide various services to the member organizations, and President Chris Cahill has met with AIP CEO Robert Brown to discuss possible ways the AIP could provide support for membership retention and recruitment, as well as administrative duties and fund raising.

Vice President Tom Terwilliger has been active in promoting the use of social media for the ACA as a means of communication with members by the appointment of Vicky Doan-Nguyen as the new social media guru, and the launch of the ACA's Twitter and Instagram accounts. He also reports that he has recruited John Helliwell to chair the Patterson Award committee, and that Yulia Sevryugina and Ilia Guzei have agreed to be program co-chairs for the 2017 ACA meeting in New Orleans.

Michael James, the Canadian Representative, reported on several Canadian meetings, including the annual *Canadian Light Source Users Meeting, the 24th Annual Buffalo-Hamilton-Toronto Symposium,* and the *6th Canadian Chemical Crystallography Workshop* (CCCW15, where 15 refers to the year held, not the number of workshops). The Canadian National Committee for Crystallography (CNCCr) is currently shifting from being organized and run by the National Research Council (NRC) to the Canadian Light Source in Saskatoon, where their new head

office will be located. A second teleconference of Canadian crystallographers was to be held in late October/November 2015.

Hanna Dabkowska, the IUCr Representative to the Council, presented the proposal being considered by the IUCr Executive Committee (EC) to establish a voluntary IUCr Associates Programme, funded by a modest dues structure. The stated goals of the Programme are in, "promoting a sense of belonging for our professional community and [to] enable us to better serve our community and support worthy activities." Key aspects would include: 1) voluntary program; 2) a way of promoting our profession and identifying and serving our professional community and Regional Associates; 3) benefits – in addition to knowing that your voluntary dues will help deliver programs and support worthy activities, there will be a reduction in costs of selected services such as open access; 4) modest dues. Specific details of the *Associates Program* will be determined at a later date and announced on the IUCr web site. In addition, the IUCr EC has approved $11,000 in support of the 2016 ACA meeting in Denver, and also to-date in 2015 had approved support for 33 International meetings, including four regional meetings.

This was Martin Donakowski's first Council meeting as the YSSIG representative, and he outlined the main goals of the SIG as recruitment/increased participation; increased diversity; increased undergraduate participation; professional development; public outreach; establishing a social media presence; increased use of the ACA web site; and fund raising. The SIG found the distribution of travel grants at the YSSIG meeting and the waiver of registration fees for the 2015 Etter Award Winners to attend the 2016 ACA meeting to be an effective means to increase SIG participation. Future meeting plans include increasing the depth of the professional development seminar, by providing a lengthier Monday evening session at the Denver meeting with assistance from the Industrial SIG, and a full-day Saturday workshop at the 2017 New Orleans meeting. The YSSIG obtained sponsorship from many companies for the 2015 ACA meeting, and they are searching for more sponsorship for future activities, including the 2016 ACA meeting. The YSSIG is also actively expanding the use of social media and the ACA web site.

Despite a slow decrease in total membership, the ACA remains financially sound. Changing the starting day of the annual meeting to Friday, has resulted in a significant savings in charges from the event hotel. Chief Financial Officer S.N. Rao suggested that the Council consider hiring a private company to conduct a fund-raising campaign in order to build up an operating expense endowment, which could help provide funds to trim costs for the annual meeting, for student travel funds and for other general outreach activities. The Council decided to form a subcommittee to address the issue of fundraising in more depth.

Many of the ACA named award funds have balances that are significantly higher than the recommended minimum amount required for generating funds for those awards, and CFO Rao recommended a reallocation of this surplus restricted awards endowment principal in order to create new awards; Council approved this action.

The annual meeting is a core benefit of membership in the ACA, and this was reflected in the results from the survey conducted at the 2015 Philadelphia meeting. The take-away from the survey is that people really do value the science presented at the meeting. Constructive criticisms included a sense that there should be a greater emphasis on professional development and value for younger scientists. With that in mind, five workshops will be provided at the 2016 meeting in Denver on the topics of serial crystallography with free electron lasers, the CSD Python API, Advanced SAXS, magnetic structure, and *SHELX*. There was much discussion about possible meeting sites for 2019 and 2020, and all agreed that incorporation of planning input from the vendors will be critical for the future success of these conferences.

At the 2016 annual meeting the ACA will present the Patterson Award and the first Rognlie Award. The Council has also approved the creation of a new award: the President's Service Award, to recognize a non-crystallographer (and non-ACA member) who has provided meritorious service promoting science in the public sphere, to be awarded at the discretion of the ACA President.

The ACA Headquarters currently resides in Buffalo, NY and is staffed by Chief Executive Officer William Duax and Director of Administrative Services Marcia Colquhoun, with Membership Secretary Kristina Vitale. Chief Financial Officer S.N. Rao, in addition to Duax and Colquhoun, have announced plans to transition out of these positions within the next 3-5 years. Council approved the formation of a Transition Committee composed of non-council members to work out details of these transitions and to make recommendations at a later date on succession plans.

Diana Tomchick - ACA Secretary

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2015 and 2014

CURRENT FUNDS (2015)		TOTALS	
		2015	2014
ASSET4			
Current Assets:			
Cash	131,807	131,807	128,727
Investments (unrestricted)	657,111	657,111	570,598
Investments (restricted)	521,967	521,967	459,592
Inventory			6,393
Accounts Receivable	0	0	0
Total Current Assets	1,254,702	1,254,70	1,165,310
Fixed Assets:			
Computers and Printers	0	0	0
Office Equipment	0	0	0
Accumulated Depreciation	0	0	0
Total Fixed Assets	0	0	0
TOTAL ASSETS	1,254,702	1,254,70	1,165,310
Liabilities:			
Unearned Revenues	75,264	12,400	12,400
Credit Card Liabilities	0	0	0
Total Liabilities	75,264	12,400	12,400
Fund Balance:			
Unrestricted	657,111	657,111	693,318
Restricted	521,697	521,697	459,592
Total Fund Balance	1179,078	1179,078	1,152,910
TOTAL LIABILITIES & FUND BALANCE	1,254,702	1,254,70	1,165,310

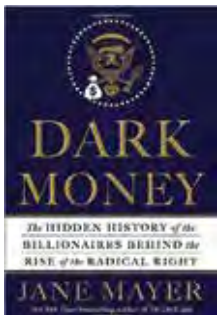
*** Current Balances in individual restricted funds -** ***as of December 31, 2015***

Bau Neutron Award	36,249
Buerger Award	38,978
Rognlie Award	60,000
Etter Award	68,549
Fankuchen Award	71,343
Patterson Award	48,786
Pauling Award	38,390
Supper Award	12,661
Student Travel Fund	21,247
Trueblood Award	40,459
Warren Award	31,094
Wood Science Writing Award	54,221

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

History Fund (unrestricted) *www.amercrystalassn.org/history_home*

For this issue's reviews we are turning to the dark side No, I'm not talking about Star Wars, but rather Jane Mayer's Dark Money and Fred Kaplan's Dark Territory.

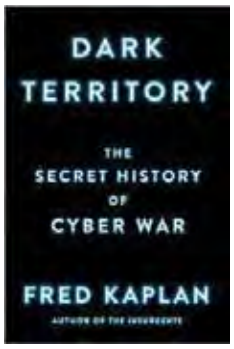


Dark Money: The Hidden History of the Billionaires Behind the Rise of the Radical Right by Jane Mayer, Doubleday, New York City, 2016, 464 pages, ISBN: 978-0385535595.

Dark Money was released in early 2016 with much fanfare. The author is a staff writer for *The New Yorker* and was interviewed on several news shows in so you may have already heard about this book. The first place I heard about was on NPR's *FreshAir*.

Mayer's book follows the libertarian money used to effect political change, mostly the Koch brothers' of Wichita, Kansas, from the early 20th century when Fred Koch built refineries for Hitler and Stalin to the massive, privately owned Koch Industries. Since the landmark Citizen's United case in 2010, there has been a huge growth in the dark funds and Mayer explains from where it came from and where it goes.

The timing of the book is also significant as we approach the 2016 election because there is so much "dark money" pouring into the coffers of certain candidates. This is a must read for the current election cycle lest we forget what happened in the years since 2010.



Dark Territory: The Secret History of Cyberwar by Fred Kaplan, Simon and Schuster, 2016, 354 pages, ISBN: 978-1476763255.

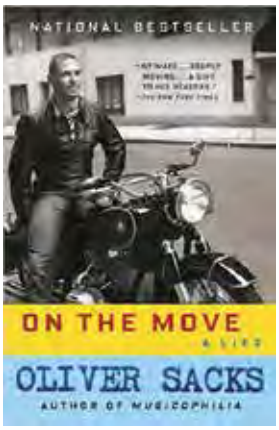
As with the previous title, I heard an interview with the author on NPR's *Fresh Air*. The book provides a detailed history of the cyberwar starting with the question posed by Ronald Reagan to the Joint Chiefs after watching the movie *Wargames* in which a teen played by Matthew Broderick hacks into NORAD and almost starts WWIII – can this really happen? A week later the answer came back: yes. This resulted in National Security Decision Directive 145 (1984) which attempted to set standards for all computers in the US but ultimately settled only on DoD computers.

Yet, in 1997 the so-called Marsh Report showed how vulnerable the military was to hackers. The NSA proved this vulnerability in a war game scenario called *Eligible Receiver* in which they hacked the DoD's command and control capability in significantly less time than they expected – hours not days. Then, in an incident called *Solar Sunrise*, Solaris computers around the world were hacked, also showing how vulnerable the US military was because there were so many in use.

Kaplan has looked at what evolved: computer network defenses, exploitation and attacks, and provided case studies for the most famous incidents. He also provides an analysis of the Snowden whistleblowing and the resultant investigation into the NSA's metadata collection. *Five Guys* headed by Richard Clarke found nothing illegal nor any abuses but also found the situation ripe for both. His report can be summarized to say that *we should respect the NSA but never trust it*.

Joe Ferrera

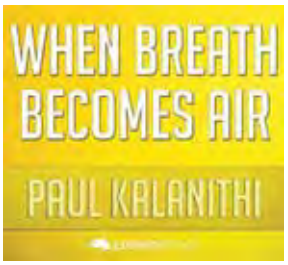
I have also recently read two memoirs written by physicians, the first, Oliver Sacks, a neurologist who lived a long life and, the second Paul Kalanthi, a neurosurgeon who barely finished his residency, both of whom passed away last year.



On the Move: A Life, by Oliver Sacks, Knopf, New York City, 2015, 416 pages, ISBN: 978-0385352543.

I remember when Sacks' book *Awakenings* came out in 1973. I was not old enough to read it, but my mother, who was also a physician practicing in New York City, talked about it with great respect at the dinner table. While I have read other books by Sacks, I have still not read *Awakenings* (although I know I should).

On the Move came out 4 months before Sacks passed away due to a metastasized ocular melanoma in August 2015. This autobiography has some explicit descriptions that I would not recommend for youngsters. The author describes his late childhood and early teens, his coming out, his study of medicine, and his love of motorcycles. He traces his path from Oxford to Montreal to San Francisco to Los Angeles and finally to New York City. He details his compassion for his patients as a neurologist and his ability to tell stories both through his expository writing and this autobiography. There are many interesting anecdotes – for example, his squat record at Muscle Beach in the early 60s and the time he strapped a dying patient to his bike to show her the sun rise at the Grand Canyon. It was his time at Beth Abraham in New York that allowed him to treat patients with post-encephalitic disease with L-dopa that led to his rise to fame. The book ends only eight months before his death, offering a nearly complete autobiographical portrait.



When Breath Becomes Air by Paul Kalanithi, Random House, New York, 2016, 256 pages, ISBN: 978-0812988406.

Paul Kalanithi was a resident neurosurgeon at Stanford Medical Center. He died March 9, 2015 of stage IV metastatic lung cancer. The prologue describes his first inkling that he might be sick, even though his tests came back negative. The first chapter then jumps backward in time, describing his youth moving from Bronxville, New York to Kingman, Arizona with his family and growing up in this forgotten valley; his days as an undergrad at Stanford; a year at Cambridge; and medical school at Yale where he met his wife, Lucy. After medical school they took residency positions in the Bay area: he at Stanford, she at USCF. Paul specialized in neurosurgery and started his residency at Stanford. The second chapter details the progression of his cancer and his daughter's birth. He officially completed

his residency, but could not attend the ceremony because he was too ill. As his health declined, he began writing the book and completed it as best he could. Lucy provides the final chapter, written after his death.

Joe Ferrara

Cristales, Un mundo por descubrir, by Juan Manuel Garcia-Ruiz and Fermín Otálora Muñoz, Triana Science and Technology, 2015, 119 pages, ISBN: 978-84-942454-1-1

Cristales, or *Crystals*, is a visually evocative and concise history of crystals and crystallography and their respective roles in our modern world. Although the majority of the book is in Spanish, there is an index at the end with an English translation of the text. The English translation matches the Spanish text with no loss of fidelity. The book is the catalogue for the titular exhibition held at in Seville, Spain in 2014.

Starting with early man's fascination with faceted objects, the first part of the book, *Paneles* or *Panels*, follows a brief history of crystals and crystallography, with each stage beautifully illustrated with photographs and digital renderings. It ends with the roles of crystals in popular culture and art, famously citing Superman's green alien crystalline Kryptonite as a classic example.

The second part of the book, *Carteles* or *Posters,* is a series of stunning digitally enhanced photographs demonstrating the beauty and pervasiveness of crystals and crystalline structures in everyday life. For example, snowflakes have a six-sided symmetry because of the way the water molecules form a solid crystalline structure at the molecular level. Even something like eggshells, which you probably do not think of as crystalline, are actually composed of very fine calcium crystals.

The third and final part of the book is a series of *Interactivos*,or *Interactives*: detailing the parts of the exhibit that allow you to interact with the concepts of crystalline structure in a more kinetic fashion. This includes standing in a room with suspended orbs, each of which represents an atom or a molecule in a crystalline structure. It helps the reader visualize the orientation of particles in a crystal that gives it such a signature shape.

Like most exhibition catalogues, *Cristales* is visually delightful and certainly a must have for any crystallographer's coffee table.

Jeanette S. Ferrara

Lab Girl by Hope Jahren, Knopf, New York City, 2016, 304 pages, ISBN: 978-1101874936

Hope Jahren's *Lab Girl* is a refreshingly honest and delightfully energetic memoir. Even though I didn't pursue a career in the sciences, I identified with Jahren's recollections of running around and playing in her father's laboratory as a young girl.

Jahren has an impressive resume. A geobiologist, she got her undergraduate degree at University of Minnesota and her PhD at the University of California at Berkeley. She has effectively built three laboratories from scratch, at three different universities: Georgia Tech, Johns Hopkins, and the University of Hawaii at Manoa. Jahren really is, as the title of her book suggests, a "lab girl."

Her work, in her own words, is not earth-shattering or life-changing. She is a geobiologist after all, not a medical doctor trying to cure cancer or Parkinson's. Her research is purely curiosity driven—any marketable or profitable side effect of her research is a perk, which makes it that much more difficult to secure funding—a struggle which consumes much of the latter half of the book. Having worked in a number of labs funded by government grants, it certainly put things in perspective to hear about the process from one of the people who actually deals with all of the paperwork and all of the stress.

Like most memoirs, Jahren's begins with her childhood in rural Minnesota, where her father was a professor at the local branch of University of Minnesota. She details her youth, playing under and around and eventually on the benches in her father's lab—to her, the lab was home.

So it is no wonder that when she went away to college, she immersed herself in laboratory work, not only in the laboratories of her professors but in the pharmaceutical laboratories of the university hospital, where she learned an important lesson: there are two kinds of people in this world—those who are sick and those who are not, and if you fall in the latter category you better find some way to help.

When she went away to Berkeley to get her PhD she met an undergraduate named Bill, a rebel of sorts who was of Armenian descent. Bill then became a steady figure in Jahren's career—her best friend and her colleague, who helped her build her various labs. Bill even lived out of a van during Jahren's earliest years at Georgia Tech, when she was only an associate professor and was unable to secure enough funding to pay him a true living wage. The depth of their professional friendship is enviable, and really drives the trajectory of the memoir's middle section.

Given the dearth of narratives regarding the achievements of women in science, save a few token exceptions like Marie Curie or more recently, Rosalind Franklin, it was nice not only to read about a woman in science, but to read about a woman in science who has the voice to tell her own story.

Jeanette Ferrara

YSSIG Activities

The ACA meeting in Denver is right around the corner and all of us at YSSIG are eagerly looking forward to it. We invite first-time attendees and young scientists with questions about the meeting to attend the ***YSSIG Orientation*** on Friday, July 22nd. This is also a great opportunity to meet some of the current officers and members of YSSIG! If you are interested in getting more involved with YSSIG and ACA, be sure attend the Young Scientists SIG meeting at noon on Sunday, July 24th.

YSSIG will once again host the extremely popular ***Networking Mixer.*** This event, sponsored jointly by ACA and Bruker, is open to all attendees of the meeting; we invite senior members of ACA to attend and meet with students in an informal setting. Admission (which includes hors' d'ouvres and tickets for beverages) is free for students and post-docs! This year's mixer will be held on Sunday, July 24th at Marlowe's Restaurant, within walking distance of the Sheraton. We hope to see you there.

In recent years ACA and YSSIG have encouraged more participation from younger members. To that end, YSSIG will be co-sponsoring the third annual ***Undergraduate Symposium*** with the Society of Physics Students (SPS) on Saturday, July 23rd. This symposium, co-chaired by Kim Stanek and Aaron Celestian, will showcase undergraduate research in the field of crystallography as students are given an opportunity to present posters of their work. We invite graduate students, post-docs, mentors, and other members of ACA to attend. Light refreshments will be provided by SPS; Bill Duax will also give a short talk.

Finally, YSSIG members George Lountos and Martin Donakowski are chairing the **Career Development** session. This session, aimed at early-career scientists, will feature resume and CV critiques and a chance to speak one-on-one with professionals from various fields. Joe York from the American Institute of Physics (AIP) will also give a talk on effective networking and identifying one's skill set that can be applied for careers. Pre-registration is required for a resume review.

Follow us on twitter *@ACAxtal* and *@ACA_YSSIG* to keep up-to-date on news regarding ACA Denver as well as the latest activities of YSSIG. We hope to see you all in July!

Kim Stanek

Net RefleXions

Social media is a ubiquitous presence in our everyday lives, especially for younger Americans .From news reports quoting politician's tweets, to reality tv stars 'breaking the internet' with their photographs on Instagram, to our friends and family updating us on their latest meals *via* Facebook. Social media is, undeniably, an important communication platform. Thus it is not surprising that the scientific community is beginning to utilize the various platforms to reach out to scientists as well as to the public. In this edition of *Net Reflexions*, I will briefly discuss the merits of Twitter as a tool for promotion and engagement.

First, for Twitter, brevity is key. After all, you only have 140 characters to work with. At first, when you just start out, it may seem that each tweet goes off into the great unknown void of the internet. But when you get your first followers (users who bookmark your page so that they can keep up do date with your latest tweets) and you begin following other users and sharing their tweets it doesn't take long for communities of hundreds, thousands, and in some cases of millions are built. Second, Twitter is versatile. By no means are you limited to the very short sentences. You can also post pictures and links and ***bit.ly*** is a great website to use to shorten links so that you still have characters to spare.

In addition, Twitter provides multiple statistics about your page. It can provide a summary of the total number of visits, called impressions, to your page as well as the total number of times all of the links on your page have been clicked. The platform also keeps track of the number of times your tweets have been shared with other users. One statistic that I find particularly useful is the rate of engagement, which is the number of clicks anywhere on your page divided by the number of impressions. All of the global statistics described above are also broken down per tweet, so as a user, you can keep track of which tweets had more impact than others, which links were clicked more often, and which tweets were shared at a higher rate.

So, with these built in features, Twitter is a fantastic platform to promote events and highlights ground-breaking research. Also, since users can follow many different topics, there is a greater overlap between communities creating a greater chance of engaging the general public. Thus, I encourage everyone to first check out ***twitter.com/acaxtal*** for all of latest news pertaining to ACA and then to make your own account to begin showcasing your research and of course the amazingness of crystallography.

Anastasiya Vinokur

Spotlight on Stamps: Early Days of X-Rays: A Tale of Two Hands by Daniel Rabinovich

There are some 25-30 different postage stamps dedicated to the German physicist Wilhelm Conrad Röntgen (1845-1923), who received the first Nobel Prize in Physics (1901) "in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him".

A few of the stamps include a picture of an early X-ray radiograph of a left hand bearing a wedding ring on the fourth digit (*i.e.*, the ring finger). Whose hand is shown on such stamps as well as in many journal articles, books, and online reports describing Röntgen's pioneering work?

The first observation of the hitherto unknown form of radiation was fortuitously made by Röntgen on 8 November 1895. He worked feverishly in the following weeks to establish the key properties of the newfangled rays and, on 22 December, he invited his wife Anna Bertha to his laboratory and showed her the fruits of his labor. He even exposed her left hand (for about 15 minutes!) to a source of X-rays and the ensuing picture became effectively the first radiograph ever recorded. Although the rather blurry image has unfortunately not been depicted on a postage stamp, it appears as a design element in a First Day Cover of the German stamp issued in 1995 to commemorate the centennial of the discovery of X-rays.

On January 23rd, 1896, Röntgen conducted the first public demonstration of the new rays in front of an animated audience at the Würzburg Physical Medical Society. Towards the end of the lecture, he obtained a radiograph of the hand of Albert von Kölliker (1817-1905), a renowned Professor of Anatomy at the local university. The radiograph of von Kölliker's left hand, much sharper than that of Anna Bertha's and showing a better-delineated wedding ring, is the one that is almost always reproduced in articles and books, and has been featured on a few postage stamps as well. Let's just say honors are divided: Röntgen's wife got the first radiograph but von Kölliker got the one that is more often reproduced.

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Dispatch from 2015-2016 American Institute of Physics State Department Science Fellow

I am delighted to follow up on my remarks from the Spring 2016 *RefleXions* dispatch wherein I introduced my participation in the American Institute of Physics State Department Science Fellowship Program. I have been fortunate enough to spend the last several months as the 2015-2016 Fellow and will continue at the Bureau of International Security and Nonproliferation's Office of Weapons of Mass Destruction Terrorism through August 2016. This has been a truly amazing experience and I encourage anyone interested in learning more about the intersection of science and technology policy, for whatever reason, to explore the AIP website or our partner society, AAAS for more details. If this is your first time reading one of my contributions, let me encourage you to dig up your Spring 2016 *RefleXions* for a more through introduction to the mission and activities of our bureau and office.

I promised some more specific details as to my activities over the past year- and here goes. In a nutshell, I work on a combination of programmatic and policy development efforts that seek to enhance the nuclear forensics capabilities of various countries of interest. Some of these countries are those with whom we have formal, bilateral Joint Action Plans, such as Georgia, Armenia, Jordan and Ukraine, whereas engagements with others may be less formal and more *ad hoc*. Programmatic efforts include activities that are budgeted and part of a bigger 'program' of engagement such as workshops, training courses and table top exercises in other countries.

This past March was particularly exciting in this regard as I was selected to support the International Atomic Energy (IAEA) as an instructor for the *Regional Training Course on Introduction to Nuclear Forensics* in São Paulo, Brazil. This was a five day course covering (almost) all aspects of nuclear forensics investigations and how countries may respond to encountering a radioactive or nuclear (RN) material outside of regulatory control (aka MORC). MORCs can come in many flavors from the more benign (mishandled medical waste), to the more nefarious (smuggled uranium). As such, governments need to develop plans for how to handle these events in terms of which agency does what, the safety of first responders and the general public, as well as how to conduct a forensic investigation that maintains the integrity of evidence such that it may ultimately support the prosecution of any wrong doers. My job in this course was to lecture on the flow of an analytical plan - which analyses to do when (mass spec, XRD, etc.) and what types of signatures might be present in a MORC. This was a transformative experience for me- having the State Department and the IAEA demonstrate faith in my abilities to deliver this information in an international forum was both flattering and inspiring. Moreover, the course had a range of participants including first responders, law enforcement, regulators, and legal advisors from 12 Latin American countries. Lecturing with an interpreter was indeed a trip as there was a trifecta of English, Spanish and Portuguese being spoken, and it was a unique experience to see the capabilities, resources, perspectives and priorities of other countries and cultures.

After the course concluded, I stuck around São Paulo for the weekend where (oddly enough) I knew some former DC folks now working at the US Embassy. From there I traveled to the University of Campinas (aka UNICAMP) to give a seminar (that featured way more crystallography than the previous week's efforts) at the Instituto de Química. I met with the staff crystallographer there and engaged with some colleagues with whom I have collaborated for the past several years, including a former student that I hosted at GW in 2013. UNICAMP is in a lovely town and has some wonderful facilities, not to mention a synchrotron.

Returning to stateside State Department activities, I have also been focusing on policy development efforts, which are perhaps a bit less tangible than the programmatic space, but seek to inform US strategy with respect to nuclear forensics globally. For example, there are a number of government agencies that may be involved in supporting nuclear forensics capabilities in a given country. As the State Department provides diplomatic top cover for these agencies and their efforts, it is of interest to have a comprehensive understanding of all of the activities of the various agencies so that one may develop synergies, avoid duplicative efforts and leverage support from across the US government. This is exciting work, yet gets sensitive fairly quickly, so I need to leave it here.

Along these lines is my participation in the 2016 Nuclear Security Summit. The Summit (***www.nss2016.org***), which was the fourth and final of the Obama administration, was held in DC in April 2016. Some 50 heads of state were in town to focus on all aspects of security. My role was that of a Deputy Liaison Officer to the European Union delegation wherein I greeted motorcades, made sure VIPs got to where they needed to be and tracked down any/all requests to make sure diplomacy stayed on track. This was interesting to say the least and I have certainly developed an appreciation for the nuance and subtleties of international engagement and protocol. I rubbed shoulders (literally) with some world leaders.

One last opportunity I will highlight is my participation in the Federal Nuclear Expertise Training Program run by Lawrence Livermore National Lab and funded by the Department of Homeland Security's Domestic Nuclear Detection Office's National Technical Nuclear Forensics Center- or the DHS/DNDO/NTNFC for those in the know. This is an amazing resource open only to properly cleared federal employees and consists of one week of coursework at LLNL followed by four days at the Nevada National Security Site (formerly known as the Nevada Test Site). This was essentially a *Nuclear Weapons 101* course aimed at developing an appreciation for the scale and history of the US weapons program, as well as the evolution thereof since the Comprehensive Test Ban Treaty in 1992. I could fill pages on this experience, yet will limit highlights to meeting an exceptional group of scientists at LLNL and traversing the Nevada desert looking at craters and other impacts of nuclear weapons testing. Sobering and fascinating all at once.

I consider myself exceptionally fortunate to have had all of these experiences. I am eternally grateful to the AIP for the

Fellowship program and for selecting me as a participant. I am eager to return to my teaching and advising duties at GW - enlightened and inspired for the classroom and as a mentor to my graduate students. I feel my perspectives have broadened on a number of fronts, including having a greater understanding as to where scientists can have an impact and feel fulfilled, as well as what skills are required to make one's scientific expertise more broadly applicable. I look forward to engaging with any of you who might be considering this or a related program and please feel free to reach me at ***cahill@gwu.edu***. Thanks for reading!

Chris Cahill

The latest addition to the ACA History website is the autobiography of Philip Coppens, *The Old and the New: My Participation in the Development of Chemical Crystallography during 50+ years*. While he is best known for his pioneering work with charge-density determinations from x-ray diffraction, his memoir describes his research contributions in other fields of chemical crystallography as well.

I regret an error in one of the figures in Cele Abad-Zapatero's Living History in the Winter (2015) issue of *ACA RefleXions*. Here is the corrected figure, right. Cele was one of the first

LDH Kendrew model built at Purdue University in the late 1960s contrasted with FRODO display of the same structure.

users of FRODO [T.A. Jones, *J. Appl. Cryst.* **11**, 268-272 (1978)], graphics software for building, optimizing and displaying protein structures in the computer rather than using physical models. The corrected figure now shows the appropriate contrast between the wire model of lactate dehydrogenase (LDH) with the computer-generated backbone display of LDH in FRODO. In addition to ease of use the new software allowed Cele to reduce the R factor for the LDH structure from 0.45 to 0.24 in a couple of months.

Virginia Pett

Why participate in IUCr2017?

1. This will be a conference with a difference in terms of content and organization. We are seriously considering parallel activities like interactive sessions between students and scientists, industry and academia. Dynamic solutions are required to combat the shortcomings of large meetings, where detachment from the program has become the order of the day especially in younger participants.

2. State of the art, highly convenient facilities at a huge convention center (HICC) will ensure the smooth running of the conference. Posters, lunch and exhibits will be in the same large hall. Electronic posters and electronic abstracts with links to IUCr journals will be freely available throughout the Congress from HICC computer monitors. All IUCr journals will be Open Access from any of the monitors within the Congress venue.

3. The Novotel, a five star hotel attached to the convention center has 225 rooms starting at USD 175, inclusive of all taxes. Many 4- and 5-star hotels are within 2 km. of the convention center, belonging to well-known international chains e.g. Radisson, Best Western, Westin and excellent Indian chains like Lemon Tree and Trident with rooms from USD 100 upwards. Shuttle buses are planned that will ply between major hotels and the conference venue to a fixed time schedule. Taxis will also be available on call outside the conference venue for reasonable rates throughout the day. Student accommodation cum registration packages will be priced very reasonably, in the range of USD 500.

4. Hyderabad is a safe city. Remaining within the confines of the venue and opting for guided city tours arranged by the organizers will keep you safer. You will not be accosted or mugged anywhere. Do not invite trouble for yourself (by going into crowded places, women getting into taxis alone at night) but these are standard precautions anywhere in the world for foreign visitors.

5. It will not be hot in Hyderabad in late August. Temperatures range from 70 to 85°F with chances of an occasional shower. The peak of summer is in April and May.

6. A completely non-spicy lunch prepared at five star standards by the Novotel for all the days of the conference is included in the registration and will be served in the exhibition cum poster area. The conference venue is neat and tidy and very safe. Mineral water and tea/coffee will be available at the HICC throughout the day at very reasonable rates. The Novotel also has several good multi-cuisine restaurants. You will find that Indian food in India tastes very different from Indian food in "Indian" restaurants overseas. It's better!

7. Hyderabad is easily accessed and it is a centrally located city within India. JFK/Newark/O'Hare non-stop to Delhi (15 hours) and then a 2 hour flight to Hyderabad is a convenient option. Alternatively one can use one of the Gulf airports as a hub.

8. Easy air access from Hyderabad to popular tourist destinations within India e.g. Agra, Delhi, Jaipur, Mumbai, Calcutta, Chennai, Goa for sightseeing before and after the conference.

9. Hyderabad is an absolute gem of a place to understand the paradox of India. It was ruled brilliantly for over two centuries by an eccentric and fabulously wealthy dynasty whose diamonds were weighed by the kilogram, pearls by the acre and gold bars by the ton. Yet, its last king was so frugal that he would save on laundry bills by bathing in his clothes!

10. India is not a strange country in which a foreigner cannot manage basic things. English is widely spoken here. There is very little problem with regards to health and sanitation issues. You do not need to take any shots before coming here, unless you are travelling *via* certain yellow fever infected regions of South America and Africa.

11. A poor country with a 7% growth rate...that has confounded its critics and economists worldwide...the scales are tilting, come and see why!

12. An ancient and complex culture that has enchanted men of letters from Romain Rolland to Max Mueller to Albert Einstein. Mark Twain famously said,

13. "So far as I am able to judge, nothing has been left undone, either by man or nature, to make India the most extraordinary country that the sun visits on his rounds. Nothing seems to have been forgotten, nothing overlooked".

See you in Hyderabad!

G R Desiraju, Chair, Local Organizing Committee

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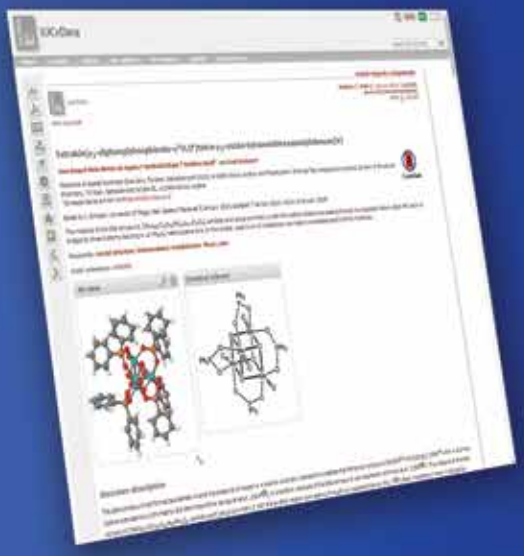

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A Random Walk in the Valley Among Giants: *Crystallography during the ACA's "Middle Ages"*

In 1961 Bruno Morosin joined Sandia Corporation, which later became Sandia National Laboratory. He continued crystallographic research there until his retirement, studying ceramics, hydrides, explosives, effects of high pressure and high temperature, magnetic interactions, ionic conductors, and one-dimensional properties, as he describes in Crystallography in North America, pp 80-83. In this Living History he emphasizes the light-hearted aspects of the many ACA meetings he attended over the years. For example, the photograph below shows Bruno's poster photo for one of the ACA meetings.

The early years of the ACA have been documented by much more knowledgeable and capable individuals than I. And this should also be true for the more recent years. The present account is really the description of the wandering of a lost poor soul among the giants of the field, attempting to recall happenings, essentially in his twilight years, that occurred many decades ago.

1990s – Promises, Promises.

Each year reminds me of the promise I made to Jenny Glusker several decades ago to write my ACA history. Upon many delays, I suggested to some of the "elders" of the Association that those memories might be a series of personal events at various ACA meetings rather than an uninteresting biographical sketch. As I put this together, I realized that occasionally some background material was necessary in order to comprehend the path I took.

2016 – January 1st – Lying Awake.

This morning caused me to think how many Januaries and New Year's Resolutions have passed without any attempt on my part to even begin something for the ACA, even though whatever will be written may very likely be read by a very minimum of individuals. I was reminded as I lay in bed that morning on the first of January that I prepared and distributed my wife's preliminary genealogy in 1995, but only completed it in 2014 after stumbling upon old (1930s) photographs which led me to some near 'cousins' of hers, one of whom recalled meeting my mother-in-law as a child during a visit with her mother in Honolulu. This eventually added some 400 new members of the extended family. I thought I better quit before I stumbled on more. That took almost two decades!! In addition I also need to prepare my own genealogy.

2016 – New Year's Resolutions and George Will.

The need to resolve the issue to write something for the ACA was reinforced by today's local *Albuquerque Journal* (January 2, 2016) with George Will's (*Washington Post* syndicated columnist) discussion on obscure political candidates. Very likely at the 1979 Clemson ACA meeting, Jim Stewart and I had one of our many political discussions over the years, which showed how naive those of us out in the Western frontier were. I only recall this because of Will's column stating the following: "According to Steven Hayward in 'The Age of Reagan: The Fall of the Old Liberal Order', Carter's obscurity was confirmed when he appeared on the syndicated TV game show *What's My Lin*e and he stumped the panel, which not only did not recognize him, but failed to guess he was a state governor. I had a similar reaction when Jim Stewart stated that our next P resident would be the peanut grower Jimmy Carter and I remarked, "Who in hell is he?" That must have been the green light for me to begin fulfilling my promise. But how much background is necessary for some understanding of my path to science and particularly crystallography?

1945 – Innocence and Periodic Table.

I grew up in southern Oregon (Klamath Falls) as one of two boys of a poor immigrant family not knowing English on my first day of grade school. Although I read many books before my fifth grade, it was only then that 'aluminum' somehow was a topic and I asked the teacher what were elements and were there others. She claimed not to know and had me write a letter to the Aluminum Company of America and eventually I received a letter from its chairman, probably a secretary, suggesting I should become acquainted with the periodic table since there were many other elements besides aluminum.

The atom bomb ended the war that year and I became more interested in science. Backing up a bit, Klamath Falls was a lumber and farming area. During WWII, there was the Japanese relocation camp some 30 miles south just below Tulelake, CA, a German-Italian prisoner camp close to Tulelake that provided workers for the farmers – potatoes were a major crop (Klamath "Gem" shipped East to better restaurants, as it was advertised) – a small air base as well as an army base in the mountains to the north (where soldiers and horses exercised in the cold snow for eventual crossing of the Alps, if required). I grew up without a family car or phone, stocked grocery shelves after school, Saturdays and Sundays beginning in grade school clear into high school. I did discover the town library, which supplemented the one at my grade school. During the sixth grade that teacher, Mrs. Foster, a local historian, interested me in Oregon history. I also spent many non-working hours reading newspapers from San Francisco and Portland, and whatever magazines that were available at that city library.

Bruno in 8th grade (1948)

1951 & 1952 – Science Trips.

My high school chemistry teacher, "Cookie" Carlson, required much memorizing of valences, compounds and inorganic reactions, but to his credit, he organized a week-long bus trip to the San Francisco Bay area for two busloads of students (Cookie and another male teacher were the bus drivers and their wives chaperoned the girls). The trip down included a stop at Shasta Dam to visit the generators, etc., while the return visited the olive groves below Red Bluff. The boys stayed in the handball courts of the Berkeley YMCA while the girls were at a nearby hotel. Our daily schedule was filled with visits to nearby facilities. These included, as I recall, the Standard Oil Refinery (tour and visit of its research facility) and Ford Company (walking next to assembly line banging out Fords).

Here, as a reader, you need to go online to the ACA History website, if you are still interested in this account. I include the ending below just to whet the appetite.

2014 – Albuquerque and Forgotten.

The most recent Albuquerque meeting illustrates how quickly one becomes forgotten and might raise the question of why I am writing these recollections. The meeting was organized to be in Albuquerque. I discovered that no one ever contacted anyone at Sandia or me. I had been an unpaid consultant ever since I retired, but my lab email was still active, my lab office phone the same for all those decades. On that basis, I decided not to bother to attend. Since no one even attempted to call me during those meeting days, I had just disappeared into the twilight. In fairness, Chuck Campana last year did visit me; I have also been contacted by the Buffalo office concerning dues and obituaries that I contributed. Perhaps similarly to Douglas MacArthur's address to Congress "Old soldiers do not die, they just slowly fade away!" old crystallographer's lives may be archived before they disappeared into the twilight, but will their written memories merely fade away unread?

Tom Workman, Bruno, Sten Samson and Dave Duchamps at the 2001 ACA mixer in San Antonio.

Bruno in a serious moment at the 2006 ACA meeting in Honolulu

2016 – January and Authorship.

"You say the name is Morrison." [the usual].
"No, Morosin."
"Doesn't ring a bell. Morison?" [according to *RefleXions*, Winter, 2015, p 23].
"No, Morosin."
"What exactly did he do?"
"Crystallography."
"[pause...] Really?? What is he known for?"
"Wandering in the field!"
"Morrison??"
"No, Morosin; mo ro ZEEN, if you wish to pronounce the name correctly!!"

2016 – February and Reflections.

Reflections: Not those of the ACA spelled with an "X", but rather some personal thoughts brought on by George Will and his discussion on obscure political candidates. I'm thinking that we need some real obscure, but capable politicos now!! Because it seems to me that this country has backed itself into a real mess and the upcoming elections, regardless of your political leanings, will not be for the faint of heart. In the past Presidential speeches have ended with "God bless America"; perhaps it should be "God save America". One of Jim Stewart's memorable XTAL error messages was, Il gioco è fatto [the game is done] – for all our sakes I hope it's not so!

Bruno Morosin

Editor's note: Bruno Morosin's complete account of his lighthearted ACA reminiscences will soon be available on the ACA History website. While humor is a long ACA tradition, the editor felt that Bruno's personal reflection on the current state of American politcs was a bit too strong – what is printed in Bruno's final paragraph titled "Reflections" are his own reflections as parsed through the editor's 'filter'. For previous examples of ACA humor see ACA Beginnings on our History website: ***www.amercrystalassn.org/history_beginnings***

Puzzle Corner

***Previous Crystal Connections** – They are all crystallographic software packages:*

1) Fossilized tree resin, *electrum* in Latin – ***Amber***

2) Felid of genus *Acinonyx* – ***Cheeta***

3) Norman ***Conquest***, 1066

4) Sound of stepping on very cold snow – ***Crunch***

5) Solids with long-range order – ***Crystals***

6) Carbon allotrope, space group 227 – ***Diamond***

7) Element or planet – ***Mercury***

The first to provide the correct solution was ***Alan Jircitano*** (Penn State Behrend, Erie, PA). ***Frances Bernstein*** submitted the correct solution for the DISORDERED puzzle.

Crystal Connections #7

What do the answers to these clues have in common?

1) Invented kindergarten

2) British Prime Minister

3) Nobel Peace Prize winner

4) Discovered radio waves from the sun

5) Communist who mapped the D-Day landing beaches of Normandy

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Guest Puzzlers are welcome!

Frank Fronczek – ffronc@lsu.edu

DISORDERED

Constructively recombine these scattered words

FERRETINE	INTERFERE
SNORTANE	RESONANT
CELISTA	ELASTIC
CLAPHRISE	SPHERICAL

The long-winded lecture on scattering theory was

Answer: INCOHERENT

As a special for the summer issue, ***Guest Puzzler, Marian Szebenyi*** (MacCHESS), has designed the new DISORDERED puzzle.

DISORDERED

Place the letters in a properly ordered arrangement

NOVELST	
SCATNOCT	
MYSTERYM	
MANEGIKE	
PRIMIDABY	

She blamed the broken vase on the movers' poor...

Answer:

SPECIAL TOPIC ISSUES

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William (Bill) Busing (1923 - 2016)

A few weeks ago we were saddened to hear that we have lost yet another of our 'founding fathers' when Bill Busing passed away on April 14, 2016. Forturnately for us Bill contributed his living history which was published in RefleXions (summer, 2011) and has been archived on the ACA History Portal (http://www.amercrystalassn.org/h-busing_memoir). What follows here are a few personal memories and notes.

Carol Brock: I first met Bill Busing at the Spring 1972 ACA meeting in Albuquerque a few months before defending my thesis and starting as an assistant professor at the University of Kentucky. Bill was legendary for having co-authored the widely used *ORFLS* and *ORFFE* programs but he turned out to be friendly and approachable. I had also used Bill's innovative program *WMIN* for doing energy calculations of molecules in crystals. While enjoying the opening reception in Albuquerque he and a few others of us wondered whether such calculations would eventually make possible reliable predictions of molecular crystal structures.

Bill was very helpful during my first years in Lexington. He invited me to give a seminar at Oak Ridge and arranged for me and a student to collect data on the ORNL diffractometer. He introduced me to his colleagues Henri Levy and Carroll Johnson, who were also legends, and he took me home for a home-cooked dinner. He was easygoing and kind.

The code in the Oak Ridge programs was lovely – efficient, logical, highly commented, and remarkably bug free. Later on I would use the printed code to learn how to do such things as calculate a cross product in a triclinic coordinate system. The code was much easier to follow than any textbook.

When my student Yigang Fu was finishing his PhD degree in 1991 he decided to take a postdoctoral position with Bill and Bernhard Wunderlich at the University of Tennessee. The plan was to measure two-dimensional x-ray diffraction patterns from partially crystalline polymer fibers and to then do a 2-D full-pattern refinement analogous to the 1-D refinements pioneered by Hugo Rietveld. A well-cited paper [(Y. Fu, W.R. Busing, Y. Jin, K.A. Affholter & B. Wunderlich (1994). *Macromol. Chem. Phys.*)] was published but the problem proved more difficult than anticipated because of the discovery of an intermediate mesophase.

In 1991 Bill officially retired from ORNL but remained active. At the April 1991 ACA meeting in Toledo Ray Young and I organized a session titled *Structure of Polymers at the Molecular Level* to honor Bill.

A few years ago Bill sent me email greetings from Oak Ridge. He had moved to a retirement home after his wife Judy had passed on but he was still driving and regularly saw a daughter who lived nearby. Several messages went back and forth and I was happy to be able to tell him that the blind tests run by the CCDC on prediction of structures of organic molecules had shown the power of lattice-energy calculations but had also revealed the problem to be more difficult than anyone had suspected. And I was able to thank him for his support during a time that it had really mattered.

Bill once told me that he had started at ORNL with little background in crystallography; as a graduate student at Princeton he had done an electrochemistry project under the direction of Walter Kauzmann. That switch in fields was an early indication of Bill's versatility. He had an orderly and inventive mind, a strong work ethic, and a wonderful way of interacting with people of all kinds. He was modest and had absolute integrity. He was a model as both a scientist and as a person.

Bryan Chakoumakos sent this black and white photograph (courtesy of ORNL) of Bill at work with the very first (as far as Bryan knows) computer –automated four-circle single crystal x-ray diffractometer. The woman in the photo is Sharron Kink, a computer engineer, and the others are J.A. Burkalter (left) and R. B. Splittgerber (right). They described the diffractometer in the following ORNL report: Busing, W. R., Ellison, R. D., Levy, H. A., King, S. P., and Roseberry, R. T. (1968). The Oak Ridge Computer-Controlled X-ray Diffractometer. *ORNL-4143 Report*, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Judy Flippen-Anderson: For the ACA meeting in St. Paul in 2000 Connie (Chidester) Rajnak and I put together an article full of vignettes from previous ACA Presidents. Bill sent us the following letter:

Dear Judy and Connie: I have been looking for photos that you might be able to use, but the only one I can find that has Henri Levy and myself in it was taken at a party in the 1950's. We look pretty young.

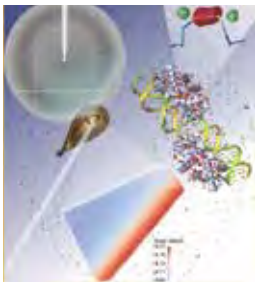
I also have a 4x6 color picture of past ACA Presidents taken at the 1986 McMaster meeting. They include (left to right): Ray Young, Jerry Karle, Isabella Karle, Dave Sayre, Phil Coppens, Sidney Abrahams, Bob Newnham, Bill Busing, Dave Shoemaker, Bill Duax, Ken Trueblood, Dave Harker, John Kasper, and Hal Wyckoff. I think this photo was sent to me by Bill Duax. .

I do remember my first ACA meeting at French Lick, IN, in 1956. At that meeting Joan Clark reported on what I believe was the first crystal structure determined entirely by direct methods. (I think the authors were Clark and Crist and perhaps Howard Evans). Someone, probably Ray Pepinsky, asked what the Patterson map looked like, and when Joan said they hadn't made a Patterson, there was a general gasp of surprise.

As President I remember the 1971 meeting in Charleston, SC. One of the presidential duties that I did not particularly like was being responsible for the protocol at the banquet. Fortunately I had Julie Roth, Secretary Walter Roth's wife, to advise me about seating at the head table. Martin Buerger was there to receive the first Fankuchen Award and Dina Fankuchen was there also. I remember having to intervene when an overly conscientious waiter tried to extract a banquet ticket from the university Vice President. Ben Post gave the banquet address. His topic seemed to be that, while everybody else was interested in information retrieval, he was more interested in information disposal. Imagine what he would have thought about the internet and junk mail!

That's about all I have for now. At this point I'm not sure of how many days I will be in St. Paul, but I will try to be there for the banquet. I'm looking forward to it! Best regards, Bill

Judy continues: Bill did show up in St Paul and was part of the ACA at 50 celebration on the riverboat cruise (see photo below - back row: Penny Codding, Connie Chidester Rajnak, Jenny Glusker, Charlie Bugg, Helen Berman, Jon Clardy, Judy Flippen-Anderson, Bill Busing, Bill Duax, Carroll Johnson, Bryan Craven. Front row: Elizabeth Wood, David Templeton, Robinson Burbank, Sidney Abraham, Abe Clearfield) . Carol's recollections of Bill are very similar to mine. However, we were not collaborators but conspirators. It started a long time ago when I was sitting next to him during a talk during which we were told that we (the younger generation) should mix and mingle with the more senior crystallographers – that they would love to talk to us. I scoffed at this remark saying that the 'pooh bahs' had no interest in meeting us. Bill took up the challenge and made it his personal pilgrimage to introduce me to as many luminaries as he could find at the meeting – and he was right! From that time forward, at each ACA meeting, Bill and I would single out some unsuspecting young crystallographer and introduce him/her to as many bigwigs as we could find. This usually took place during the cocktail hour before the banquet (back in the days when we had an 'open' bar) and then we would sit together and at the banquet and 'critique' the after dinner speaker. It was great fun and provided me with some of my best memories of what it meant to part of the ACA family. When I was elected vice-president Bill sent me a hand-written note of congratulations. He was as outstanding as a person as he was as a scientist. He will be missed.



Elspeth Garman (University of Oxford) will receive the ACA Fankuchen Award in Denver.

Seeking to understand the physical and chemical basis of radiation damage on macromolecular crystals, Elspeth's group focuses on developing improved methods that will enable problems not previously accessible to structure solution to be tackled. They are currently studying 100K and room temperature (RT) radiation damage and are optimizing the data collection strategies for dose spreading in macromolecular crystals.

The image at left, kindly provided by Jonathan Brooks Bartlett and Charles Bury in Elspeth's group, depicts a visualization of a macromolecular diffraction experiment showing the x-ray beam (white) hitting a ~80 micron long cryo-cooled crystal of an RNA-protein complex. The dose was 1.31 MGy (MGy, pronounced mega grey, is the energy absorbed per unit mass. 1 Gy = 1 Joule of energy / 1 kilogram; 1MGy = 1,000,000 Gy). Emanating from the crystal is a representation of the crystal shape used in RADDOSE-3D to calculate the dose distribution (bottom right with color key bar) in the crystal during measurements of a dataset series for a radiation damage study. A structure of a DNA-protein complex (C.Esp1396I) is shown on the right of the image. The sizes of the red balls are proportional to the extent of electron density loss due to damage to the protein, and the blue balls represent the damage to the much more radiation resistant DNA following a dose of ~46 MGy. Top right shows an difference electron density map illustrating the radiation damage to a disulphide bond in insulin which is broken during the diffraction experiment (red and green respectively are regions of negative and positive difference electron density contoured at + / - 6s).

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Experimental Determination of the Radiation Dose Limit for Cryocooled Protein Crystals by Robin Owen, Enrique Rudiño-Piñera & Elspeth F Garman. (2006) *PNAS* 103, 4912-4917.

RADDOSE-3D: Time- and-Space-Resolved Modeling of Dose in Macromolecular Crystallography by Oliver B Zeldin, Markus Gerstel & Elspeth F Garman. *Journal of Applied Crystallography* (2013) 46, 1225-1230.

RNA Protects a Nucleoprotein Complex Against Radiation Damage by Charles S Bury, John E McGeehan, Alfred A Antson, Ian Carmichael, Markus Gerstel, Mikhail B Shevtsov & Elspeth F Garman (2016) *Acta D* (in press), May.

Radiation Damage to Nucleoprotein Complexes in Macromolecular Crystallography by Charles Bury, Elspeth F Garman, Helen Mary Ginn, Raimond B.G. Ravelli, Ian Carmichael, Geoff Kneale & John E McGeehan (2015) *J. Synchrotron. Radiation* 22, 213–224.

Candidates for ACA Offices in 2017

The Nominating Committee (Ward Smith, Martha Teeter and Louise Dawe) proposes the following candidates for the 2017.

Officers:

Vice-President: **Lisa Keefe & Winnie Wong-Ng**

Canadian Rep to Council: **Gerald Audette & Tomislav Friscic**

***Committees*:**

Data, Standards & Computing: **Thomas Proffen & Nick Sauter**

Continuing Education: **Kay Onan & Charlotte Stern**

Communicatons: **Martin Donakowski & Brian Patrick**

To nominate write-in candidates for any office, write to the ACA Secretary: Diana Tomchick, Dept. of Biophysics, University of Texas, Southwestern Medical Center, Irving, TX 75061 (diana.tomchick@utsouthwestern.edu). Letters must be received by September 15, 2016 and must be signed by five ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in October 2016.

Lisa J. Keefe - Vice-President

Director of Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT), Vice-President of Center for Advancing Therapeutics, Hauptman-Woodward Medical Research Institute @ Advanced Photon Source, Argonne National Laboratory

Education: AB in chemistry, Vassar College (1983); PhD in biophysics and biophysical chemistry, The Johns Hopkins University School of Medicine (1992); DOE Alexander Hollaender Distinguished Postdoctoral Fellow jointly at Argonne and Brookhaven National Laboratories (1992-1996); Argonne Scholar (1992-1998)

Professional Activities: Member Biological & Life Sciences Pillar Review Committee, Canadian Light Source (2015); Canadian Macromolecular Crystallography Facility Peer Review Committee (2010-present); Life Sciences Council, APS (2007-present); HHMI Beamline Upgrade Technical Review Committee, ALS (2006); General User Program Advisory Committee, APS (2003-2004); Partner Users Council APS (2002-present); Users Organization Steering Committee APS (2001-2004). ACA - Secretary (2003-2008); Chair YSSIG(1994)

Research Interests: macromolecular crystallography; molecular recognition; high-throughput structural biology for drug discovery; automation and technique development for data acquisition in the synchrotron environment.

IMCA-CAT, located at APS, Argonne National Laboratory, operates a high-throughput macromolecular crystallography beamline aimed at accelerating drug discovery serving the pharmaceutical industry. The facility has expanded in its services for IMCA industry members and now non-member pharmaceutical companies. As a result of this growth, the Center for Advancing Therapeutics was recently established and focuses on synchrotron-based structural biology for pharmaceutical drug discovery programs. Learn more at ***www.imca-cat.org.***

Statement: The ACA is a rich and vital part of our scientific mission. While providing core services including hosting enriching annual meetings, recognizing the groundbreaking research achievements of members, and publishing the notable journal *Structural Dynamics* and informative *ACA RefleXions*, the ACA also serves to advocate for structure-based science, educate future generations of researchers, and provide professional guidance and development as we journey through our careers. We connect with each other as crystallographers and that connection transcends our varied scientific interests that are becoming increasingly diverse, driven by technological advances and expanding research frontiers. Our scientific disciplines are dynamic and thus our scholarly approaches are constantly shifting. The ACA is continually challenged to keep pace with these changes and respond to the evolving needs of crystallographers across the spectrum of Special Interest Groups, across generations, and across academia, government, and industry research environments. As our science grows and becomes more global and more collaborative, we rely on the ACA to provide intellectual space for us to share knowledge, discoveries, and ideas.

I truly am honored to have been nominated as a candidate for vice president of the ACA and enthusiastically embrace the potential opportunity to serve our community. I was introduced to crystallography in the early 1980s during my senior year of college and attended my first ACA meeting a few years later. The exciting science and supportive community of crystallographers shaped my course of graduate study and guided my career. As our science has advanced and our community has grown, the ACA has proven responsive to our expanding needs. Early in my postdoctoral appointment, I and several fellow postdocs had a vision for promoting young scientists and we collaborated on a proposal to ACA for establishing a new special interest group targeted to students, postdocs, and early-career scientists. The ACA was overwhelmingly supportive and, in 1994, the Young Scientists SIG was launched. Over the years, it has been gratifying to observe the growth of the YSSIG and witness the positive impact it has had in propelling the career of so many young crystallographers.

We are fortunate that the ACA is strongly committed to maintaining relevance to our growing scientific interests and fostering cooperative and collaborative environments. My scientific career began in

small molecule crystallography before migrating to macromolecular crystallography. Currently, I work with industry, at a government laboratory, and under the umbrella of an academic research institute. Regardless of the perspective, the ACA has demonstrated flexibility by listening to members, drafting new strategies, and implementing change while traversing the boundaries. Council, the governing body of the ACA, leads this progress. Reflecting on my experience serving as secretary of Council for six years, the committees, Canadian Division, and SIGs are integral components of Council's stewardship of the ACA. Collaboration between these components is essential as the ACA confronts significant challenges in today's limited funding climate, namely increasing the engagement of the crystallographic community, providing relevant benefit to individual scientists across the full spectrum of special interest groups, and ensuring sustainability for future generations. These challenges may seem enormous, but the opportunities are abundant.

As a member of Council, I would lead the ACA by focusing resources on strengthening and growing ACA's core services to members, advocating for structure-based science, educating future generations of crystallographers, and providing the value expected from membership. Specifically, I would foster a collaborative climate in which Council, committees, the Canadian Division, and the SIGs could thoroughly explore and effectively implement innovative approaches to engaging more members. Great benefit can be realized by bridging the crystallography disciplines and connecting with academia, government, and industry researchers. There is no substitute for the annual ACA meeting where we have the opportunity to strengthen our research through face-to-face discussions and advance our careers through networking. As the climate for research funding becomes ever-more limiting and negatively impacts attendance, the ACA can creatively adapt by implementing mechanisms for increasing participation in ways that enhances professional value. While we rely on the ACA to connect with our peers to discuss and debate our research and advance our careers, the ACA relies on us to contribute our time and expertise to advocate, educate, and advance crystallography. As a member of Council, I would guide the ACA on a course for sustainability that would be inclusive across the spectrum of special interests, collaborative between the diverse research environments, and valuable at all career levels.

Winnie Wong-Ng -Vice President

Materials Measurement Science Division, National Institute of Standards and Technology (NIST), Gaithersburg, MD

Education: BSc, Chemistry/Physics, Chinese University of Hong Kong. PhD, Inorganic Chemistry, Louisiana State University (with Steve Watkins); Postdoctoral Fellow/Research Associate/Lecturer in Chemistry Department, University of Toronto, Canada (with Stan Nyburg).

Professional Activities: ACA - Local chair, 1998 meeting, Arlington, VA. Chair/member, Continuing Ed Committee (2001-2003); Data, Standards & Computation Committee (2007-2010); Chair, Warren Award Committee (2005); Chair/member: Nominating Committee (2002-2003); Co-organizer of four scientific sessions (1989, 1992, 1993, 1998). Secretary/treasurer, USNCCr (2000-2003); ICDD - Board of Directors Member-at-large (2010-2014); Chair, Membership Committee (2001-2004); Chair, Ceramics Subcommittee, (1994-2000, 2015-present); Member, Awards and Scholarship Committees (2004-present); Chair, Thermoelectric Task Group, (2006-present); Chair, High-Temperature Superconductors Task Group (1994-2006). Trustee, Electronics Division, American Ceramic Society (ACerS, 2014-2016) and chair (2005-2006); Member, Board of Directors, Applied Superconductivity Conference (ASC) (2006-2010); Editor, *Powder Diffraction* (International reports, 1999 - present); Assoc. Editor, *J. American Ceramic Society* (2012-present); Co-organizer of more than 40 symposia/workshops at various scientific meetings; Co-leader of the "Measurements, Standards, and Data for Energy Conversion Materials" project and member of the CO_2 mitigation team at NIST. Honors and Awards: Fellow ACA (2014); ICDD (2001); ACerS (2002). Bronze Medals from Department of Commerce (2002 & 2008); McMurdie Award from ICDD (2004); Spriggs Phase Equilibria Award from ACerS (2007).

Research Interests: crystallography (single crystal, powder, synchrotron and laboratory x-ray, and neutron diffraction); crystal chemistry and phase equilibria; standard reference materials, reference x-ray powder patterns; materials databases; non-ambient diffraction; structure/property modeling; thermoelectric materials; photocatalysis; CO_2 capture and sequestration; high-throughput combinatorial thin film metrology.

Statement: I am honored to be a candidate for Vice-president in the forthcoming ACA election. ACA is the first scientific organization that I joined when I was a graduate student, so it is an organization that I 'grew up' with. Over the years, I have served ACA in several roles such as organizing symposia and serving on committees. In 1998, I enjoyed the experience of serving as the local chair of the meeting in the greater Washington DC area. With that fond memory, I am delighted to have the possibility of serving ACA again as your Vice-President. As ACA plans its strategies and opportunities for the years ahead, I would like to share my views concerning the future.

ACA is facing many new challenges and opportunities. First, we must keep abreast of the latest technological advances. For example, there are exciting recent developments in the fields of materials science, nanoscience and bioscience that require new techniques for characterization. Having worked in a standards/metrology organization for many years, I recognize the importance of crystallographic metrology. In addition to practicing traditional crystallography, we should encourage the increased use of new scattering metrologies to meet the challenges of nanoscience. As the recent rapid progress in electron diffraction/spectroscopy has the potential to

revolutionize the materials community, we need to embrace electron microscopy and emphasize the role of crystallography in its development. Local structure determination using x-ray absorption spectroscopy combined with x-ray and neutron pair distribution function analysis is another example of where new methods will become more prominent. This also deserves our increased attention. We must encourage our members to make the best of the x-ray synchrotron, neutron- and electron-based national research facilities, particularly with their state-of-the-art *in situ* capabilities.

In addition to maintaining the health and growth of the macromolecular crystallography component of the organization, on the materials front, we also need to advocate and build up the strength of the components that are related to small molecule research, including more subfields of materials science such as liquid crystals and complex minerals; others that are of current technological importance should also be integrated. We also need to expand ACA membership among our industrial colleagues by paying more attention to the materials industries, including those actively researching and developing bio- and nano-materials, and micro- and mesoporous materials. In this way, the harmony between the macro- and small-molecule components of the ACA could reach a higher level. My experience and knowledge of materials science will be important for leading the effort of integrating materials science with the existing program, in order to benefit all members.

In order to meet the needs of our members as well as attracting new members, we must work closely with the Scientific Interest Groups (SIGs) to build a strong and balanced scientific program during the annual meetings. The SIGs are vital components of the ACA. We should work closely with the SIGs to explore opportunities for funding invited speakers to provide us with the best possible meeting content. We might think about adding new SIGs to reflect the latest technological advances (for example, an electron microscopy SIG). At these meetings, we should also take the opportunity to increase our visibility by contacting the scientific press to showcase our publications and programs. We should strengthen the special *Transactions* symposia and plenary lectures to reflect state-of-the-art crystallographic research. We should plan strategies to obtain the funding and sponsorship necessary to achieve this, while continuing to maintain individual member subscription fees at a level that provides one of the best values of any professional organization.

Our institutional health relies heavily on continuing and promoting crystallographic education. We must continue to build upon this important aspect for both our young members as well as for our established professionals. It is our responsibility to ensure the strength and skills of the next generation of crystallographers by providing them with the necessary education and training. We will strive to increase resources (i.e. more fund raising) for supporting attendance of more young people at ACA annual meetings. We will investigate possible ways of establishing more scholarships for crystallographic studies. We might consider the formation of an education SIG. We will make sure our annual meetings will continue to meet the needs of our members by providing ample networking opportunities, mentoring by senior members, and employment opportunities. We must also continue to support, encourage, and if possible, expand both the macromolecular and small molecule summer schools.

In recent years, there has been tremendous progress in the area of *database development*. In addition to the availability of macromolecular information, a vast volume of various diffraction data will soon be available partly due to the increasing importance of the combinatorial approach in materials research, an area that I am also currently involved in. To be able to access this large volume of diffraction data, various computational strategies and standards are critical for data collection, storage, transport and exchange. Communication and cooperation between creators/producers of crystallographic databases and those responsible for other property databases are important in order to maximize research opportunities for all. We should emphasize the potential of combined use of these databases for enhancing research opportunities to the maximum possible extent.

An effective way to achieve the growth/retention rate of an organization is through *focused membership drives*. New members will provide us with new scientific insights and resources. We need to design strategies to gain new members, for example, adding new fields of crystallographic interest to our programming could attract new members. The best example of how this can benefit the ACA can be seen in the evolution of our own gold open-access journal, *Structural Dynamics*. The journal focuses on structural determination and dynamics of chemical and biological systems and solid materials, enabled by the emerging new instruments. Many of our current members are already engaged in research that would fit perfectly in *Structural Dynamics* but, more importantly, it should help us attract new members working in these emerging areas, especially with the 40% discount on page charges that is available only to ACA members! Promoting the journal will be a high priority for the ACA Council going forward and I would welcome the opportunity to be part of it.

There are also many scientists who have crystallographic knowledge and are currently participating in other scientific societies, but they are not members of ACA. Many of these societies may also have interests in structural science or crystalline materials. We need to cooperate with these organizations to identify potential new ACA members, to ensure that structural data is appreciated, and to raise the profile of our organization. We need to provide potential new members with effective opportunities to join us. The form of cooperation between societies could include joint symposia/sessions, and cross-links on the world-wide web.

Financial stability is important to ensure the survival of our organization. It will be important to investigate different ways to bring in more income, including possible new products, and expanded efforts in fund raising, in addition to increasing/retention of the membership. The accumulation and maintenance of funds for long-term investment and financial security will be essential.

I believe a well-planned *outreach* program is also important for the growth and visibility of the organization. In addition to continuing support of research and education, and meeting the needs of the membership, we need to increase our outreach to other countries. We should also facilitate educational opportunities for the public

in general, for example, by encouraging our members to give talks about crystallography at local high schools. We should encourage teachers from local schools to introduce students to crystallography. To do this we need to develop appropriate publicity materials, create attractive website information, and when appropriate, invite teachers to attend selected sessions on crystallographic education during the annual meetings.

We should look into the possibility of establishing avenues to help *influence public policy*, particularly those related to the support of national resources such as the synchrotron, neutron and electron-beam research facilities, as they are vitally important to many of our members. We will investigate the possible creation of a mechanism to bring the members' concerns to the attention of the policy makers. We should initiate and support efforts to increase public funding of all components of crystallographic research.

I recognize that the vice-president position comes with many key responsibilities. I know I can bring to this office an appreciation for the diverse and exciting field of materials crystallography. If honored with your election, I pledge to commit my best abilities to fulfilling the responsibilities of the office. As your vice-president, I will apply the experience that I have gained in working at academic, industrial and government institutions, and also the leadership positions at ACerS and ICDD to serve the ACA. I will seek important opportunities and issues, and work with the ACA officials, ex-officials, and members. Together, we will strive for the continuous prosperity of our organization, and the steadfast advancement of the field of crystallography.

Gerald F. Audette
Canadian Representative to Council

Associate Professor, Centre for Research on Biomolecular Interactions, Department of Chemistry, York University

Education: BSc, University of Alberta; PhD, University of Saskatchewan (L.T.J. Delbaere & J.W. Quail); Postdoc, U. Alberta (B. Hazes)

Professional Activities: Director, Centre for Research on Biomolecular Interactions (2014-15); Undergraduate Program Director, Dept. of Chemistry, York University (2014); Subject Editor, *Crystallography and Structural Chemistry, FACETS Journal* (2015-Present); Chair, Canadian Division of the ACA (2012-13); Canadian Light Source User Advisory Committee (2002-2004); Co-Editor in Chief, *Journal of Bionanoscience* (2006-2010). I was also awarded the Faculty of Science's Graduate Mentorship Award in 2014.

***Research Interests*:** Broadly speaking, my research interests lie in the application of x-ray crystallography and other methods to understand how microorganisms utilize multi-protein complexes for transferring genetic material and effector molecules across membranes, and facilitate adherence to a variety of surfaces. I am interested in how these systems are assembled from their component proteins, as well as their effects on infection, adaptation to varying environmental conditions and the development of multi-drug resistance. I am also interested in how these secretion systems assemble fiber-like pili for surface and cellular adherence, motility etc. In particular, we are examining how the relatively simple structure of an engineered pilin can direct protein nanotube assembly in the absence of a hydrophobic helix used to drive native pilus assembly, and are exploring the development of pilin-derived protein nanotubes for biosensor applications.

Statement: I am honored to have this opportunity to represent the Canadian crystallographic community as a candidate for the Canadian Representative on Council. The ACA was the first association I joined as a student, and has been my professional home for over 20 years. Indeed, many of my friends and colleagues of diverse scientific backgrounds, both in Canada and North America, I met through the ACA. It is incredibly beneficial for Canadians to be members of the ACA, where chemists, physicists, biochemists, mineralogists etc. come together through the common language of crystallography. This commonality of language allows for the removal of "silos"; crystallography bridges disciplines and the ACA is our venue. I am excited about the opportunity to give back to my community in a leadership role.

Perhaps the main reason I'm standing for election to represent our community as Canadian Representative on Council is engagement. Mike James has been an excellent voice on council for the past 3 years. He and Louise Dawe (when she was Chair of the Canadian Division) developed a questionnaire for Canadian crystallographers to help understand our needs and thoughts about the ACA. I will continue this work to increase the "Canadian content" in the ACA through engagement of the community to "reintroduce" my colleagues to what the ACA can offer. We have a diverse spectrum of interests, and often get focused on our particular sub-discipline, be it inorganic catalysts, minerology or structural biology, when we are considering meetings to attend. If you peruse the programs of the ACA meetings, most of these areas are covered, as well as sessions touching on crystallographic education and career development, in addition to learning about the latest technological developments from the vendors of our instruments. The ACA meeting allows us to build broader connections and relationships within the North American community and beyond. With the ACA meeting coming back to Toronto in 2018, I look forward to working towards an excellent meeting where we can (re) engage Canadian crystallographers within the ACA. I would also look to promote my Canadian colleagues to consider further engaging with our community through submitting manuscripts to our society's journal, *Structural Dynamics*. Reaching

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out to those of us in the field as well as the next generation of crystallographers, through the annual meetings and promotion of our society's journal, is critical to keeping the ACA vibrant and strong.

In summary, I would be honoured to serve at the Canadian representative on Council. I'll be an active voice for Canadian crystallography in the Americas, encourage more Canadian involvement in the ACA, and lend my experience and enthusiasm to the position.

Thomislav Frisic
Canadian Representative to Council

Assistant Professor, Department of Chemistry, McGill University, Montreal, Quebec, CA

Education: BSc University of Zagreb (Croatia); Phd University of Iowa (USA); Postdoc University of Cambridge (UK)

Professional activities: CEMWOQ Organizing Committee (2013 -2014 Montréal, 2015 Guelph, 2016 Windsor); Co-organizer *Mechanochemistry and solvent-free chemistry symposium* (Pacifichem 2015); *Crystal Engineering Form & Function symposium* (ACA 2015); *Growth, Structure and Application of Multi-Component Crystals symposium* (ECM-29, 2015), Co-Chair *170th Faraday Discussion on Mechanochemistry* (Montréal, 2015); Co-organizer *International Symposium on Mechanochemistry in Synthesis and Nanoscience*"(Warsaw-Ossa, 2015); *Contemporary Crystal Engineering* (ACA 2013); *Green Chemistry Symposium* (96th Canadian Society for Chemistry Meeting, 2013); Session Chair *Symposium on Gas Capture Materials* (95th Canadian Society for Chemistry Meeting, 2012); Social Media Editor for *Crystal Growth & Design* (ACS, 2015-); Editorial Board Member for *CrystEngComm* (RSC, 2013-); Associate Editor for *Molecular Crystals & Liquid Crystals* (Taylor & Francis); Executive Committee of Canadian Thermal Analysis Society (2014-). RSC Harrison-Meldola Medal (2011); *ChemComm* Emerging Investigator Award (2014); McGill Tomlinson Scientist Award (2014); McGill W. J. Dawson Scholarship (institutional CRC equivalent, 2015) and McGill Principal's Award for Outstanding Emerging Investigator (2016).

Research Interests: My research is focused on application and, to a certain extent, re- discovery of solid-state chemistry in modern chemical synthesis. Inspired by the growing need for and interest in new, sustainable approaches to making molecules and materials, my research group is developing mechanochemistry (i.e. chemical reactivity induced or sustained by mechanical force) and other, solvent-free and low-energy approaches for improving chemical transformations, such as vapor-induced "accelerated aging" reactions. The ultimate aim of my research is to demonstrate efficient, clean and, importantly, generally applicable solid-state alternatives to conventional solution-based or solvothermal synthetic approaches. Crystallography and x-ray diffraction play a central role in this research, by enabling the direct structural characterization via methods for structure solution using x-ray powder diffraction data, and studies of reaction mechanisms via *in situ* x-ray diffraction. In particular, the application of highly penetrating synchrotron x-rays at the ESRF and, recently, DESY and PSI, enabled the first real-time and in situ observation of the course of structural and chemical transformations in a ball mill, leading to the discovery of a new topology for a tetrahedral structure, named katsenite (kat). In a desire to not only understand solid-state reaction mechanisms, but also demonstrate the generality of such reactions, we target a wide diversity of popular molecules and materials, specifically microporous metal-organic frameworks, pharmaceutical cocrystals and the synthesis of active pharmaceutical ingredients themselves. In a different aspect of our research, we also investigate 'smart' materials responsive to stimuli (heat, light). We have been using x-ray single crystal diffraction to monitor the crystal-to-crystal transformations of azobenzene-based crystals in real time, providing the first *in situ* evidence for cis to trans azo isomerization in a crystalline solid.

Statement: The greatest asset I can provide to the ACA and its Canadian members is a dedicated, dynamic attitude, directed towards promoting crystallography and its ability to solve wonderfully different problems. I offer diverse research and international experience, and a broad perspective of how crystallography fits in the colourful fabric of science. I joined the crystallographic community >20 years ago (while in high-school). Working with Branko Kaitner at the University of Zagreb, I received my first formal training in x-ray diffraction and crystallography – and still remember those fun and chilly winter mornings in the lab, figuring out unit cells and space groups, while the buzzer on a Picker machine announced peaks! This is really when my connection to Canadian crystallography started, as Branko got us all running NRCVAX, reminiscing over his visits to the Ferguson lab at Guelph. My first scientific collaboration: George Ferguson and Alan Lough helped us with a disorder problem, resulting in a joint *Acta C* paper. Since then I have been jumping in and out of different labs (in Croatia, USA, UK, Canada) and different research areas, making me realize how crystallography can be a key element of seemingly most diverse activities, from structural determination via x-ray powder diffraction and crystal engineering, to reaction mechanisms monitoring and organic synthesis! I have been a member and supporter of a number of crystallographic communities around the world, not only of ACA, but also of ECA, the Croatian Society for Crystallography, and also the Canadian National Committee for Crystallography - where am honored to serve as the Vice-Chair. I want to broadly present crystallography as a powerful and all-pervasive effort, as seen from my activities as the Social Media Editor of *Crystal Growth & Design*, Editorial Board member of *CrystEngComm* and Associate Editor of *Molecular Crystals & Liquid Crystals*. One might say that things are too busy (sometimes it certainly feels that way), but this is what I strongly and sincerely believe in.

At the level of ACA, the first and foremost important question that I want to address is the membership of the Canadian

crystallography community. I would like to know how we can be more important, how can we contribute more and how can we encourage more Canadian crystallographers – and solid-state and materials scientists – to join this community? And I don't mean only membership numbers - I mean events, workshops and summer schools. I also mean publishing and participating in the ACA publications – such as *Structural Dynamics*. And I know that I am not the only one thinking along these lines – the fantastic IYCr 2014 meeting in Montréal organized by Mirek Cygler and Albert Berghuis demonstrated the interest and dedication of the crystallographers in Canada. And now strictly talking to Canadian crystallographers: I would like us to find out how we can increase our numbers and broaden our scope. How do we engage researchers in x-ray crystallography, crystal engineering, solid-state NMR spectroscopy or crystal structure prediction and modeling to participate? How do we engage brilliant Canadian researchers living abroad to join scientific events in Canada? This may sound very broad – true - but I strongly believe in a crystallography as a dynamic, inclusive and continuously growing discipline.

I like to think that I have a good presence within the ACA community. I have never refused an invitation to participate at the ACA event (even if it meant very a tight car and airplane trip from the *Crystal Engineering Gordon Conference* to the ACA meeting at Albuquerque) until this year when, alas, a scheduled beamtime at DESY overlaps with a fantastic event spearheaded by Jason Benedict. I have organized two *Crystal Engineering Symposia* at the ACA meetings, once with Travis Holman (USA) and once with Pete Wood (CCDC, UK) which, I believe, reflect my view of crystallography as a broad and diverse discipline. I also enthusiastically participate in the Canadian crystallography community – starting from a modest workshop supported by NSERC and FRQNT we have spun off a new tradition in Canada: the *Crystal Engineering and Emerging Materials Workshop* (CEMWOQ), taking place this year in Windsor with 70 participants. As a guest Editor, I have encouraged the participation of Canadian researchers in special issues of *CrystEngComm* dedicated to the IYCr (2014), and *New Talents in Crystal Engineering* (2016).

Since arriving in Canada and joining McGill University in 2011 I have been wonderfully welcomed and supported by colleagues across Canada. I would like to return this support by serving as a dedicated and dynamic representative of Canada's great crystallographic community as part of the ACA council, and would strive to the utmost of my abilities to grow the importance and activity of Canadian crystallography in this association.

Thomas Proffen
Data Standards and Computing

Director Neutron Data Analysis and Visualization Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN.

Education: Diploma Physics, Ludwig Maximilians University, Munich (1992); PhD Crystallography, Ludwig Maximilians University, Munich (1995); Postdoc Research School of Chemistry, Australian National University, Canberra (1995-1998); Postdoc Michigan State University, East Lansing, MI (1998-2001).

Professional Activities: Co-Editor *Journal of Applied Crystallography* (since 2014); Member of Advisory Board for *Zeitschrift für Kristallographie* (since 2004); Member, ACA Communications Committee (2009-2011); Member, NeXus International Advisory Committee (2003-2010); Various positions in ACA Scientific Interest Groups and organizer of sessions at ACA meetings.

Research Interests: My main research focus has been the study of disordered and nano-crystalline materials and extracting structural information from scattering data. My goal has always been the quantitative analysis of single crystal diffuse scattering or the Pair Distribution Function (PDF). As part of my quest, I have upgraded the neutron powder diffractometer (NPDF) at the Lujan Neutron Scattering Center dedicated to PDF studies of disordered materials as well as worked on a number of analysis codes such as DISCUS (***tproffen.github.io/DiffuseCode/***) and PDFGui (now part of ***www.diffpy.org***). More recently my interests have broadened to more generally integrating materials modeling and neutron scattering experiments across science problems that can be addressed using current and future neutron sources.

Statement: It is very exciting to be considered for the ACA committee on Data, Standards and Computing at a time where advances in computing, detectors and the amount of data we are able to collect is truly revolutionizing how we conduct science. Growing up as a crystallographer has shown me first hand the benefits of a well-defined data standard such as CIF and as staff member at neutron sources in Los Alamos and Oak Ridge, I have helped develop the NeXus file format now used at many of the neutron and light sources. On the computing side, I remember my early work in analyzing diffuse scattering and putting aside many ideas as just not practical given the computing resources at the time. Today, many of the ideas can come back and open new opportunities to understand the defect structure of materials. Similar advances are happening across many fields from using massive Molecular Dynamic simulations to understanding bio-molecules to refining the detailed structure of nano-materials. Having helped to develop the field of Pair Distribution Function (PDF) analysis through building a user friendly neutron powder diffractometer (NPDF at the Lujan Center at Los Alamos National Laboratory) and developing the corresponding PDF refinement software has clearly proven the critical importance of scientific software and the need for access to higher performance computing resources. The crystallographic community often serves as a shining example of integrated workflows from data collection to publication and deposition of the resulting data. At the same time, opportunities around us are developing rapidly from 'big data' to high performance computing and in my current position I am connecting these opportunities to the scientific potential of current and future neutron sources at Oak Ridge National Laboratory. As a member of the committee on Data, Standards and Computing, I would be dedicated to helping to continue

advancing our crystallographic community and take full advantage of all the data we collect and extracting the most information possible from it. There are many ways an organization such as the ACA can help from publishing best (data) practices to hosting workshops, hack-a-thons and topical sessions at the annual meetings to name just a few. As far as I am concerned, very exciting times are ahead of us.

Nicholas Sauter
Data, Standards & Computing

Computer Staff Scientist, Lawrence Berkeley National Laboratory, Berkeley, CA (Photo courtesy of LBNL)

Education: AB Physics, University of Chicago (1983); PhD Biophysics with Don Wiley, Harvard University (1991); Damon Runyon-Walter Winchell Cancer Research Foundation Postdoctoral Fellow with Keith Yamamoto and David Agard, UCSF (1992-1994).

Professional Activities: Acting Head of the Berkeley Center for Structural Biology at ALS (2011-2012); Reviewer for *Acta Cryst. D*, *J. Appl. Cryst.*, *IUCrJ*, *J. Sync. Rad.*, *Nature Communications* and *PNAS*; Lecturer at the SBGrid/NE-CAT Computing School: Quo Vadis Structural Biology (2014), and *Rapidata* at SLAC: Data Collection and Structure Solving (2015-2016); Co-organizer of workshops on *Can Diffuse X-ray Scattering Reveal Protein Dynamics* (ALS User Meeting, LBNL, 2013), *Workshop on Bio-XFEL Data Analysis* (LBNL, 2014), *Challenges in Crystallography* (HHMI Janelia Research Campus, 2015), and *High Data-Rate MX* (BNL, 2016); Session Chair on *Chemistry and Biology with Novel Scattering Techniques* at ACA 2014 Meeting.

Research Interests: I'm one of the principal developers of the *DIALS* software package, which aims to create new algorithms to best process data from the latest detector technologies deployed for structural biology at new lightsources. I've been focused particularly on x-ray free-electron laser sources, with their capacity to expose the crystal in a matter of femtoseconds, thus avoiding specific structural damage known to occur at side chains and metal sites. Also, as the experiments are largely performed at room temperature, the diffraction potentially reveals more about the dynamic ensemble of internal motion (such as alternate rotamer conformations) relevant to understanding biological function, and allows us to follow reaction pathways in the time domain. However, in order to bring out these fine details in the electron density map, account must be taken of the "diffract before destroy" arrangement, merging data from tens of thousands of still-shot diffraction patterns instead of single-crystal rotation data as collected at synchrotron sources. My colleagues and I introduced new parameter fitting and post-refinement techniques to optimize these multi-crystal experiments. We are also continuing to address the challenges of data scale for both XFELs and synchrotrons, where the newest pixel array detectors can frame images at rates of 20 terabytes/hour.

Statement: Thank you to the Nominating Committee for suggesting I stand for election. The subject is fortuitous because "Big Data" challenges are foremost in my mind as well as for other developers of primary data processing software for biosciences. I am heartened that creators of all the major macromolecular processing programs, plus beamline scientists, are gathering at three community meetings this summer that I am co-organizing, including satellite sessions at the ACA and ECM, to look for common approaches for handling the expected deluge of data. One future issue to consider is whether beamlines can partner with national supercomputer facilities to provide real time processing coverage for the expected burst data rates.

I'm very supportive of the widely accepted practice of archiving structure factors to the PDB, aside from atomic models, for this assures that structure solution and refinement can be repeated in the future as algorithms improve. However, this reasoning also extends to unmerged data from multi-crystal experiments that are gaining popularity generally, not just at XFEL sources. With multi-crystal processing algorithms still a matter of active research, there is great potential benefit in the future from reanalyzing subtle measurements from unmerged data that are not usually considered, such as the polarization anisotropy of anomalous scattering. The ACA should actively encourage standard approaches, such as the inclusion of enough metadata to accurately describe experimental conditions.

Likewise, it is encouraging to see growing community interest in archiving the raw diffraction images for successful structure solutions. While the details of data reduction may often be treated as a black box, improvements in detectors and light sources also mean that algorithms are in constant flux, so for example we may shortly see better profile fitting of Bragg spots leading to greater detail in the electron density. Also, there has been recent interest in drawing structural conclusions from diffuse scattering. Unless the complete diffraction pattern is archived, this information from photons outside the Bragg spots might otherwise be discarded when disks are cleared after publication. While archiving data takes effort and is not cost-free, there is a benefit to having post-publication public access, as readers can double check conclusions and form alternate hypotheses.

On a broader level, I'm always glad to see scientists question the computation, and feel that it is important to train beginning crystallographers to seek a deeper understanding. In as much as the ACA can take a role, perhaps the annual meeting's agenda could place an increased emphasis on methods workshops. I'd be honored to participate in this process as part of this committee.

Kay D. Onan
Continuing Education Committee

Assoc. Professor, Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA

Education: BA Chemistry and German, Concordia College (1971), Moorhead, MN; PhD Physical Chemistry, Duke (1975), Durham, NC; MBA., Northeastern (2007), Boston, MA

Professional Activities: ACA Continuing Education Committee (1989-1991); Chair (1991-1992); ACA Communications Committee (2001-2004 -Chair in 2005); Numberous academic administrative positions at Northeastern overseeing academic affairs, faculty affairs, graduate education and undergraduate education at the college level in a university setting and special assistant for academic policies for our past university president.

Statement: I am honored to have been nominated for the Continuing Education Committee. My journey through academe has taken me into administration for some long time and now I am back in the Department of Chemistry and Chemical Biology. When I was a practicing crystallographer I always found the ACA to be a supportive and rewarding presence in my professional life. No small part of the richness of this crystallographic community came from the fact that practitioners and developers of new techniques tended to want to share their knowledge. I believe that this is no less true today than it was then. This enthusiasm is what makes the ACA such an enriching community. There is much to learn and there are engaged crystallographers excited to share their expertise. Participating on this Committee is one way I feel I can give back to the ACA, an organization that has meant so much to me.

Crystallographic results are extremely valuable to many different kinds of scientists, some number of whom do not completely comprehend how to understand, and therefore best utilize, their results. This committee is charged with continuing professional development for crystallographers. Because new techniques, software packages and best practices appear regularly there is a need for workshops to keep interested scientists abreast of new and developing techniques. There is also a need to engage those who might want to use crystallography as a complement to the rest of their science. I posit that non-structural scientists are interested in exploring the best ways to use databases of structures and learning the potential pitfalls of crystallographic data.

It is important to me that interest in, and knowledge of, crystallography be shared with the next generation of scientists. I would like to ensure that undergraduate students get at least an introduction to crystallography. I think that the multi-year series of sessions on *Engaging Undergraduate Students with X-ray Crystallography* organized by K. Wheeler and R. Rowlett for ACA meetings was a good model of the kind of sessions that should be encouraged.

Though the International Year of Crystallography (2014) has passed, we should not let the many, very useful outreach pieces that were developed for it sit on the shelf. Public outreach, while not an explicit mandate of this committee, could easily be seen as a part of how the ACA provides continuing education. The promotion of crystallography more broadly could bring this structural science into the eyes of the public, including into high school systems.

I would be honored to serve the ACA as a member of this Committee.

Charlotte Stern
Continuing Education Committee

Staff Crystallographer Dept of Chemistry Northwestern University 2145 Sheridan Rd Evanston Il, 60208

Education: BS Chemistry (1985) University of Illinois, Champaign, Il.

Professional Activities: ACA member since 1990, Co-organizer of the ACA Summer Course for chemical crystallography since 2012; PLATON workshop (ACA 2009); OLEX2 workshop (IUCr 2014) *Things We No Longer Need to Know* (ACA 2016)

Research interests: Structure elucidation of complex small molecules via single crystal diffraction

Statement: I am honored to be nominated to the Continuing Education Committee. As it has become easier to obtain crystallographic data, the understanding of the fundamentals of x-ray diffraction has diminished. The ease of use and speed of the new instruments allows a novice to use this technique without fully understanding its capabilities and limitations. It is my job as a crystallographer to ensure that the next generations of chemists have the tools and foundations of this technique. This technique cannot become a "black box" where just the desired outcome is met, where problems are not just swept under the rug, but are looked at.

At Northwestern I have had the opportunity to help develop courses in crystallography for both undergraduates and graduates. It is always exciting to see the undergraduates choose a crystallographic project for their independent research. It is just as exciting to see the graduate students learn to solve their own crystal structures. I have been very involved in coordinating ACA educational workshops on programs that can assist professional crystallographers in their tasks. I get excited working with individual students from around the world at the ACA summer course when a difficult concept is finally understood.

The duties of this committee provide a crucial service to the ACA and the crystallographic community. Committee members develop new workshops, provide professional development, and encourage student travel to the meetings. Many crystallographers are alone at their place of work. We need to be a center for them. Having an opportunity to go to a workshop to learn a new technique or look up a teaching manual from the ACA webpage to help understand a concept can make a big difference to them. These resources are indispensable to both novice and professional crystallographers alike. If elected, I will work enthusiastically to support these vital educational opportunities and try to facilitate others for the crystallographic community.

Martin Donakowski
Communications Committee

Department of Chemistry; Naval Research Laboratory; Washington, DC

Education: National Research Council Postdoctoral Fellow (2014–Present), PhD Chemistry (2014) Northwestern University, and BS Chemistry (2008) University of Minnesota.

Professional Activities: ACA - member sin 2012; 2016 Twitter *Updater*; YSSIG Concil Representative (2016–2017); Chair (2016); Chair, *Career Odyssey Panel* (2014). ICDD – Student Affiliate; NRL Colloquium Organizer (2014–2016). and reviewer for several journals.

Research interests: Structures of semicrystalline / nanocrystalline materials, small molecule crystallography, optical materials, functional electrodes and structure-property relationships thereof for batteries, capacitors, and catalysts. My background is in small molecule and synthetic strategies for noncentrosymmetric materials for use as piezoelectrics and frequency doublers with hydrothermal chemical techniques. My current postdoctoral research is the analytic study and development of advanced electrodes of semi-crystalline materials in 3D batteries. To study these materials I employ a variation of pair distribution function (PDF) to quantify metal oxide components and develop models from reverse Monte Carlo simulations and PDF fitting. The structures of these materials help to explain electrochemical behaviors and allow strategies to obtain optimal battery performance based on phase, crystal size, habit, and porosity.

Statement: I would first like to thank the nominating committee for the honor of being considered for the communication committee. I first became interested in being involved with ACA governance because I found the overall ACA community to be warm and welcoming and I was especially impressed with how approachable the YSSIG was. I wish to continue this practice and encourage increased membership amongst early career scientists. To do this, I will work with the ACA to examine emerging crystallography studies and translate this to the communications committee to increase advertisement of the ACA via a larger web presence. I am currently the Chair of the YSSIG and the YSSIG representative to council wherein I work as the ACA twitter *Updater*. I would like to increase the frequency and depth of our social media (and apply analytics to evaluate effectiveness). Based on an idea from the vice-president and CEO, I would like to begin a blog community for ACA that will increase the activity of ACA between conferences, provide scientists a platform to write on current science topics, advertise the ACA, and provide public outreach on the importance of crystallography. I have previously worked in social media via Twitter, video editing, and photography. Helping the ACA increase membership while simultaneously assisting in public discussions on the importance of crystallography would be a great pleasure; I believe I have a strong background to support an initiative of increased web presence.

Brian Patrick
Communications Committee

Dept. of Chemistry University of British Columbia, Vancouver, BC, CANADA

Education: BSc Chemistry (1992) University of Waterloo PhD Chemistry (1997) University of British Columbia Postdoc (1998-99) University of Kentucky

Professional Activities: ACA member since 1998; Chair, Small molecule SIG (2002); Secretary, Service SIG; Treasurer, Canadian Nation Committee on Crystallography; Secretary, ACA-Canadian Division (2014-16)

Research Interests: Small molecule single-crystal x-ray crystallography

Statement: I was very pleased to be nominated to serve on the Communications Committee, and would welcome the opportunity to serve. As an ACA member for over 15 years, I owe it to the community to contribute to its continued success. One of the most satisfying things I've done this year was to visit my 7 year-old's 2nd grade class and spend half an hour telling them about what I do every day. It reminded me of how science can inspire, and also of how relatively invisible scientists are in general, and crystallographers are specifically. Teaching crystallography for the past 8 years has shown me that, even at the undergraduate and graduate levels, students are not fully aware of the role crystallography of one sort or another has played in the way science shapes our lives. The role of getting the word out, of making the public aware of the important work being done by ACA members falls, in part, to the Communications Committee and I would be honored to help the ACA with this part of its mission.

Contributors to this issue: Cele Abad Zapetero, Gerald Audette, Carol Brock, Chris Cahill, Bryan Chakoumakos, Gautam Disiraju, Martin Donakowski, Joe Ferrara, Jeanette Ferrara, Thomislav Frisic, Frank Fronczek, Michael-James, Lisa Keefe, Bruno Morison, Kay Onan, Chiara Pastore, Brian Patrick, Virginia Pett, Thomas Proffen, Dan Rabinovich, Connie Rajnak, SN Rao, Nicholas Sauter, Kim Stanek, Charlotte Stern, Marian Szebenzy, Tom Terwilliger, Diana Tomchick, Anastasiya Vinokur, Winnie Wong-Ng, , Eddie Snell,

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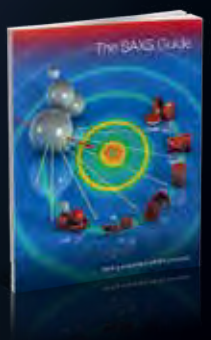

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Report from Canada by Mike James

Before I introduce our featured crystallographers in this issue of *RefleXions*, I would like to make a few comments about the work of our Canadian National Committee for Crystallography. They are required to submit an annual report of their performance to International Affiliations of the Canadian Government. These Annual performance reviews provide a means whereby the impact of Canadian scientific bodies can be assessed by the Canadian Government. This is a mandatory review and failure to comply could result in the cancellation of the Government support which in our case amounts to annual dues of 6000 Swiss francs. Each year the performance review amounts to approximately 20 or more pages detailing what our crystallographers have achieved on the world stage. The report for 2015 was submitted at the end of January 2016 and was put together by the members of the CNCCr. We are deeply indebted to Patrick Mercier, Michel Fodje, and other members of the CNCCr for their hard work in putting the report before the International Affiliations Committee in a timely fashion. Copies of their report can be obtained through Michel Fodje, the secretary of the CNCCr ***(michel.fodje@lightsource.ca)***.

Also I would like to briefly summarize the workshop on *Automation in Macromolecular Crystallography* that was held as part of the 19th Annual Users Meeting at the Canadian Light Source in Saskatoon, SK on May 2nd, 2016.This year the meeting was organized by Pawel Grochulski (CLS) and Tom Caradoc-Davies (Australian Synchrotron). The meeting was devoted mainly to a discussion of developments in the Stanford Automated Mounting (SAM) system, The 7 presentations were given by: Jinhu Song (Stanford Synchrotron Radiation LightSource); Masahiro Hiraki (Graduate University of Advanced Studies, KEK, Japan); Tom Caradoc-Davies (the Australian Synchrotron); Alex Soares (National Synchrotron LightSource); Raphael Richaud (from the custom engineering firm IRELEC); Michel Fodje (Canadian LightSource); and Aina Cohen (Stanford Synchrotron Radiation LightSource). The presentations were followed by a round-table discussion led by Tom Caradoc-Davies. Abstracts of the speakers talks can be found at: ***www.lightsource.ca/pages/speaker_abstracts#Caradoc***. This was a popular workshop with ~27 people in the audience.

Marie Fraser is one of three Macromolecular Crystallographers at the University of Calgary. She is an Associate Professor in the Department of Biological Sciences in the Faculty of Science. Marie started her academic career at Queen's University in Kingston, Ontario where she received a BSc (Honors Chemistry) and a PhD under the supervision of Suzanne Fortier. Her PhD.thesis was on Direct Methods Phasing of Macromolecular Crystal Structures using single isomorphous replacement data. She then went out west to Alberta and did a variety of protein structure studies before settling in on structural studies of the citric acid cycle enzyme, succinyl Coenzyme A synthetase with Bill Wolodko in Bill Bridger's laboratory (Biochemistry Department, University of Alberta). Some of the key structures that Marie has solved were the Shiga toxin that is the cause of hemolytic uremic syndrome that is the result of severe infections of *E. coli* 0157:H7. This is an AB_5 toxin having the cell surface recognition B pentamer and the catalytic A subunit that is responsible for shutting down protein synthesis in the infected cell. Another protein structure that has been determined in Marie's lab is the multi-domain human ATP-citrate lyase. This is a key metabolic enzyme that links energy metabolism from glycolysis to the production of fatty acids. It has an "ATP grasp" domain that is in common with the succinyl CoA synthetase enzyme from *E. coli*. ATP-citrate lyase catalyzes the conversion of citrate and Coenzyme A into acetyl-CoA and oxaloacetate powered by the hydrolysis of ATP and the formation of a phosphohistidine residue that is a key residue in the reaction pathway (Figure 1).

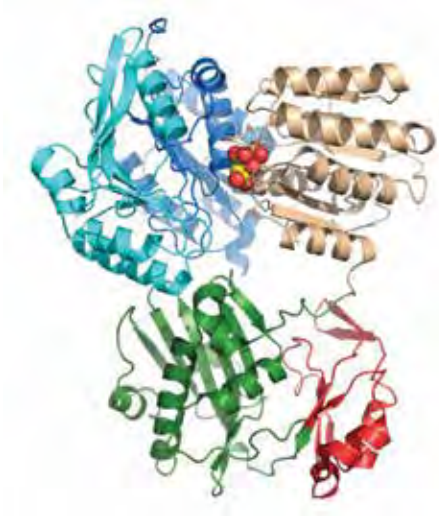

Figure 1: ATP-citrate lyase in complex with citrate. The bottom 2 domains (green and red) form the ATP-grasp fold. The citrate (represented by spheres) is bound to the wheat-coloured domain the upper portion of the figure.

Succinyl CoA synthetase is an enzyme of the citric acid cycle. It is an $\alpha_2\beta_2$ tetramer in *E. coli* and it's crystal structure was solved and published in 1994. Subsequently, approximately 12 more structural papers have been published by Marie and her colleagues on this interesting enzyme and there is more still to

come. The α subunit has the binding site for Coenzyme A and the reactive site histidine H246α is also located in that subunit (coloured blue in Figure 2). The β subunit (coloured salmon in Figure 2) has the ATP-grasp fold and it has been shown to be the ADP binding site in SCS by crystallographic studies. In succinyl CoA synthetase the residue that is phosphorylated by ATP is His246α. This residue is ~35Å away from the ATP-grasp binding site in the β subunit (Figure 2). There still remains the question of how does this phosphorylation take place when the substrate (His246α) is ~35Å from the reaction site in the β subunit? What is the driving force for this conformational change and reaction? His246α is on a flexible loop (coloured magenta in Figure 2) that could refold to bring the imidazole ring of His246α close to the binding site for ATP and to the phosphorylation reaction. The search for the answers to these exiting questions occupy the present research efforts in Marie's laboratory.

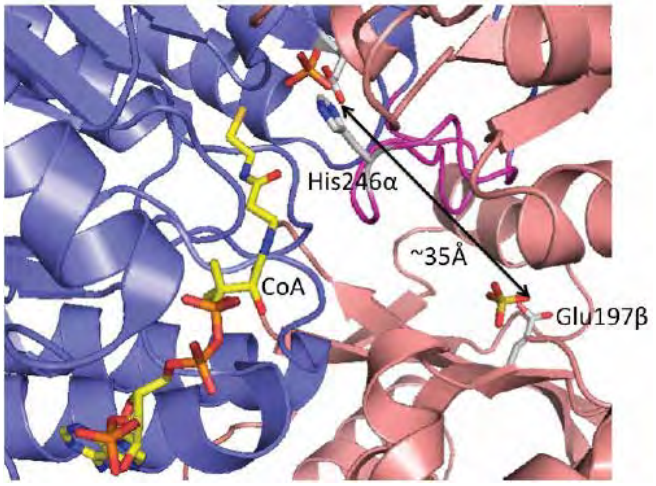

Figure 2: A close up view of the αβ dimer of E. coli succinyl CoA synthetase. The α-subunit is coloured slate and the β-subunit is salmon. The 2 glutamates, 208α and 197β, are separated by ~35 Å. The histidine in the α-subnit, His246α, has to move from its observed position in the figure to the ATP-grasp fold site in the β subunit in order to be phosphorylated. The carbon atoms of the CoA molecule bound in the α-subunit are coloured yellow.

Not only has Marie been intimately involved in the research that I have briefly discussed above, but also she has been very active in the Canadian Crystallographic Community. Marie has served as Treasurer for the Canadian National Committee for Crystallography (CNCCr) as well as being the one responsible for providing funds for those students to help them to travel to International and National Crystallographic Meetings. Marie has also been a long time member of the American Crystallographic Association and the Canadian Institute for Synchrotron Radiation.

My second selection for this issue of ACA RefleXions is ***Lynne Howell*** (Senior Scientist and Associate Chief, Research Integration and Communication, Research Institute of The Hospital for Sick Children, Toronto and Professor, Department of Biochemistry, University of Toronto). Like Marie, Lynne has been and continues to be a stalwart supporter of Crystallographic activities in Canada. She is a long-standing member of the American Crystallographic Association. Lynne has a 22-year history (1992-2014) as co-organizer of the Buffalo-Hamilton-Toronto Crystallographic Annual Meeting; she was a member of the International Program Committee for the IUCr Congress held in 2011, Madrid, Spain; a member of the IUCr Commission on Biological Macromolecules since 2008, a member of the Canadian National Commttee for Crystallography (2011-present) and a member of the Board of Directors of the Canadian Light Source (2014-present).

Lynne began her academic career by doing a B.Sc. (Honors) in Biophysics at the University of Leeds in the UK. There she did an undergraduate research project with Professor A.C.T. North on the degradation of the heme group in myoglobin and hemoglobin. Following her Ph.D. studies with Julia Goodfellow at the University of London, Lynne travelled across the Atlantic to do Postdoctoral Studies with Greg Petsko when he was at MIT in Chemistry. This was followed by a second PDF at the Institut Pasteur, Paris with Roberto Poljak and Andre Menez. She finally settled down by crossing the Atlantic once again and landed a position at The Hospital for Sick Children, Toronto, where she has been ever since.

Lynne's fascination with structural biology almost certainly began with her time in Leeds doing an undergraduate research project with Tony North, a member of the team that determined the structure of the first enzyme, hen egg white lysozyme. As her interests evolved she has recently turned to the study of bacterial and fungal proteins involved in the formation and regulation of biofilms. Biofilms are exopolysaccharides that in some systems are synthesized intracellularly and subsequently secreted through the inner membrane into the periplasmic space and then through the outer membrane to the external environment. Others are synthesized extracellularly by enzymes that are anchored to the outer membrane or the cell wall. Perhaps the most well know exopolysaccharide is dextran produced by *Leuconostoc meserentoides*; it was originally discovered in wine by Louis Pasteur and it has now become a very useful column support for size exclusion chromatography known as Sephadex

The aspects of biofilm formation that Lynne and her group study are the adhesion of bacteria to surfaces using an organelle called a Type IV pilus and the synthesis of the extracellular biofilm matrix that protects the bacteria from host defences such as the immune system and render the bacteria more tolerant to various antimicrobial agents. Examples of biofilm infections include

those that suffer from periodontitis caused by gram negative anaerobic oral pathogen; nechrotizing fasciitis caused by group A *streptococci*; and perhaps the most well-known biofilm protected bacterial colony is *Pseuomonas aeruginosa* involved in chronic wounds, burns and cystic fibrosis. Lynne has been working on trying to understand how the polysaccharide matrix of a variety of different microbes is made and is making great strides in the development of ways to treat P. aeruginosa biofilms in order to make antibiotics effective against these infections.

P. aeruginosa produces several exopolysaccharides that have been implicated in biofilm production. The structural study to be highlighted here is the glycoside hydrolase encoded by the psl (polysaccharide synthesis locus) operon and known as PslG. The biological function of PslG is not fully established but recent work by Lynne's group published in *J. Biol. Chem*, 290 (47), 28374-87, 2015 revealed that contrary to previous findings, pslG is not required for polymer production but its over expression does impair biofilm formation. PslG is located in the periplasm and bound by an N-terminal transmembrane helix to the inner membrane. The PslG enzyme was cloned from *P. aeruginosa* PAO1 and expressed in *E. coli* cells. The structure of purified PslG (31-442) was solved from data collected from crystals grown in the presence of CdCl2 using the anomalous signal from Cadmium for phasing.

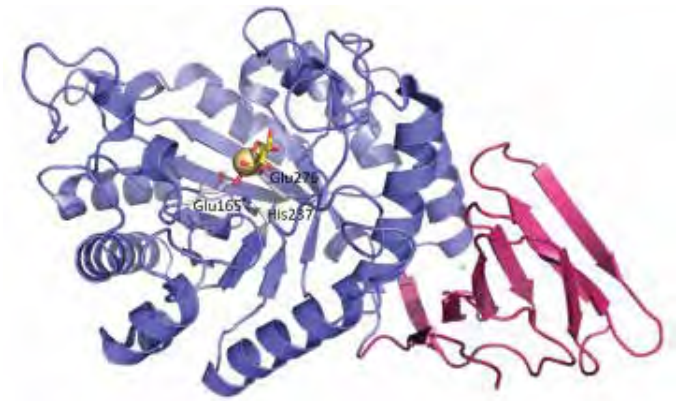

Figure 3: The structure of the glycoside hydrolase PslG from Pseudomonas aeruginosa. The catalytic domain (β/α)8 is coloured slate and the β-sandwich domain is in pink. The active site has a Cd++ ion and a mannose bound (the C atoms of the mannose are in yellow). Also represented are the general acid/base Glu165 and the nucleophile Glu276 as well as a highly conserved histidine residue His237. This enzyme belongs to glycoside hydrolase family GH39 (J. Biol. Chem, 290 (47), 28374-87, (2015)).

PslG is a 2 domain enzyme belonging to the glycoside hydrolase family, GH39 (Figure 3). There are 2 glutamate residues responsible for catalysis; Glu165 is the general acid/base and Glu276 is the nucleophile. Domain 1 is the catalytic TIM barrel and domain 2 is a β-sandwich. The Psl polysaccharide is a repeating mannose rich pentamer with 3 D-mannose residues, an L-rhamnose, and a D-glucose. As the polymer is not readily available co-crystallization with Cd^{++} and 3M mannose was successful. Several mannose monosaccharides were bound to an electronegative groove on the enzyme's surface enabling identification of key catalytic residues. Modeling of the pentasaccharide repeat suggested that the bound mannose residues come from adjacent repeat units.

The very exciting results of this structural study are contained in a recent paper published in *Science Advances* May 20 2016 (Vol. 2, no. 5, e1501632). This paper details a comprehensive study showing that the exopolysaccharide glycoside hydrolases such as PslG can be used to prevent *P. aeruginosa* biofilm formation and more importantly from a treatment perspective be used to disrupt existing biofilms. Two glycoside hydrolases PelA and PslG were able to reduce the *P. aeruginosa* biofilm mass of clinical and environmental isolates by 58-94% *in vitro*.

Not only do biofilms play an important role in pathogenic bacterial infections, but also exopolysaccharides play an important role in fungal infections such as *Candida albicans* and *Aspergillus fumigatus* (Sheppard, D.C. and Howell, P.L., J. *Biol.Chem*. 2016) In fact, the Howell group has determined the structure of one of the enzymes required for the biosynthesis of galactosaminogalactan in *A. clavatus* (Sph3). It turns out that Sph3 is also a glycoside hydrolase with an $(\beta/\alpha)_8$ fold. The structure of the catalytic domain is similar to the glycoside hydrolase families GH18, GH27, and GH84. As GH family classification is based on primary amino acid sequence, Sph3 actually defines a new family of hydrolases, GH135. While Lynne and her team have been able to demonstrate hydrolase activity using purified polymer, the role of general acid/base and nucleophile have yet to be assigned

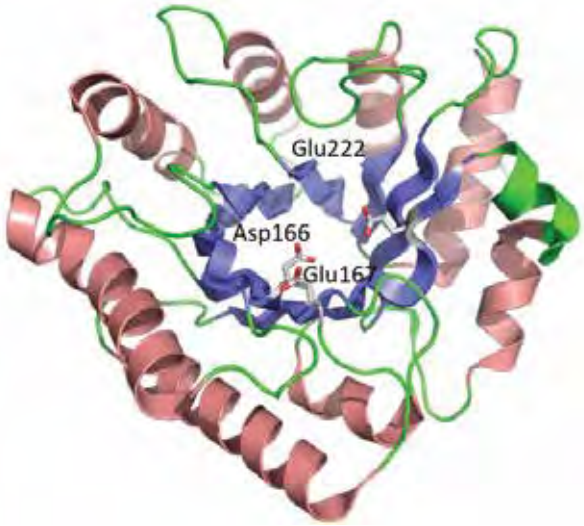

Figure 4: A rendering of the structure of the Sph3 glycoside hydrolase from Aspergillus clavatus. The eight strands of β structure are central and coloured slate. The eight helices of the $(\beta/\alpha)_8$ are on the outside of the molecule and coloured salmon. The connecting loops are green. There are three carboxyl groups that are implicated (but not yet proven) in a mechanism of catalysis: Asp166, Glu167 and Glu222. (Bamford N.C. et al. J. Biol. Chem. 290 27438-27450 (2015).

Both functional characterization of the enzymes in vitro and microbiological experiments *in vivo* provide hope that in the future we will be able to combat and effectively treat microbial biofilm infections. Sixty-five to eight-five percent of all chronic infections involve microbes growing in a biofilm state.

My sincere thanks to Michelle James for transcribing my almost illegible handwriting to typescript.

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FRAGMENTS

Zbignew Dauter Selected to Receive the 2017 ACA Patterson Award

For over 30 years, Zbignew Dauter has been one of the leading proponents of the use of synchrotron radiation for advancing the methodology and speed of macromolecular crystal structure determination and for enhancement of the quality of the results. Zbigniew Dauter's career has been centered at synchrotron beamlines, including those at the EMBL Outstation in Hamburg, at the National Synchrotron Light Source at Brookhaven and at the Advanced Photon Source at Argonne, where he has played a significant role in supporting users at these facilities. More importantly, in the larger picture, he has been an innovative developer of methodology with highly influential studies on the use of anomalous diffraction in structure determinations and in biomolecular structure analysis at true atomic resolution. He has strongly influenced the development of phasing methods based on native anomalous scatterers. He has analyzed many structures at exceptional resolution and detail that provided new insights in biological chemistry.

Dauter's work on utilizing anomalous scattering, has helped to develop methods for phasing using both light atoms such as sulfur and phosphorus, and also halogen atoms. Sulfur is intrinsic to most proteins, and advances in instrumentation and software have enabled phasing of more and more complicated structures. He is among the leaders in this area, with an emphasis on obtaining high quality diffraction data at what are referred to as 'non-heroic x-ray wavelengths' i.e. without resorting to the longer wavelengths where these light atoms' anomalous scattering are set to increase but at the 'cost' of sample absorption and where the experiment has the challenge, in the ideal, of working in vacuo. Zbigniew Dauter has also pioneered the application of phosphorus anomalous scattering to solve nucleic acid structures. In a separate development one of his most important contributions was the introduction of fast soaks of macromolecular crystals with high concentrations of halide ions (Br- and I-) for phasing by anomalous dispersion. This latter method has been adopted by many subsequent investigators to solve novel macromolecular structures, including ones intransigent to other methods.

He is a sought-after lecturer and workshop instructor, and indeed he has assisted even the most experienced crystallographers in their work through his insights presented in his keynote and plenary lectures. Along with his colleagues he applies his crystallographic exptertise to indentify / correct errors in published macromolecular crystal structures. His extraordinary depth of understanding also comes to the fore in his longstanding work as a Section Editor of the biological crystallography section (D) of *Acta Crystallographica*, where he handles papers expeditiously and provides substantial insight. He is, as well, very much involved in advisory committees for synchrotron facilities. Zbigniew is also an extraordinary teacher. He has answered the call to take part in numerous workshops on data collection where he has left an indelible imprint on the minds of emerging crystallographers. He has also delivered many plenary lectures at international conferences where, in his inimitable style, he both educates and entertains.

Zbigniew is an exceptionally productive scientist working in diverse areas of crystallography; indeed he is one of the very rare examples of a crystallographer who has published in all the sections of *Acta Crystallographica*. Zbigniew Dauter embodies the positive spirit of scientific research at all levels, in depth and in breadth, and fulfils the vision of the ACA Patterson Award *To recognize and encourage outstanding research in the structure of matter by diffraction methods, including the methodology of structure determination and/or innovative application of diffraction methods*.

Selection Committee: John R Helliwell (Chair), A. Brunger, W. Hendrickson, A. Sarjeant, Ton Spek, J. Britten, M. Nespolo, Vivian Stojanoff

Helen M. Berman Selected as Receipient of the 1st ACA David Rognlie Award

Helen Berman received her PhD in Chemistry in 1967 from the University of Pittsburgh under the direction of George Jeffrey, and stayed on for postdoctoral training as a National Institutes of Health Trainee. In 1969, she joined the Fox Chase Cancer Center, where her research program focused on nucleic acid crystallography. In 1989, she joined the faculty at Rutgers, The State University of New Jersey, where she is now a Board of Governors Professor of Chemistry and Chemical Biology. At Rutgers, she studied collagen and protein-nucleic acid complexes in addition to nucleic acids, and at the same time developed structural databases and ontologies.

Helen has been a champion for open access to scientific information since the concept of data sharing was in its infancy. Beginning in 1971, she played an influential role in the initiation and early development of the Protein Data Bank (PDB), first operated by Brookhaven National Laboratory. For nearly five-decades she has been committed to ensuring that the PDB archive has been a resource created by, and for, the community. As head of the Research Collaboratory for Structural Bioinformatics (RCSB), Helen became the Director of the PDB in 1998, and developed the RCSB PDB into a vital and key resource for biology and education (***rcsb.org***). The primary reference for the RCSB PDB (*Nucleic Acids Research, 2000, 28: 235-242*) has been cited over 20,000 times and was included in Nature's 2014 list of the 100 most-cited papers as tracked by the *Web of Science*. Today, she serves the RCSB PDB as Director Emerita and Associate Director.

In 2003, Helen formed the Worldwide PDB with groups in the UK and Japan to ensure that a single PDB archive would continue to be freely and publicly available to the global community (***wwpdb.org***). Her passion for making structural data accessible and understandable by a broad community has driven the development of other bioinformatics resources,

ontologies, and community-driven validation standards. Other biological data management projects include EMDataBank, a global deposition and retrieval network for 3DEM maps, models, and associated metadata, and the Structural Biology Knowledgebase (SBKB), an online resource that combines the results from the NIH-funded Protein Structure Initiative research with external data annotations to provide comprehensive information about proteins. As part of the SBKB, the BioSync resource provides up-to-date information on over 130 beamlines at worldwide synchrotron radiation facilities where biological macromolecules are studied.

In parallel to her research, Berman is extremely active in the community, and serves on a variety of advisory committees, professional societies, and editorial boards. Helen has already garnered significant national recognition and numerous awards, including a Fellow of the International Society of Computational Biology (2016); the DeLano Award for Computational Biosciences from the American Society for Biochemistry and Molecular Biology (2013); the Carl Brändén Award from the Protein Society (2012); a Fellow of the American Crystallographic Association (2011); the Department of Chemistry Alumni Award from the University of Pittsburgh (2010); the Distinguished Lecturer Award from Sigma Xi (2007–2009); the Martin J. Buerger Award from the American Crystallographic Association (2006); and a Distinguished Service Award from the Biophysical Society(2000).

Selection Committee: Simon Billinge (Chair), Bobby Barnett, Denny Mills

James O'Brien Named to Receive Elizabeth Wood Science Writing Prize in 2017

James F. O'Brien began his academic career as a physical chemist at Missouri State University (then Southwest Missouri State College) in 1969. O'Brien was a highly respected faculty member as noted by both his peers and his students. He won three teaching awards during his career including the Governor of Missouri's Award for Teaching Excellence (2001). He earned two terms as a distinguished scholar between 1991 and 2001. In 2002 he was granted the status of Distinguished Professor – the highest status awarded to faculty at Missouri State University. During his academic career he published thirty-one papers in peer-reviewed journals and presented 84 times at professional chemistry conferences. Early in his career O'Brien began presenting general lectures as part of the American Chemical Society speaker series. He has given two hundred ninety-three invited talks at seminars, banquets, meetings, etc., including 135 Sherlock Holmes lectures and 136 "Famous Mad Hatter" talks. The "Famous Mad Hatter" talks are about mercury poisoning.

He retired in 2003 and in 2010 he was elected the Missouri State University Wall of Fame. This recognizes and honors employees who have excelled at Missouri State and significantly contributed to the success and positive collegiate experience of students. While Missouri State University has had many outstanding employees during its long history, the intention of the Wall of Fame is to recognize those faculty and staff members who have had an impact on students that is considered truly noteworthy.

O'Brien's writing for the general public has focused on Sherlock Holmes. The book *The Scientific Sherlock Holmes* (J. F. O'Brien, Oxford University Press) won a national award - an Edgar Award from the Mystery Writers of America as the best book of 2013 in the critical/biographical category. In addition O'Brien has written three articles that have appeared in The *Baker Street* Journal and an invited piece for the *Encyclopedia Britannica* - ***www.britannica.com/topic/Sherlock-Holmes-Pioneer-in-Forensic-Science-1976713***. Other Holmes articles were featured on the cover of the June 1993 issue of the science journal *Chemistry and Industry* and in the *Huffington Post* - ***www.huffingtonpost.com/jim-obrien/sherlock-holmes-a-science_b_2549834.html***. A chapter on Holmes was included in the book *Chemistry and Science Fiction* (1998). O'Brien's latest work - a chapter entitled *Sherlock Holmes: Forensic Science Pioneer* has been accepted for a forthcoming book (2016).

Christine Dunham to Receive 2017 ACA Etter Early Career Award

Christine Dunham, Assistant Professor of Biochemistry at Emory University and ACA member, is the recipient of the 2017 Margaret C. Etter Early Career Award, which recognizes "outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career."

At Emory Christine and her group use structural techniques, mainly x-ray crystallography and cryo-EM, to understand how proteins are synthesized in bacteria and how the process is regulated in conditions of stress. In particular, she is interested in unraveling the molecular basis of frameshift errors, which arise when the ribosome reads a shifted sequence of the messenger RNA, thus producing an alternative protein sequence. She is also investigating the role of a specific protein pair, the toxin-antitoxin system, in persistency, a latent state that bacteria enter when they are in specific stress conditions and that is characterized by repression of protein translation. Finally, her lab is also keen on understanding RNA modification and its link to antibiotic resistance.

Christine obtained a bachelor's degree in biochemistry at Barnard in New York City, and later pursued her PhD from the University of California Santa Cruz, under the mentorship of William Scott. She then moved across the pond to take up an extremely productive post-doctoral position in structural biology at the MRC in Cambridge, UK, with Venki Ramakrishnan, after which she started her independent career at Emory.

Chiara Pastore

Karena Chapman Receives MRS Awrad

ACA member Karena Chapman received one of the two 2015 Materials Research Society (MRS) Outstanding Young Investigator Awards "for her contributions to understanding the coupled structure and reactivity of energy-relevant systems and for developing the incisive experimental and analytical tools needed to interrogate these complex materials systems."

Karena works as an x-ray chemist at the Argonne National Laboratory, which she joined in 2005 as the Arthur Holly Compton Post-Doctoral fellow, after completing her PhD in chemistry at the University of Sydney. She became a staff scientist in 2009, and she now researches on materials with energy-related applications; she also manages a dedicated instrument for the Pair Distribution Function analysis of crystalline, nanoporous and amorphous materials that are challenging to study with conventional crystallography. She is co-editor of the *Journal of Applied Crystallography*.

Ian Wilson Elected to the National Academy

Ian Wilson, Professor of Structural Biology and Chair of the Department of Integrative Structural and Computational Biology at The Scripps Research Institute in San Diego, has been elected as a foreign associate of the National Academy of Sciences. This honor is only the most recent of a the long list of awards and prizes that Ian has received during his career; among the others, he was elected Fellow of the Royal Society of London (2000), Member of the American Academy of Arts and Sciences (2002), and Fellow of the Royal Society of Edinburgh (2008).

Ian started his professional journey (1971) with a Bachelor's degree in biochemistry from the University of Edinburgh. He then moved to Oxford, to work with David Phillips, who had then just solved the structure of lysozyme. He spent six years in Oxford, obtaining his PhD (1976) with a thesis reporting the crystal structure of triose phosphate isomerase, an enzyme that plays a key role in glycolysis. He then moved to Harvard, where he stayed (1976 to 1982), to work with Don Wiley on the structure of the influenza virus hemagglutinin, which they published in *Nature* (1981).

He became an Assistant Professor at The Scripps Research Institute (1982), where he set up the first structural biology laboratory of the institute and continued his quest to understand the immune system and its interaction with viral pathogens. Over the years his laboratory has produced an impressive number of structures of antibodies and antigens and their complexes, which have led to invaluable insights for the development of vaccines and immunization strategies against pathogens such as influenza and HIV

2016 ASBMB DeLano Award to Todd Yeates

Todd Yeates, Professor of Biochemistry at the University of California, Los Angeles, is the recipient of the 2016 DeLano award from the American Society for Biochemistry and Molecular Biology (ASBMB). The award has been established in honor of Warren DeLano, an advocate of open source scientific technologies, and recognizes scientists that have achieved "the most accessible and innovative development or application of computer technology to enhance research in the life sciences at the molecular level."

Highly praised by the colleagues who nominated him for the award, Todd's approach to structural problems is extremely interdisciplinary and creative. He contributed to the advancement of protein crystallography with several computational tools, which are aimed at assisting structure determination and which he made freely available to the scientific community. One of these software tools, ERRAT, is used to validate a crystallographic structure, and can be easily accessed on the UCLA website. Another helps detecting twinning, a widespread phenomenon in protein crystallography that arises when two different crystals intergrow with each other. More recently, he and his group have developed CrowdPhase, a citizen science online game where players have to solve the phase problem of macromolecular crystal structures.

Other ongoing projects in his lab focus on protein engineering and have a more applicative nature. Besides protein engineering for crystallography, one major theme in his lab is protein nanotechnology, a field that Todd pioneered and that entails the design of proteins that self-assemble into complex structures with well-defined architecture, useful as building blocks for new biomaterials.

Todd obtained his bachelor's degree from UCLA (1983), and then pursued his PhD at the same institution with Prof. Douglas Rees, being part of the team that determined one of the first membrane protein structures. He then moved to The Scripps Institute for his post-doctoral studies with James Hogle, working on the structure of poliovirus. He returned to UCLA in 1990 as a faculty member of the Department of Chemistry and Biochemistry

Small Grants To ACA Members for Outreach

The ACA Outreach Task Force is awarding small grants (average $400 with maximum $1000) to ACA members for demonstration outreach projects that can be replicated by other members. The intent is to strengthen each member in crystallography, generate enthusiasm for crystallography and engage K-12, local communities, organizations or politicians in exciting activities (e.g. growing crystals) and in understanding the relevance (applications) of crystallography today. Long range goals are attracting students to crystallography, combating anti-science attitudes, and raising the status of crystallography in the academic community. The successful proposal should:

◊ Impact a large group of people in appreciating crystallography

◊ Include matching funds from outside sources equal to the award by the deadline if over $400 is requested

◊ Specify follow-up and evaluation of the event impact

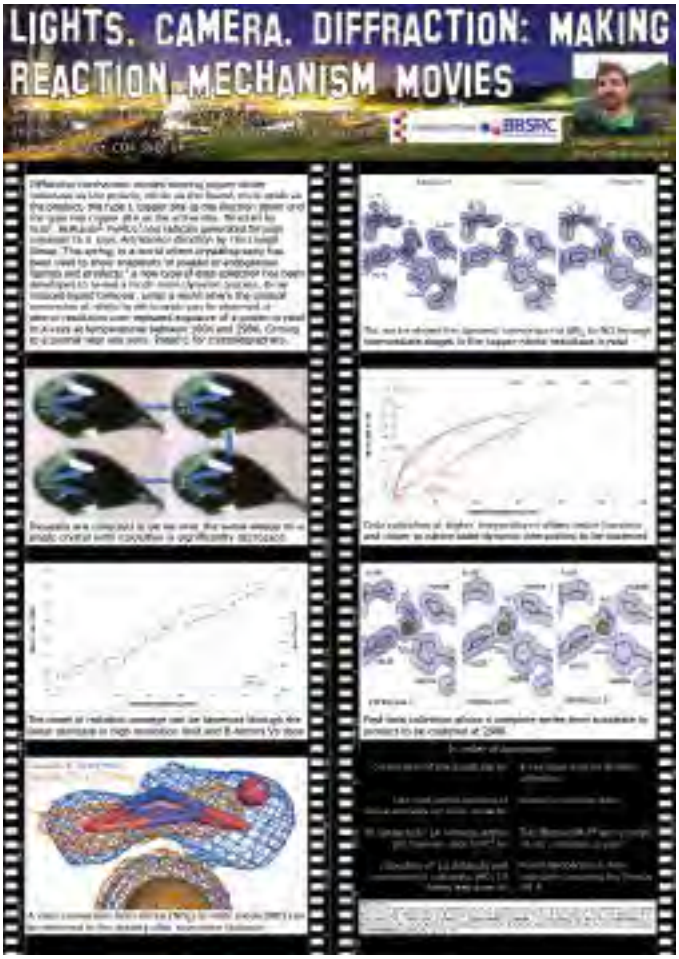
◊ Delineate a plan for replication by other ACA members

Proposals should be sent by July 20, 2016 by email to ***martha.teeter@gmail.com*** with the subject header "Small Grants for Outreach". Proposals are limited to three pages, including the budget. Awards will be made in August. Projects should be completed in calendar year 2016 and a report submitted in early January 2017. Presentations of the projects will be made at the 2017 ACA meeting.

Martha Teeter

Structural Dynamics Poster Prize at BCA Meeting

John Helliwell (Chair), Ben Bax, Matthew Bowler, Hazel Sparkes, and John Spence constituted the judging panel for the 2016 ACA Structural Dynamics Journal Poster Prize at the British Crystallography Association April meeting at the University of Nottingham. The panel awarded the prize to Sam Horrell from the University of Essex for his poster titled *Lights, Camera, Diffraction: Making Reaction Mechanism Movies*.



2016 ACA Fellows

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

Gerard Bricogne

Gerard Bricogne is one of the giants of crystallographic theory. He has made unique and exceptional contributions to our understanding of crystallography and in exploiting crystallographic relationships to solve the crystallographic phase problem. His most important contributions to crystallography have been the development of a comprehensive theoretical treatment of crystallography using Bayesian and maximum-entropy approaches, the recognition and application of the power of using non-crystallographic symmetry in solving the crystallographic phase problem, and the development and widespread distribution of exceptional algorithms and software for calculation of crystallographic phases and refinement of macromolecular structures.

Within Bricogne's treatment of crystallographic theory, one particular element stands out: His understanding of the power of non-crystallographic symmetry and his development of theoretical approaches to use this symmetry to solve the phase problem. Bricogne recognized in 1974 that the presence of multiple copies of a molecule in the asymmetric unit of a crystal not only led to the phase relationships previously identified by others, but that these were formally equivalent to real-space symmetry in density that could be used in an iterative procedure to determine crystallographic phases. This relationship is one of the most important aspects of the *density modification* procedures now used routinely in macromolecular crystal structure determination. Bricogne used this approach with 5-fold averaging to greatly improve the density map for Tomato Bushy Stunt Virus in 1978.

In 1984 Bricogne wrote a seminal paper, *Maximum entropy and the foundations of direct methods* that lays out a deep mathematical description of direct methods that explains their power and extends their potential to macromolecules. He followed this in 1988 with *A Bayesian statistical theory of the phase problem*, a classic paper that describes how Bayesian approaches can be used to analyze not just a single structure but related structures, non-crystallographic symmetry, and contributions of fragments to structure factors, as well as how to combine phase information from a variety of sources with Bayesian approaches.

In addition to his theoretical contributions, Bricogne has made a systematic effort to develop tools that apply his theory and allow others to more effectively carry out macromolecular structure determination. Bricogne's 1988 paper on Bayesian approaches provided the theoretical basis, and over the past 20 years he has developed the widely-used SHARP and BUSTER software distributed by his non-profit company, Global Phasing.

Bricogne's major contributions to crystallography are well known around the world and he has been the recipient of the Swedish Academy of Sciences Aminoff Prize, the ACA Patterson Award, and the BCA Dorothy Hodgkin Prize. He held a Howard Hughes International Fellowship while working at LMB Cambridge and has been Director of Research at LURE (Orsay, France).

Despite his residence in the UK, Bricogne has been a regular attendee at ACA meetings. He co-organized the 1993 ACA *Transactions* session on Bayesian approaches, and led a workshop at the 2010 ACA meeting on software available from Global Phasing and he served on the ACA selection committee for the 2003 Buerger Award. Gérard has also been involved in instructing and assisting many young crystallographers at numerous workshops, such as CCP4 weekends, and symposia making him one of the key people involved in training new generations of crystallographers.

I. David Brown

David studied for two BSc degrees and a PhD (with Jack Dunitz) at the University of London, England. Together with Dunitz he published two papers on the structures of copper (I) complexes in *Acta Crystallographica* that set the tone for much of David's future work on inorganic complexes and minerals. He took a postdoctoral fellowship in metallurgy at McMaster University, Hamilton and remained there, rising through the ranks to full professor in the Department of Physics until he retired in 1996. He also had joint appointments in the Departments of Metallurgy and Chemistry. During his time at McMaster many students had the pleasure of having David as their graduate supervisor or on their supervisory committee. He supervised 11 graduate students for MSc or PhD degrees and mentored 11 postdoctoral fellows.

When working as a Section Editor for *Structure Reports* (IUCr 1964-1975) David was one of the first to realize the importance of databases and started collecting information for inorganic crystal structures solved by x-ray crystallography. At the International CODATA Conference Kyoto (1980), David, together with his friend and collaborator G. Bergerhoff, reported for the first time the official existence of the *Inorganic Crystal Structure Database (ICSD)*. This database was a new aid in studying

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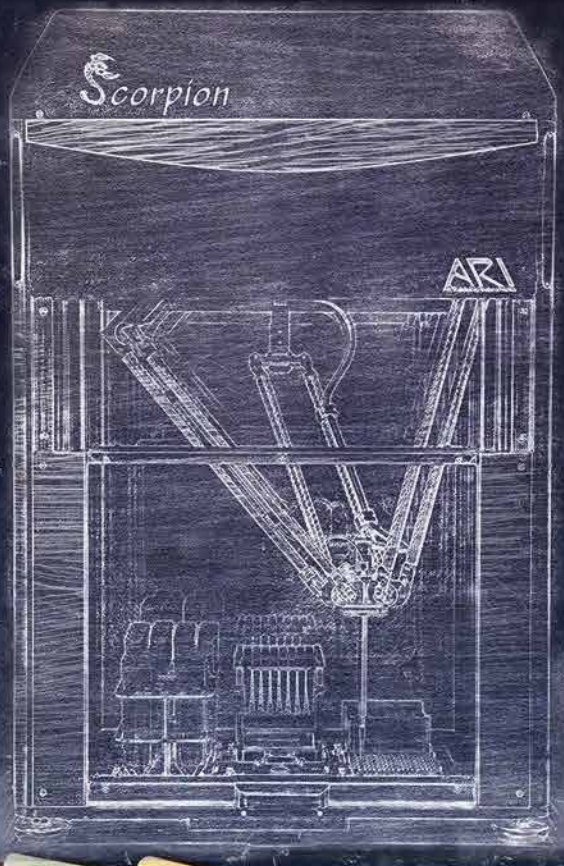
- ✓ Build screen blocks
- ✓ Optimize screen conditions
- ✓ Room for 96x 15 ml reagent tubes
- ✓ Access 1.5, 15 and 50 ml tubes
- ✓ Aliquot and normalize salt screens for LCP reactions
- ✓ Aspirate and dispense 1 ul to 1 ml
- ✓ Build multi-dimensional grids, pH, concentrations & titrate additives
- ✓ Set up 24-well plates, protein + screen
- ✓ Anything you can do with a handheld pipettor



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inorganic materials, it offered direct searchable access to structural details through keywords, chemical elements, structural values, *etc*., and it formed the basis on which one could apply new algorithms to detect relationships between structures and new properties of materials.

During his active academic life David examined a large number of unknown structures of inorganic solids and deduced empirical rules of atomic interaction in crystals, which he developed in to the concept of bond valence model [*Chem. Soc. Rev.* 7 (1978) 359-376]. His Bond Valence Method (often referred to as the *Brown Method*) is taught at many universities around the world. David published his experiences in this field in the book *The Chemical Bond in Inorganic Chemistry, The Bond Valence Model*, Oxford, 2001. The second, updated edition will be available in 2016.

David was also involved in developing the CIF dictionary for inorganic structures, the Crystallographic Information File (S.R.Hall, F.H.Allen, I.D.Brown, *Acta Cryst.* A 47(1991) 655-685), which helps researchers and users create more up-to-date databases automatically and cheaply. The *dictionary* allows calculations and logical operation on crystallographic information.

David has served the crystallographic community in Canada by being on the Canadian National Committee and representing Canada on the Data Commission of the IUCr. When the ACA held a meeting at McMaster University David served as the local chair (1986). He also served the IUCr as a member of the Teaching Commission; as well as the Commissions on Crystallographic Computing and Inorganic and Mineral Structures. He was a member of the ACA Computing and Data Committee (1988-91) and served as the first the Canadian Representative on the ACA Council (1991-1995). All of these positions were done on a volunteer basis.

Yu-Sheng Chen

For quite some time Yu-sheng Chen has been involved with the Consortium for Advanced Radiation Sources (CARS) at the Advanced Photon Source, Argonne National Laboratory. Although most of his responsibilities have been in ChemMatCARS (the component of CARS that concentrates on chemistry and materials science), he also had responsibilities in BioCARS, the structural biology component. He shares an interest in time-resolved x-ray scattering that combines his more materials science perspective with others that have a structural biology perspective. These interactions have always worked well since there is substantial overlap in experimental approaches, in data analysis, in the day-to-day running of large, national and international user facilities such as ChemMatCARS and BioCARS, and in interactions with demanding and frequently stressed users of these facilities.

Chen has organized a number of workshops at APS with lectures and hands on experience to train new users of the facilities. They include a Synchrotron Charge Density School in 2013 and a School for Synchrotron Crystallography: *Introduction and Experimental Methods at ChemMatCARS/APS*. Yu-sheng has always been a calm, solid presence whose large and diverse publication record attests to his interactions with users who effectively deploy a wide variety of experimental techniques under his guidance. While he is generally a junior co-author in these publications; he is a top-notch facility scientist whose support is often critical to others as they pursue their research problems. Without his experience and guidance, the users, and ChemMatCARS itself, would be much less successful.

Chen has also managed to attract a large number of first rate scientists and their research groups from abroad to perform experiments at APS. Collaborators and their research groups include Iversen from Denmark, Stalke, Luger and Scherrer from Germany, Spackman from Australia, Toudec from France, and Wang from Taiwan to name a few. All have used the Chem/Mat Cars beamline 15-ID at the Advanced Photon Source on which Chen is the Principal Scientist.

This work has resulted in a large number of excellent publications and it is clear that his contributions have been crucial to the published research. 15-ID is now one of the prime stations at APS for a wide range of innovative small molecule and material science work and continues to attract users from all over the world. These efforts should be recognized as they greatly promote the non-routine use of crystallographic methods, which are the future of the field.

Charles Campana

An organometallic chemist by training, Chuck Campana held an assistant professor position at University of New Mexico, Albuquerque (1976-80) before becoming an application scientist with Nicolet Instrument Corporation. Nicolet eventually transitioned into Syntex, Siemens, and now Bruker, Inc., and Chuck has remained with them as an application scientist and software developer for over 35 years.

Throughout his career he has distinguished himself with teaching and scientific and technical contributions to the field of single-crystal x-ray diffractometry. He excelled at sales support duties (instrument demonstrations, technical presentations, and preparation of brochures and application notes), research and development projects (e.g., design and testing of new instrument hardware and software), and customer support (e.g., customer training and consultation on problem crystal structures). He was largely responsible for establishing the company collaboration with George Sheldrick and played a key role in the development of revolutionary CCD detectors for use on x-ray diffractometers. Suffice it to say that George Sheldrick's programs are the most widely used crystallographic programs in the field of small-molecule crystallography and Chuck's feedback and software testing have been of tremendous help to George in particular and the scientific community in general.

Chuck has attended and presented papers at nearly all ACA and national ACS meetings since 1980, as well as at numerous regional ACS meetings and most national meetings of the Canadian Society of Chemistry. He has given talks at many international

crystallographic conferences, including IUCr congresses, BCA meetings, PacifiChem, and specialized meetings on charge-density, high-pressure crystallography and powder diffraction.

His professional duties required extensive domestic and international travel, allowing him to serve as an instructor in many ACA and Canadian summer schools as well as at problem structure workshops in China, Taiwan, Hong Kong, India, Mexico, South America, Germany, and England. Chuck's teaching and mentoring activities have helped several generations of crystallographers, chemists and mineralogists learn how to use crystallography as an indispensable tool in their research. He has been very generous with his time and always enjoyed helping young scientists overcome crystallographic problems in pursuit of their scientific research. Chuck's willingness to travel, exceptional people skills, and profound knowledge of crystallography put him in an enviable position that allowed him to collaborate with numerous scientists around the globe and work on the most interesting crystallographic problems. The latter, in turn, enriched Chuck's knowledge that he has always generously shared with anyone who approached him for assistance.

Chuck has worked on countless crystallographic projects and solved and refined thousands of crystal structures with no expectation of co-authorship. Nevertheless, he has co-authored over 300 publications in a wide variety of research fields, where non-routine techniques were required for successful project completion. His publication record, widely accorded recognition and respect by scientists across the globe, remarkable interest in crystallography and chemistry, service to the scientific community, service to the ACA, and dedication to promoting excellence in structural science make him a excellent addition to the cadre of ACA fellows.

Bryan Chakoumakos

Bryan's career combines excellence in research, as exemplified by his many careful structural studies of important materials, with great service to the crystallographic community, and to those who study neutron scatterers in particular. Bryan's research focuses on structure property relationships and spans a wide range of important materials. He has worked extensively on radiation damage mechanisms, high temperature superconductors, phosphors, thermoelectrics, gas hydrates and a variety of mineral and magnetic materials. His work at the High Flux Isotpoe Reachtor (HFIR) has consisted of a very large number of collaborations on neutron diffraction studies, as well as his own research focused on structure-property relationships in technologically important materials. He is very well known for his contributions in the area of crystal chemistry and crystallography of inorganic materials, where his structural investigations inevitably involve neutron diffraction. This work has resulted in over 250 entries in the ICSD database. Overall this body of work is documented in ~150 peer reviewed papers ~29 of which have 100 or more citations.

His service to the community of (neutron) crystallographers is very impressive: He was a member of the committee charged with identifying key instruments to be built at the SNS. He served on the instrument development team for the SNS single crystal neutron diffractometer TOPAZ. He was a Co-PI on the funded NSF proposal to build the quasi-Laue diffractometer Imagine at the HFIR, which focuses on studies of biological macromolecules. He served for extended periods as an instrument scientist for both the powder diffractometer HB-2A and the 4- circle single crystal neutron instrument HB-3A at the HFIR. He provided leadership for the crystallographic team at ORNL, while serving as group leader for both the *Single Crystal Diffraction* and *Structure of Matter* groups. The bottom line is that if you have done a crystallographic experiment (powder or single crystal) at the HFIR or a single crystal experiment at the SNS, you have probably benefited from Bryan's efforts to build and operate a high quality crystallographic instrument suite at Oak Ridge National Laboratory.

Bryan's activities with the ACA are extensive. They include numerous talks at ACA meetings, serving as Chair for a SIG and for meeting sessions, organizing workshops and, most notably, as a member of the local organizing committee for the Knoxville ACA meeting in 2008. Bryan is also passionate about crystallographic education serving on the board of directors for the annual *National School on Neutron and X-ray Scattering*. This annual school provides invaluable hands-on and classroom training in neutron and synchrotron x-ray methods to graduate students from around the US *via* a two week experience split between HFIR/SNS at ORNL and the Advanced Photon Source at ANL.

Frank Fronczek

Frank Fronczek is a generous and gregarious scientist. He has trained innumerable graduate and undergraduate research students in the practical aspects of x-ray diffraction and structural chemistry. He has a long standing tradition of providing crystal structure determinations or diffraction data sets (perhaps numbering in the thousands) to investigators who do not have local facilities or expertise, especially in developing countries. This includes researchers at 14 Louisiana universities, and colleges and government labs in 13 other states and in 11 other countries, most notably India and Turkey. He has also provided copper wavelength x-ray data for the determination of absolute configuration of chiral organics to several crystallographers who did not have that radiation available. Frank's record of scientific publications is legendary. As of Feb 2015, he had an amazing number of publications, 992, among which 373 have been published in IUCr journals. According to *SciFinder*, he is in the top 20 authors in the CSD, second in USA among currently active researchers, and is among the top professional service crystallographers in the US.

Frank has been in charge of the Departmental X-ray Facility of the Chemistry Department of Louisiana State University (LSU) for almost 40 years. He has also been an adjunct professor of the Department of Pharmacognosy, University of Mississippi (2003 to the present). His expertise has been

The AIP Congressional Science Fellowship Program

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

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

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

The **2017 Annual Meeting** will be held at the Hyatt Regency Hotel in New Orleans, Louisiana. The meeting will begin on Friday, May 26 and end on Tuesday, May 30. Ilia Guzei (Univ. of Wisconsin-Madison) and Yulia Sevryugina (Texas Christian Univ.) are Program Chairs.

Want orgnaize a session? The SIGS will plan sessions for 2017 during the SIG business meetings in Denver.
Schedule of SIG Meetings at the 2016 Meeting:

Biological Macromolecules: Saturday, July 23 at 5:00pm
Fiber Diffraction: Sunday, July 24 at 12:00pm
General Interest: Saturday, July 23 at 5:00pm
Industrial: Saturday, July 23 at 5:00pm
Light Sources: Sunday, July 24 at 5:00pm
Materials, Neutron & Powder: Sunday, July 24 at 12:00pm
Service & Small Molecule: joint meeting, Monday, July 25 at 12:00pm
Small Angle Scattering: Monday, July 25 at 12:00pm
Young Scientists: Sunday, July 24 at 12:00pm
Canadian Division: Saturday, July 23 at 5:00pm
All Member Business Meeting: Monday, July 25 at 5:00pm

The **2018 Annual Meeting** will be held at the Sheraton City Centre Hotel in Toronto, Ontario, Canada.

The meeting will begin on Friday, July 20 and end on Tuesday, July 24.

sought after not only by the faculties and students at LSU, but also around the world. He has taught many students the art and science of crystallography and has molded the career of many young educators. In addition, many of his colleagues have benefited greatly from his knowledge, expertise and friendship.

Frank has been an ACA member since 1971 and has an extremely impressive list of contributions to ACA, IUCr, and other crystallographically oriented organizations. He has been a co-editor for *Acta Crystallographica C* (1996-2005) and for *Acta Crystallographica B* (1996-1999). He served on the editorial board of *Journal of Chemical Crystallography* (1994-present). For ACA, he was the Chair of the Service Crystallography SIG (1993); member of the Continuing Education Standing Committee (2010-2013); Chair of the Patterson Award Committee (2007); member of local committees for two New Orleans meetings; a perennial poster judge, and the *Puzzle Editor* of ACA RefleXions since 2011. In addition, he was a member of USNC/Cr (2004-2006) and was on the organizing committee for the USNC/Cr Education Summit (2005). In acknowledgement of his tremendous crystallographic contributions, Frank received the LSU Foundation outstanding Service Award (1984), and the ACA Oxford Cryosystems Prize in (2007) and, much to his chagrin, he was also awarded the *ORTEP of the Year* prize by Dick Harlow in Montreal (1995).

Michael James

It is no exaggeration to say that Michael is the founding father of macromolecular crystallography in Canada, and one of the first in the field in North America. Following his DPhil with Dorothy Hodgkin in Oxford (1966), Michael began his long career at Alberta, beginning as a postdoctoral fellow (1967) and subsequently joining the faculty in the Department of Biochemistry at the University of Alberta, where he is now a Distinguished University Professor Emeritus.

Michael's transition to proteins started immediately on his appointment to the faculty, with his first protein publication appearing (1974) not long after the lysozyme structure. Within a couple of years, he had transitioned almost fully to proteins, with his seminal work on serine proteases. His publication record of over 320 peer-reviewed papers (with an h-index at least 65 (hard to know for sure, as many papers were published before the development of the indexing process) include several that laid the foundation for the understanding of acid protease mechanisms and, by extension, all proteases. He has obviously gone on to investigate many other proteins systems as well,

Michael's list of trainees is a Who's Who of Canadian macromolecular crystallography that spans several generations. His scientific children and grandchildren run major laboratories nationally and internationally. The list includes such people as Delbaere (former ACA President), Read, Brayer, Strynadka, Fraser, Mosimann, Ng, Allaire and many others.

In terms of the ACA, Michael has been a member for over 30 years, having been Chair of the Macromolecular SIG (1985-86), and Canadian Representative on Council for the past three years. He received the ACA Buerger Award (2009) for his lifetime of contributions to the establishment of protein crystallography in North America. He was elected a Fellow of the Royal Society of London (1989) and a Fellow of the Royal Society of Canada (1985). Most recently, he has been awarded the National Research Council of Canada Research Press Senior Investigator Award, which recognizes a record of outstanding achievement in research in one or more of the fields of biochemistry, molecular or cellular biology undertaken in Canada by a Canadian scientist

He currently sits on the Canadian National Committee for Crystallography, where he has been facilitating a greater dialogue between this group and the ACA. He has also been spotlighting Canadian crystallographers in his regular *RefleXions* column, further bridging crystallography in North American countries. This foundational work is essential to new directions for both the Canadian National Committee, and for the ACA.

Brian Matthews

At the University of Groningen in late 1966, important papers by Brian Matthews were already being discussed in great detail. These included methods to combine isomorphous and anomalous scattering in experimental phasing, described in *Acta Crystallographica*. At about the same time, while working at the Laboratoroy for Molecular Biology in Cambridge, UK, Brian authored several papers on the structure of chymotrypsin.This was one of the earliest enzyme structures reported and had a tremendous impact on our understanding of protein structure and enzyme catalysis. The analysis of this structure led to the famous catalytic triad in the active site of a major class of serine proteases which has inspired enzymologists for decades. One of Brian's most enduring contributions has been his work on the solvent content of protein crystals, which led to the use of the *Matthews Coefficient* to estimate the number of copies of a molecule in the asymmetric unit of a crystal. Based on this work he published the classic paper (1968), entitled *Solvent Content of Protein Crystals*, cited more than 8000 times.

In the early 1970s, back in Eugene, the Matthews group solved the crystal structure of lysozyme from the bacteriophage T4. This was not only a major achievement on its own but proved to be the start of a major line of future research in his lab. By combining site directed mutagenesis, thermodynamic methods and crystal structure determinations of an immense number of T4 lysozyme variants, his group made tremendous contributions to science and Brian became one of the founding fathers of protein engineering. The importance of those studies can hardly be exaggerated. These investigations have been incredibly influential in our understanding of the stability of proteins. These fundamental insights have stimulated numerous practical applications, ranging from improving enzymes in household applications like laundry washing powders to increased stability of enzymes used in bioreactors.

In addition to these ground-breaking protein engineering studies, Brian's group solved many other crystal structures. One of these, a bacteriochlorophyll protein from *Chlorobium limicola,* was stunning at the time. Determined in 1975 without knowledge of the amino acid sequence, the structure revealed an all-β protein which held seven bacteriochlorophyll molecules together in a quite disorganized arrangement, surrounded by numerous β-strands. The capability of proteins for non-conventional ligand binding was demonstrated in a splendid way by this structure.

Brian is also a very stimulating personality, who has given splendid lectures all over the world captivating audiences with new results, insights and gentle humor. His service to the crystallographic community and structural biology in the USA has been, and still is, extensive. He was chair of the NAS Subcommittee on Macromolecular Crystallography, part of an effort to evaluate the potential of crystallography (1975-76). He started as a member of the Editorial Board of *Protein Science*, then became Associate Editor and has been Editor-in-Chief since 2007. He chaired the NIH committee overseeing the field of Structural Genomics (2001-2009). He has been an active member of the IUCr and ACA and has been a frequent attendee at the West Coast Protein Crystallography meetings. Through all this Brian has been exceptionally supportive of the work of his many colleagues and students

Arnie Rheingold

Arnie Rheingold continues to have a distinguished career as a productive teacher-scholar highly engaged in the crystallographic community; as a prominent advocate of crystallographic education and the training of next-generation crystallographers; and as one of the foremost crystallographers who advocates for and collaborates with a broad spectrum of scientists. His reputation as a world-class crystallographer is supported by his considerable research productivity and four decades of service to the community. The enormous demand for his expert counsel and use of his state-of-the-art xray facility are key indicators of the respect he has earned. He has not only created a crystallographyic enterprise that is modeled around the globe, he epitomizes the ideal ambassador of our discipline who actively seeks to support the research and teaching initiatives of both junior and senior scientists.

Arnie's education began at Case Western Reserve where he completed an AB degree (1962) and an MS (1963). He completed his PhD (1969) in inorganic chemistry at the University of Maryland working with volatile reactive organometallic compounds. His first faculty appointment was at the State University of New York Plattsburgh. His passion for crystallography was nurtured during these early years, where he used a sabbatical to learn foundational techniques and theory from Melvyn Churchill at the State University of New York at Buffalo (1980-81). Leaving behind tenure and a senior faculty position, he then moved to the University of Delaware (UD) in 1981 as a visiting professor and senior scientist. Arnie's research and teaching aptitude quickly launched him into a permanent faculty appointment. This partnership proved immensely successful for raising the prominence, research capacity, and small-molecule presence of both Arnie and UD. After 33 years as a faculty member on the east coast, he migrated to the University of California San Diego (UCSD) where he has extended the capacity of his x-ray facility (small-molecule and macromolecular crystallography) and continues his research interests with main-group and transition-metal organometallic chemistry and gas-phase cluster synthesis.

Arnie is an active member of both the ACA (1990-present) and the ACS (1964-present). For the latter, his service includes the Joint Board-Council for *Chemical Abstracts* (1998-2002), as well as several capacities within the Inorganic Division and various journal editorial boards [*Organometallics* (1990-2015), *Inorganic Chemistry* (1994-1996, 2001-2006), *Journal of Cluster Science* (1993-1995), *Inorganica Chimica Acta* (2001-present), and *Polyhedron* (2001present)]. Arnie's awards and honors are numerous. He has secured in excess of $3,000,000 in external funding with significant effort directed to the development and operation of the x-ray facilities. He is a Fellow of the AAAS (1988) and the ACS (2011) and was honored by Sigma Xi (1999). He also received the prestigious ACS National Award: Distinguished Service in the Advancement of Inorganic Chemistry (2012). Since 1977, Thomas Reuters has identified Arnie as the *Most Highly Cited Researcher* with nearly 59,000 citations averaging 29.6 citations per article. The breadth of his activities and accolades span journal editorial boards and multi-disciplinary professional societies with unrivaled research productivity, all culminating in considerable national recognition. Without question, Arnie's highly decorated accomplishments are firmly attached to his many pursuits in the field of x-ray crystallography.

It is not an overstatement to assert that, through his effors, research programs across the US and beyond have undergone transformational change due to the direct use of x-ray crystallography. Over the years, his open door policy has attracted collaborators from all areas of the science community: academia to industry; research intensive PhD granting to principally undergraduate institutions; as well as Nobel Laureates to faculty just beginning their academic careers. It is not surprising that these same partnerships now number in the thousands and continue to this day because of Arnie's ability to help investigators rapidly move forward with their research endeavors.

The environment he created, wherever he was, offered fertile ground to nurture the scientific aptitudes of students and scholars by providing comprehensive experiences in the essential principles and hands-on techniques of single-crystal x-ray diffraction. Many of these individuals moved on to productive careers in scientific disciplines with several pursuing productive careers as staff crystallographers at major facilities. A few examples include Kraig Wheeler (UD), Steven Geib (Univ. of Pittsburgh), Ilia Guzei (Univ. of Wisconsin Madison), Lev Zakarov (Univ. of Oregon and Oregon State University), Antonio DiPasquale (Univ. of California Berkeley), Glenn Yap (Univ. of Delaware), and Curtis Moore (Univ. of California San Diego). This remarkable record of training next generation scientists and crystallographers has had an immensely positive influence on the crystallographic community.

Meeting logo designed by John Aspinall

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Hotel Reservation Deadline: June 28, 2016

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

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Fankuchen Award in honor of Elspeth Garman
Bau Award in honor of Benno Schoenborn
Trueblood Award in honor of Axel Brunger

Jason Benedict
Etter Early Career Award

Elspeth Garman
Fankuchen Award

Benno Schoenborn
Bau Award

Axel Brunger
Trueblood Award

Amy Sarjeant
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Program Co-Chairs

Poster Chair
Ilia Guzei
iguzei@chem.wisc.edu

Photographer
Peter Müller
pmueller@mit.edu

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
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Evening Sessions

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Planning your talk: Each session room will be have an LCD projector and laptop. You are encouraged to bring your talk on a memory stick and to use the provided laptop. You should review your presentation in the Speaker Ready Room the day before your presentation. Please arrive at your session room 30 minutes before the session begins or during the coffee break to connect computers and/or copy files to the laptop.

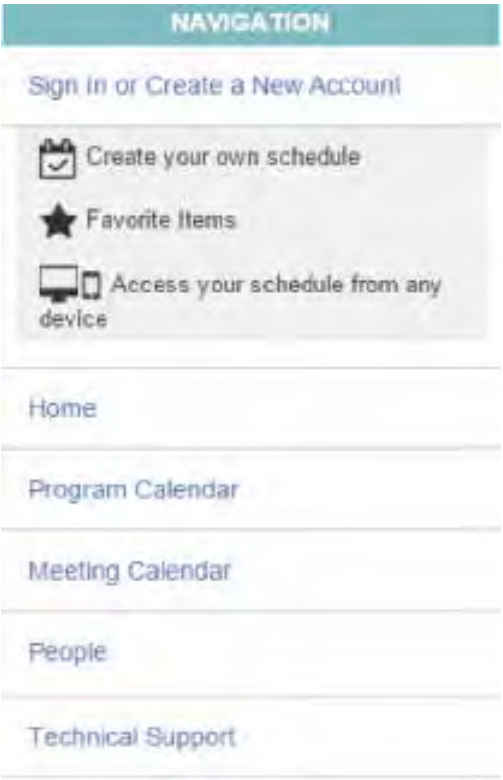
Planning your poster: Each poster will be 4' x 4'. There will be three evening poster sessions: Saturday, Sunday and Monday. Push pins will be provided. Authors will be assigned dates and times to be present at their board.

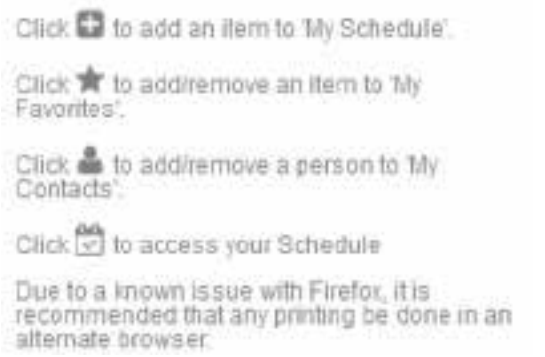
Poster by Robert Evans
receipent of 2014 IUCr Poster Prize
Albuquerque, New Mexico

Welcome to the Denver Meeting App

Visit ***aca.confex.com/aca/2016/meetingapp.cgi/Home/0*** to view the 66th Annual Meeting schedule.

To find a session, either check the *Program Calendar* link on the left or use the *Meeting Calendar* section to browse by day. Once you find a session, you can click on it for more details. For oral and poster sessions, click on presentation titles to access the abstracts and author information. See the left navigation bar (shown below) for instruction on how to create your own schedule





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Congratulations to the following 2016 SIG Etter Lecturers: Powder Diffraction - Dan Taylor; Small Molecules - Victoria Hall; Service - Claudia Wandtki; General Interest - Jens Luebbben; Light Sources - Charles Bury; BioMac - Stefan Imseng; YSSIG - Jose Olmos; Neutron - Amber Larson; Materials - Daniel Mast; Industrial - Mikaela Pyrch; Fiber - Brandan Sullivan.

AUGUST 2016

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

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

DECEMBER 2016

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

FEBRUARY 2017

11-15 **Biophysical Society. 61st Annual Meeting.** New Orleans, LA *www.biophysics.org*

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

JULY 2017

24-26 **Ninth International Conference on Borate Glasses, Crystals. and Melts.** St. Anne's College Oxford, UK. *www.borate-.phosphate.sgt.org*

26-28 **Second International Conference on Phosphate Materials.** St. Anne's College Oxford, UK. *www.borate-.phosphate.sgt.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, Ontario, Canada *www.AmerCrystalAssn.org*

1st Pan African Crystallography Meeting, Cameroon, October 6- 11, 2016

The Cameroon Crystallography Association and the University of Dschang, invite you to participate to the First Pan African Conference on Crystallography (PCCr[1]) in the city of Dschang, Cameroon. The theme of the conference is *Crystallography for Sustainable development in Africa*.

The topics of the conference are organized around seven microsymposia: Inorganic Materials and Mining Industry; Inorganic Materials and Industry Minerals; Crystal engineering and structural chemistry: function through design (2 sessions); Crystallography data bases; Crystallography for life sciences; and Large Facilities for emerging countries.

The four regional Associates of the IUCr are endorsing the Pan African Conference and welcome the African crystallographic community to our world wide family. The ACA encourages its members to support the growth of crystallography in Africa by attending the conference and establishing contacts with African crystallographers. The conference organizers are also requesting donations to support the attendance of young researchers. Donations can be made payable to American Crystallographic Association, (include a note stating what the funds are to be used for) and mailed to ACA, P.O. Box 96 Ellicott Station, Buffalo, NY 14205-0096

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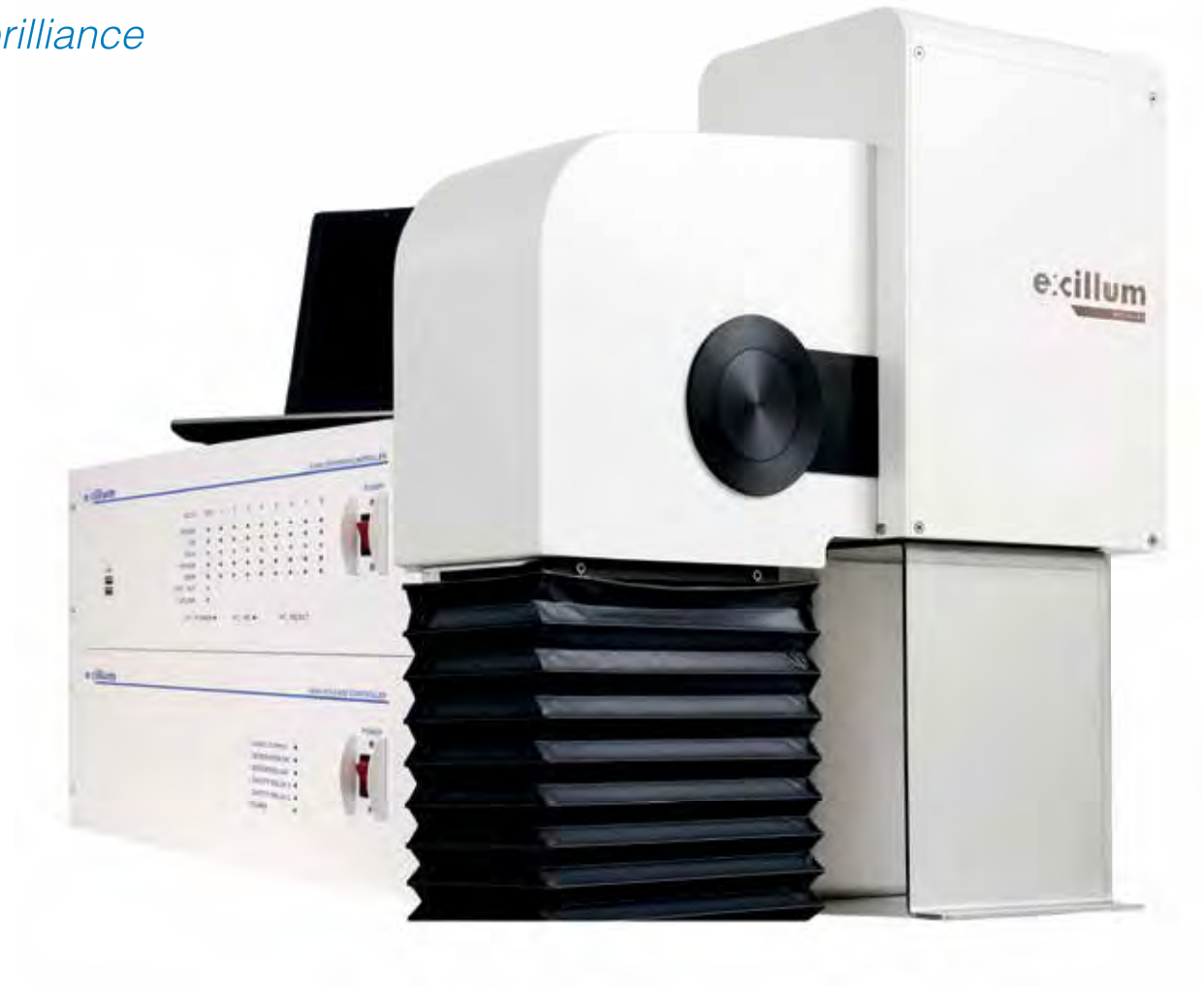

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