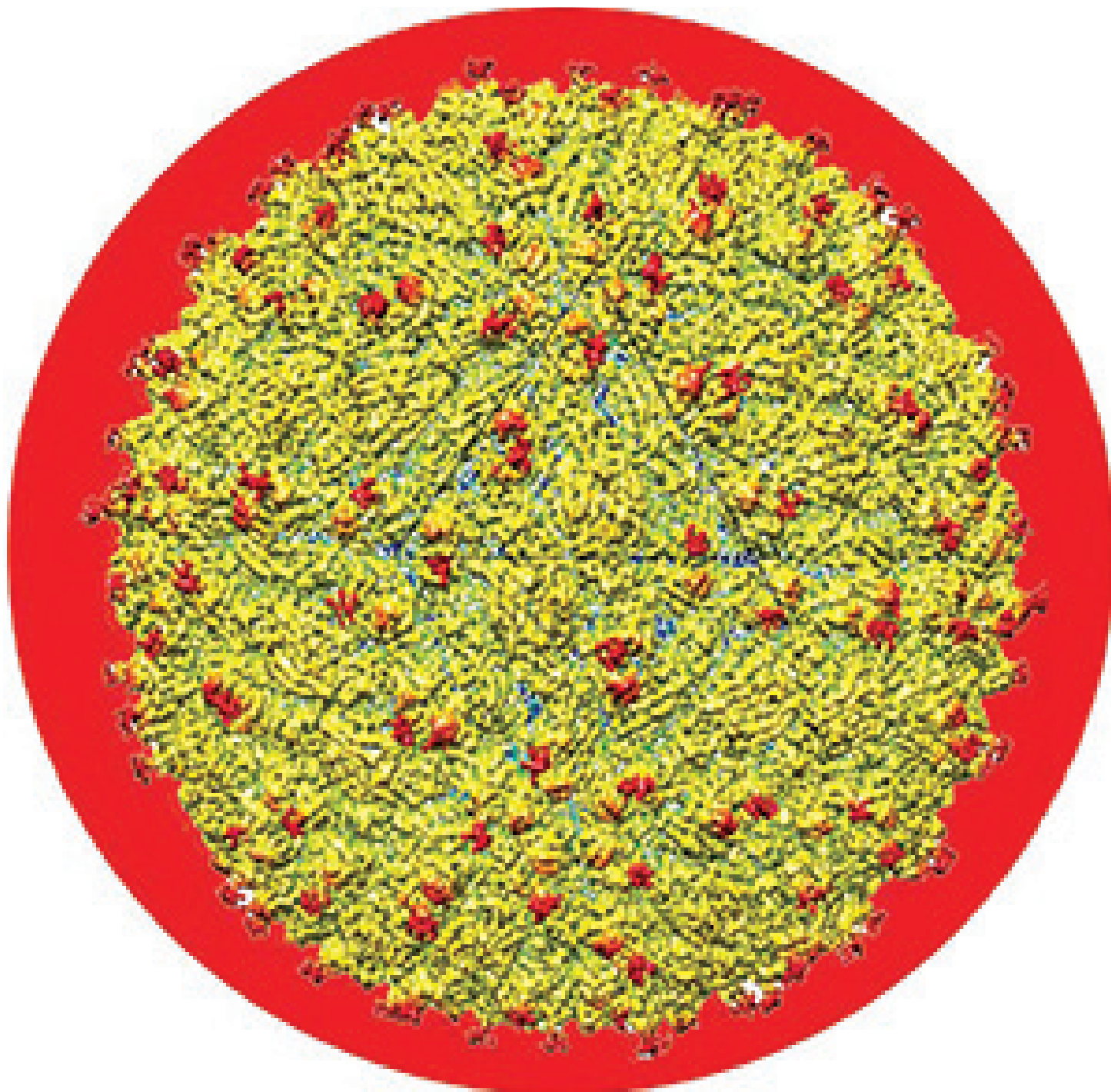


ACA RefleXions

*American Crystallographic
Association
Structure Matters*

Number 4

Winter 2018



***ACA Summer Meeting
July 20-24, 2019
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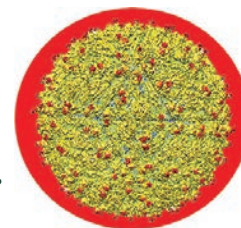
Joseph Ferrara
2019 ACA President

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What's on the Cover?

In the Fall, 2017 issue of ACA Reflexions on page 22, there is a Transactions Symposium in which Michael Rossmann described the structure of the Zika Virus and it's effects on human health. It was obvious that this should have greater exposure, so Michael Rossmann was contacted with a notice that this virus would be featured on the Cover. See page 5.



2019 ACA Award Winners



Bryan Chakoumakos
Bau Award



Efrain Rodriguez
Etter Award



Eaton Lattman
Frankuchen Award



Brian Toby
Trueblood Award



Robert Von Dreele
Trueblood Award

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President's Column



Joseph Ferrara

At the 2014 Annual Meeting in Albuquerque, I stood up at the business meeting and commented how badly the meeting had turned out for the vendors. Judith Flippen-Anderson suggested that I could be part of the solution and recommended I join the site selection committee. I had been Books Editor for *RefleXions* for many years,

but I had never been very active in the ACA. With this column, I am starting my year as President. I would like all of you to think about how you can help change the ACA for the better. The only way for this to happen is for you to become active as well.

Council has decided to form three *ad hoc* committees to address some of our ongoing challenges. The first is a Strategic Planning Committee. Council applied for funds from AIP through the Venture Partner Fund to create a strategic planning template for small member societies like the ACA. We failed to get the funding we asked for, but will try again in 2019. Nevertheless, strategic planning is needed, especially as our membership is changing. Council also wants to ensure diversity in our awards and so will form an *ad hoc* Awards Oversight Committee. The remit of this committee is self-explanatory. The third and last *ad hoc* committee is the By Laws Review Committee. The remit of this committee is also straightforward: review the By Laws and make sure they are consistent with the needs of the society moving forward. If you are interested in serving on one of these three *ad hoc* committees, please contact me.

The *ad hoc* Finance Committee will remain active, and we have some challenges ahead. One of the most difficult has been balancing the budget. Lisa and I have been going through the books in an attempt to understand the income and expenses of the society. We have reached the conclusion that that it is time to move bookkeeping to headquarters. In addition to saving some money, Council will be able to monitor expenses more closely and to make adjustments as needed. The good news is that with a lot of help from Rao, Sue, Ilia and Kristin we have presented a balanced budget to Council for 2019.

We can reduce expenses to a certain point, but then there will be little left of the society to keep us as

members. In the business world, there is an adage "nothing solves problems like sales". This paradigm applies to the ACA. Nothing will solve our problems better than more members and higher meeting attendance. I would like to borrow an idea Elspeth Garman used to increase the roll of the BCA after a purge of non-existent members. We will provide a free member renewal for every five referrals[†].

The member survey suggests that meeting content is the most important factor to bring people to the Annual Meeting. Steve Ginell, Vivien Yee and Kristin Stevens have been working extremely hard putting together a fantastic technical program for the Annual Meeting. They also have a few surprises in store for the opening ceremony and the banquet. Please see pp. 10-12 of this issue of *ACA RefleXions* for meeting details.

Speaking of surveys, Lisa mentioned in her last column we completed the membership survey. The good news is that representation of women in the society is consistent with STEM careers overall. The bad news is that while the ACA does promote women in its ranks, we don't do a good enough job of keeping younger women and minorities involved. If we are going to survive, we must nurture all young crystallographers. This means all older members must be good mentors.

One of the issues that has become a real problem for crystallographers is the lack of recognition in publications. One colleague I spoke to indicated that he was given no recognition for some very difficult structures he solved and refined. I did quick survey of fellow crystallographers and found this practice to be widespread. I find this unacceptable, and with Council's advice, decided to task the Data Standards and Computing Committee with the task of contacting some major publishers and convincing them to abide by the ACA code of ethics with respect to publications.

I would like to congratulate Brian Toby on being elected Vice President and Ilia Guzei on being elected Treasurer. I would also like to congratulate all the new committee and SIG members.

Finally, my year as vice president has been a true learning experience. I thank Amy, Lisa, Diana, Sue, Rao and especially Kristin for their help introducing me to the inner workings of Council.

Joe Ferrara

[†]New member must not have renewed in the last three years. Free membership will be based on lowest class of the members referred. To get a full membership you must refer 5 full members. Any student referral will result in a free student membership.

2018 Fall ACA Council Meeting Highlights



Diana Tomchick

The 2018 Fall Council Meeting was held at the Hauptmann-Woodward Institute (HWI) in Buffalo, NY on October 25. Voting members in attendance were President Lisa Keefe, Vice President Joe Ferrara, Treasurer Sue Byram, Past President Amy Sarjeant, Canadian Representative Tomislav Frišćić and Secretary Diana Tomchick. Non-voting members in attendance were IUCr Representative Hanna Dabkowska, YSIG Representative George Lountos, Director of Administrative Services Kristin Stevens, CEO William Duax and CFOS.N. Rao. Visitors included Stephan Ginnell (2019 Annual Meeting Program Co-Chair) and Michael Moloney (American Institute of Physics CEO). In addition to this meeting, Council held two online Council meetings (one in August, another in September) to decide various pressing issues, which will also be described below.

Preparations for the annual meeting in 2019 in Cincinnati/northern Kentucky are well underway, and there was much discussion regarding various details of the program as well as the meeting budget. The ACA Council decided to set the registration fees for the meeting at \$595 for regular attendees, \$325 for postdoctoral students and retirees, \$275 for all other students and \$150 for guests. During the meeting, the ACA will present the Fankuchen, Trueblood, Bau and Etter Early Career Awards, as well as announce the new ACA Fellows. The ACA President will work to get the ACA Nominating Committee to finalize candidates for office in 2019 prior to the ACA meeting, so that candidates may volunteer in the meeting booth to help out the ACA Headquarters staff and meet ACA members.

S.N. Rao, the ACA Chief Financial Officer, presented a draft 2019 budget which generated much discussion about methods to increase revenue and cut expenses. Approval of the 2019 budget was delayed to the December 2019 Council teleconference meeting.

President Lisa Keefe outlined plans to form an *ad hoc* Strategic Planning Committee to address future plans for the ACA. To address the lack of diversity (for example, in gender, nationality, etc.) of past ACA Awardees and Fellows, Lisa and VP Joe Ferrara will recruit members to an *ad hoc* awards oversight committee, that will be charged with encouraging

members to nominate diverse candidates for awards and Fellows. Lisa also recommended that monthly ACA Council teleconference meetings continue to be held in the future in order to more efficiently and promptly handle business. She also recommended a few teleconference meetings be held at the beginning of the year to be held jointly with Council and the members of standing committees and SIG officers, as a forum for two-way communication of duties, questions and new ideas.

Vice President Joe Ferrara discussed plans for the 2019 ACA annual meeting banquet and the ACA Fellows reception. A tentative plan was made to hold the General Business Meeting during the lunch hour (actually, 1.5 hours) one day during the meeting rather than at 5 PM, which conflicts with the 5:30 PM poster session. Joe presented and discussed the results of the ACA member survey, which was conducted online, and approximately 50% of the membership responded. Joe also presented a report from the ACA representative to the American Institute of Physics (AIP) Committee on Diversity, Krystle McLaughlin, who provided recommendations to the ACA (and specifically, the Meeting Planning Committee) for achieving “diverse, equitable, and inclusive professional meetings.”



ACA Council, Fall 2018 meeting.

Front Row, from Left: Diana Tomchick, Sue Byram, Lisa Keefe, Joe Ferrara, Amy Sarjeant, Bill Duax. Back row, from left: S. N. Rao, AIP CEO Michael Moloney, Hanna Dabkowska, George Lountos, Tomislav Frišćić, Kristin Stevens.

Tomislav Frišćić, the Canadian Representative, provided a recap of recently held Canadian meetings, including the 11th Canadian Powder Diffraction Workshop in Hamilton, Ontario, July 25-29, 2018; the 9th Canadian Chemical Crystallography Workshop (CCCW18) as a satellite meeting of the 101st

Annual Meeting of the Canadian Chemical Society in Edmonton, Alberta, May 22-26, 2018; the 8th Annual CLS Mx Data Collection School at the Canadian Light Source in Saskatoon, Saskatchewan, June 4-8, 2018; the 19th Sagamore 2018 Conference on Quantum Crystallography in Halifax, Nova Scotia, July 8-13, 2018; and the 5th Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec (CEMWOQ-5) in Montreal, July 16-19, 2018. Upcoming meetings include the 12th Canadian Powder Diffraction Workshop organized by Louise Dawe for May 2019 in Montreal and the 6th Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec (CEMWOQ-6) planned for late May-early June 2019 in Montreal.

Hanna Dabkowska presented highlights of IUCr activities, including the provision of \$7,500 in support for student travel grants to the 2019 ACA meeting; the support for 25 international meetings in 2018, and 6 confirmed meetings for 2019; the support of the IUCr Outreach and Education Fund of initiatives in Africa, the IUCr-UNESCO OpenLabs and crystallographic schools around the world; the winners of the 2018 IUCr Crystal growing competition for schoolchildren will be announced soon; and the next IUCr Executive Council meeting will be held prior to the ACA Meeting in Covington, Kentucky, July 2019.

Highlights of the report from George Lountos, the Young Scientists Interest Group (YSIG) representative, included a recap of the successful events the YSIG sponsored during the 2018 meeting and details about the plans for the 2019 meeting. These include a Friday afternoon Career Development workshop, A First Time Attendee meeting, a Three Minute Thesis Competition, a Diversity and Inclusion Session, the YSIG Mixer and co-sponsorship of several scientific sessions. The YSIG members are looking forward to providing active input to the new ACA web site, with the goal of improving communication between members and the ACA on topics such as travel grants, career opportunities and locating affordable lodging at the ACA meeting.

The new AIP CEO, Michael Moloney, spoke to Council about the strategic planning the AIP is undergoing to address its changing relationship to its member societies, specifically that the AIP was originally a publishing society primarily, and that has changed. The AIP will no longer provide international shipping for printed copies of *Physics Today*, and member societies can decide whether they wish to subsidize those costs, or pass them on to the individual member. The AIP has instituted an initiative known as TEAM-UP in order to investigate why they aren't

attracting and retaining diverse students. Michael recommended that Council invites the AIP Publishing CEO to the Spring Council meeting to discuss issues that the ACA may have with the retirement of Bob Finnegan, who was responsible for organizing the ACA meeting exhibitor show.



Amy Sargeant (right) receives a certificate of appreciation from Lisa Keefe for her service as ACA Vice-President, President, and Past President.

The August and September Council teleconference meetings primarily covered organizational details related to the 2019 ACA meeting, the web site redesign, outreach funding requests, the ACA member survey, an update to the ACA Council Handbook and appointments of ACA members to AIP Liaison Committees.



Sue Byram(left) receives a certificate of appreciation from Lisa Keefe for her service as ACA Treasurer.

The main topic of the November Council teleconference meeting was ACA finances, and the 2019 Vice

President Brian Toby and Treasurer Iliia Guzei joined the discussion. Lisa proposed that the ACA will no longer outsource bookkeeping services, as Director of Administrative Services Kristin Stevens will do the accounting, and also to base the 2019 ACA Meeting budget on an attendance of 550 rather than 600. The ACA CFO's duties will be reduced which will result in additional savings.

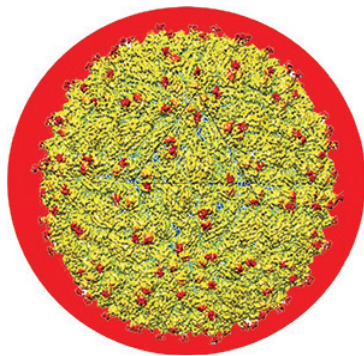
Last, but not least, considerable thanks are due to the services of the outgoing ACA officers: Lisa Keefe as President, Amy Sarjeant as Past President and Sue Byram as Treasurer.

The next in-person Council meeting in Buffalo, NY will be in early 2019.

Diana Tomchick

On the Cover

The 3.8 Å resolution cryo-EM structure of Zika virus.

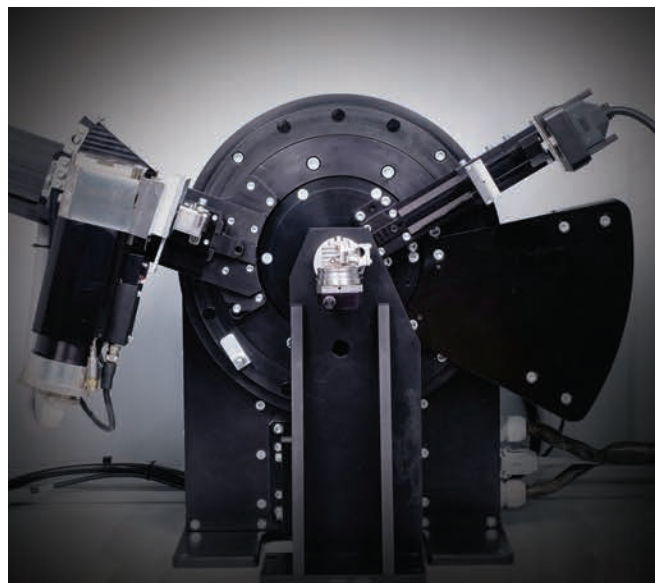


The recent rapid spread of Zika virus and its unexpected linkage to birth defects and an autoimmune neurological syndrome have generated worldwide concern. Zika virus is a flavivirus like the dengue, yellow fever, and West Nile viruses. The cover

image shows the 3.8 Å resolution structure of the mature Zika virus, determined by cryo-EM. The image is a surface-shaded depth-cued representation of the virus, viewed down the icosahedral twofold axis. The asymmetric unit is identified by the black triangle. The structure of Zika virus is similar to other known flavivirus structures, except for the ~10 amino acids that surround the Asn¹⁵⁴ glycosylation site in each of the 180 envelope glycoproteins that make up the icosahedral shell. The carbohydrate moiety associated with this residue, which is recognizable in the cryo-EM electron density, may function as an attachment site of the virus to host cells. This region varies not only among Zika virus strains but also in other flaviviruses, which suggests that differences in this region may influence virus transmission and disease.

From Devika Sirohi, Zhenguo Chen, Lei Sun, Thomas Klose, Theodore C. Pierson, Michael G. Rossmann, Richard J. Kuhn, *Science*, **352**, 467-470(2016). Reprinted with permission from AAAS.

Connie Rajnak



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ACA History Project Update

As you've no doubt noticed the ACA website has undergone a face-lift! The migration from the previous website software to the newly adopted MemberClicks version required a lot of unseen work in the background by Kristin Stevens, Kristina Vitale and Vanessa Reitz to design the new ACA web pages. History Webmaster Vanessa Reitz is adapting the 250 or so history pages to make them as attractive and user-friendly as they were before the changeover.

While the new web pages were being planned, Webmaster Reitz had time to make a new video of Helen M. Berman's 2006 Buerger Award lecture. In her lecture Helen described the early history of the PDB – showing how technology, science, and community can synergize further science. It is an inspiring story. The video is available from the ACA History pages at http://www.amerocrystalassn.org/h-berman_videos.



ACA President Robert Bau presenting the 2006 Buerger Award to Helen Berman



Bust of Rosalind Franklin in The College of Wooster Science Library

Speaking of inspiring stories, The College of Wooster Science Library (Wooster, OH) has added exhibits celebrating the contributions of women and non-western scientists. Called "Hidden Science Superstars," six people are featured: Rosalind Franklin (crystallographer), Chien-Shiung Wu (physicist), Maryam Mirzakhani (mathematician), Ibn Sina (philosopher and physician), Mae Jemison (physician and NASA astronaut) and Martha Chase (molecular biologist).

It was the research of Franklin and her student Raymond Gosling that led to the famous Photograph 51 – the diffraction pattern that showed the double helical structure of DNA and allowed them to calculate the helical parameters. (See what students said about her career here: <https://bit.ly/2DcWMo0>).

Regarding Franklin, James Watson commented in his book *The Double Helix*, "By choice she did not emphasize her feminine qualities. Though her features were strong, she was not unattractive and might have been quite stunning had she taken even a mild interest in clothes. This she did not." On the other hand, Gosling described Franklin as elegant when she dressed to go out in the evening.

Jenny Glusker knew Franklin in the 1950s. "I went to the International Union of Crystallography Meeting in Paris in July 1954. I was a graduate student and Dorothy Hodgkin was my supervisor, and that was when she lectured on the chemical formula of vitamin B12 that we had been working on. Her talk generated great excitement among the audience. At one stage Rosalind Franklin came up to me and asked me if I wanted to come to a fashion show with her. I explained that I was a scientist and had planned to attend the scientific sessions that afternoon. She replied that the sensible thing to do at a meeting of this kind was to look at the scientific program and also at the program for accompanying members and attend the one that was the more exciting. She thought the fashion show sounded more interesting. So I accepted her invitation and off we went. The fashion show was in Rue Faubourg St. Honoré and there was a lovely display of autumn hats, some of which I liked very much, and several elegant dresses. We had a very pleasant afternoon together."

Virginia Pett
pett@wooster.edu

Bryan Chakoumakos Selected to Receive the 2019 Robert Bau Award



Bryan Chakoumakos, Group Leader of the Structure of Matter, Quantum Condensed Matter Division at Oak Ridge National Laboratory, is the recipient of the ACA's 2019 Robert Bau Neutron Diffraction Award. This award recognizes "exceptional research achievements in neutron diffraction."

Chakoumakos has spent his career at Oak Ridge National Laboratory (ORNL), starting as a staff scientist and, in 1993, transitioning into the Neutron Scattering Sciences Division where he became responsible for the oversight and development of many neutron powder and single-crystal neutron diffractometers. Between 2006 and 2011, Bryan served as Group Leader of Neutron Single-Crystal Diffraction at ORNL, overseeing the Spallation Neutron Source (SNS) instruments, as well as the diffractometers at the High Flux Isotope Reactor (HFIR). For many years, as group leader of diffraction at ORNL, Bryan has overseen the strongest suite of neutron diffractometers in the world.

Bryan Chakoumakos is a productive researcher whose scientific achievements in the neutron sciences span a number of fields, as he leverages his profound knowledge of single crystal and powder diffraction to extract detailed structural information to aid in determining structure-property relationships in novel and technologically important materials.

Perhaps his most durable legacy to the field of neutron diffraction took place in the early 1990's. Bryan served as chair of the Single-Crystal Diffraction Working Group for the "Workshop on Instrumentation Needs and Performance Metrics for the National Spallation Neutron Source". This event essentially kick-started what is today the SNS, the flagship neutron scattering facility in the U.S. Bryan then headed, as group leader, the next generation of instrument

scientists in the construction, commissioning and operation of the suite of state-of-the-art, single-crystal diffractometers at the SNS.

Bryan has been an engaged member of the ACA community, as chair of sessions, as invited speaker and as Chair of the Neutron Scattering and Powder Diffraction SIGs. Throughout his career, Bryan Chakoumakos has been a true ambassador for the neutron sciences.

Kay Onan

Efrain Rodriguez Selected to Receive the Margaret C. Etter Early Career Award



Efrain Rodriguez is the recipient of the 2019 Margaret Etter Early Career Award, an award given "to recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career." Efrain is Associate Professor of Chemistry and Biochemistry at the University of Maryland. He heads a solid state chemistry laboratory that combines chemical synthesis with advanced characterization of physical properties and atomic structure to tackle ways of controlling the physical properties of solids. At the heart of his group's efforts to discover new functional materials through the preparation of inorganic compounds is structural characterization by x-ray and neutron diffraction.

The educational path taken by Efrain started at MIT, where he earned his undergraduate degree in Materials Science and Engineering. He then moved west to the University of California, Santa Barbara (UCSB) for a PhD in Materials, carrying out his PhD research between UCSB and Los Alamos National Laboratories. He won a competitive National Research Council Postdoctoral Fellowship to join the diffraction group of Mark A. Green at the National Institute of Standards and Technology (NIST) Center for Neutron Research. He then moved to the University of Maryland. He has already established a very productive program in solid

state sciences that is having high impact. He received an NSF CAREER award that supports his interest in looking for non-iron superconductor systems that display the specific magnetic behavior closely related to superconductivity. This award is “NSF’s most prestigious award in support of junior faculty members who exemplify the role of teacher-scholars through outstanding research, excellent education and the integration of education and research.” And, in 2016, he was recognized as an Emerging Investigator by the Royal Society of Chemistry in the Journal of Materials Chemistry C for “carrying out work with the potential to influence future directions in materials chemistry.”

Efrain is technically competent, thinks deeply about problems, is very innovative and has a great deal of drive. He is defining a new age in solid state and materials chemistry and is a pioneer in having a skill set in synthesis and characterization that will allow the scientific community to move into hitherto unknown areas. *Kay Onan*

Eaton (Ed) Lattman Selected to Receive the 2019 Isidor Frankuchen Award



Ed Lattman is the recipient of the 2019 Isidor Frankuchen Award, an award that is given “to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography.” He is the Director of the BioXFEL Center, an NSF Science and Technology Center focused on applying new X-ray laser technology to further our understanding of the structure and function of biomacromolecular machines. He is also Professor of Structural Biology in the University of Buffalo School of Medicine and Biomedical Science.

His scholarly achievements have contributed fundamentally to macromolecular crystallography and other diffraction methods. Ed was the first to articulate the currently used approach to molecular replacement, in which a known molecular structure is placed into an unknown cell. Today, almost five

decades later, roughly 75 percent of all new protein structures are determined using this technique; few other advances achieve this degree of influence. Perhaps more importantly, Ed has contributed to the advancement of crystallography by thinking broadly and with deep insight into issues; for instance, he has written profoundly about conceptual problems in protein folding.

Ed’s teaching of crystallography comprises a number of modalities over the years. His formal lectures have a clarity that helps his audience understand complex issues. At Johns Hopkins, in the laboratory and in Friday afternoon beer sessions, he thoughtfully and clearly discussed the nuances of crystallographic theory and practice making him a wonderful mentor. Ed brought his skills of teaching to IMCA with remarkable impact. He has provided a vision for growth and expansion of their scientific capabilities and of their thinking; for instance, he educates on new technologies. One of his wonderful qualities is his interest in the advancement of each scientist. At IMCA this has manifested itself by his talking to all of the IMCA staff and board members about science and about scientific growth and development.

As a testament to the significant and prolonged impact that Ed has had and will continue to have is the authorship, with Patrick Loll, of a graduate text Protein Crystallography, a masterpiece of clarity. His impact goes far beyond that provided by his own publication list. *Kay Onan*

Robert B. Von Dreele and Brian H. Toby Selected to Receive the 2019 Kenneth N. Trueblood Award



Robert B. Von Dreele



Brian H. Toby

The Trueblood award is given “to recognize exceptional achievement in computational or chemical crystallography.” Bob Von Dreele and Brian Toby, like Kenneth Trueblood, have both been pioneers in computational crystallography and, as a team, have had an unmatched impact on the progress of powder diffraction crystallography.

Bob is known for being a co-author of the General Structure and Analysis System (GSAS) suite of programs, the first to allow refinement of crystallographic models to either single-crystal or powder diffraction data and to utilize x-ray or neutron data. Before that, the analysis of crystal structures from powder data using the Rietveld method remained the domain of experts willing to, and capable of, delving into Rietveld's refinement program. Though GSAS did make studies easier, the learning curve for using it was steep, especially for those just starting out with Rietveld refinement. Brian responded to this difficulty by writing a widely-used front-end to GSAS called EXPGUI that made GSAS more user-friendly and accessible to thousands of users. Brian's amazing helpfulness to users all over the world has been instrumental to the impact that is seen from this suite of programs (GSAS-EXPGUI). It has been approximated from a survey carried out by the DANSE project that about 75% of users in the US who do Rietveld refinement use GSAS, of whom about 90% use the EXPGUI interface.

More recently, Bob and Brian have, together, created GSAS-II that takes the functionality of GSAS+EXPGUI to a whole new level. It is a nearly completely new code, written using modern programming language, and with a greatly extended scope; it now includes area detector data reduction, structure solution, powder diffraction indexing, microstructure characterization and small-angle scattering analysis. The impetus for developing this new package was to provide a modern code that would integrate visualization in all stages of crystallographic analysis, better facilitate the needs of novices, and provide a platform for analysis of parametric diffraction studies. Part of the value of these pieces of software to the entire world is that they are distributed free of charge.

Individually, both Brian and Bob have also contributed to the design and construction of diffractometers, Bob at Los Alamos and Brian at NIST. Teaming up they produced the most prolific beamline at the Advanced Photon Source and, arguably, the leading powder diffraction instrument in the world, known as 11-BM. Bob co-wrote the initial proposal that obtained the funding to build the instrument. Brian oversaw the construction but his most high profile contribution was in writing the software and interface for sample management that has allowed the instrument to be so efficient. Bob wrote the user interface for the on-site use of 11-BM.

While not stated in the description of the award, it is nice to remember that Kenneth Trueblood was a superb teacher. Therefore, it is particularly satisfying to note that the impact of Bob and Brian's work has

been greatly enhanced by their willingness to devote large amounts of time to the training of novices in powder diffraction. They have done so in workshops and short courses offered around the world. Brian has been a stalwart lecturer at the ACA Summer Course while Bob has been teaching at the Erice Crystallographic School in Europe. Brian has also put together a series of tutorials that allow novice x-ray diffraction users to develop background on the technique.

Both Brian and Bob have provided valuable service to the crystallographic community; Bob as ACA President and as a member of the US National Committee and Brian as a member, vice-chair and chair of the US National Committee. Brian has also spent years on extending the IUCr's Crystallographic Information File electronic standard for exchange of crystallographic results to powder diffraction data.

Together Bob and Brian have led significant advancements in the field of crystallography and played a pivotal role in the widespread community adoption of powder diffraction crystallography. They have changed the face of powder diffraction in the United States.

Kay Onan

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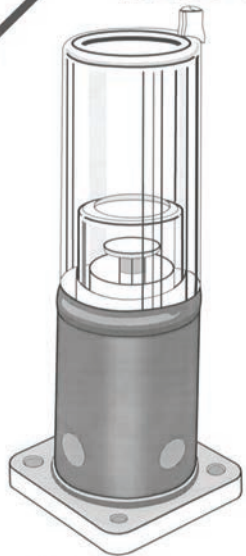
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Winnie Wong-Ng named Academician of the World Academy of Ceramics

Winnie Wong-Ng of the National Institute of Standards and Technology (NIST) was honored as an Academician of the World Academy of Ceramics (WAC) in recognition of her outstanding contribution to the advancement of ceramics science. The award ceremony took place during the 14th International Ceramics Congress (CIMTEC) in Perugia, Italy (June 4-8, 2018). WAC is connected to the International Ceramic Congress (CIMTEC).

Those named as Academicians are individuals who have made an international, noteworthy contribution to the advancement of ceramic culture, science, technology, industry or art. *Kay Onan*



Award Ceremony (June 5, 2018). Left to right: Takashi Goto (Tohoku University, Japan), Winnie Wong-Ng (National Institute of Standards and Technology, USA), Gary Messing (Pennsylvania State University, USA). Goto and Messing were co-chairs of CIMTEC 2018.

From the Editor's Desk:

Late word has been received of the passing of four notable crystallographers.

On October 9, **Thomas A. Steitz** (1940-2018),
2009 Nobel Laureate.

On November 20, **Aaron Klug** (1926-2018),
1982 Nobel Laureate.

On November 22, **Håkon Hope** (1930-2018),
ACA Fellow.

On January 2, **Joel Bernstein** (1941-2019),
AAAS Fellow.

Friends and colleagues are invited to submit remembrances to either of the Co-Editors for publication in the Spring 2019 issue of *ACA RefleXions*.
Ed Stevens

ACA CINCINNATI/NORTHERN KENTUCKY

Saturday, July 20 - Wednesday, July 24, 2019

Travel Grant Application Deadline: March 29, 2019

Abstract Deadline: March 29, 2019

Early Registration Deadline: May 31, 2019

Hotel Reservation Deadline: June 28, 2019

ACCESS UPDATED MEETING INFORMATION:

<http://www.amercrystalassn.org>

Abstract submission - Meeting registration - Full call for papers

**Sponsorship opportunities
Information for exhibitors**

Abstracts accepted online only

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

WORKSHOPS

*Advanced Structural Characterization of
Nanomaterials*

Accelerating Your Career Development

*Introduction to PHENIX for electron
cryo-microscopists*

*Serial Crystallography: Obtaining Protein Structure
from Many Crystals*

CryoEM I : Image Processing II : Reconstruction

YSIG Sponsored/Co-Sponsored Sessions

Three Minute Thesis Sessions I & II

Structure Without Structure

General Interest Sessions I & II

Solid State Supramolecular Chemistry I & II

Diversity & Inclusion Session

YSIG Orientation and Networking Mixer

EDUCATION ORIENTED SESSIONS

Open Exchanges in Crystallographic Education

Would You Publish This?

Sustaining Crystallography Education and Training

ACA AWARDS

Robert Bau Award honoring Bryan Chakoumakos

I. Frankuchen Award honoring Eaton (Ed) Lattman

*Kenneth Trueblood Award honoring Brian Toby
and Robert Von Dreele*

*Margaret C. Etter Early Career Award honoring
Efrain Rodriguez*

2019 ACA MEETING - CINCINNATI/NORTHERN KENTUCKY



Program Chair - Stephan Ginell
slginell4aca@gmail.com



Program Chair - Vivien Yee
Vyee.aca@gmail.com



Posters Chair - Louise Dawe
ldawe@wlu.ca



Posters Chair - David Rose
david.rose@uwaterloo.ca

SCIENTIFIC SESSIONS

ACA Transactions Symposium - Data Best Practices: Current State and Future Needs

Applications of Anomalous Techniques for MX

Cancer: Structure and Mechanics I & II

Cool Structures: Important Science from Small Molecule Crystallography I & II

Crystal Structure Solution from Powder Data

Crystallography at Extreme Conditions

Crystallography in the Geosciences

Cutting Edge Studies in CryoEM

Diffuse Scattering in Crystals

General Interest Sessions I & II

Growing Crystals in the Industrial Space Station

Home Built Software and Hardware

In-situ/Operando Methods

Locating and refining H atoms using X-rays, Neutrons, and Solid-State NMR

Materials for Sustainability

The Meaning of Resolution

Micro-Electron Diffraction

New Toys: Sources, Beamlines and Detectors I & II

Physiology Temp

Radiation Damage in X-ray and EM

SAS Contrast Methods in Biology and Soft Matter

Solid state NMR Crystallography

Solid State Supramolecular Chemistry and Crystal Engineering I & II

Structural Biology Combining SAS and high resolution methods

Structural Parameters of Porous Materials

Structure Based Drug Design

Structure/Local Structure of Thin Films, Interphases and Surfaces

Structure Without Structure

Time-Resolved @ XFELS

Understanding Polymer Dynamics

What is a Crystal, In Time and Space?

Would You Publish This?

	Regular Room Rate	Student Room Rate
Cincinnati Marriott RiverCenter	\$159 Per Night Plus Customary Taxes & Fees	\$129 Per Night Plus Customary Taxes & Fees
Embassy Suites Cincinnati RiverCenter	\$159 Per Night Plus Customary Taxes & Fees	\$129 Per Night Plus Customary Taxes & Fees

General Meeting Information

Venue:

All scientific sessions, workshops and poster exhibits will take place at the Northern Kentucky Convention Center, 1 W Rivercenter Blvd., Covington, KY 41011, <http://www.nkycc.com/>.

Hotel:

There are two hotels with dedicated ACA room blocks: the Cincinnati Marriott RiverCenter (10 West Rivercenter Blvd., Covington, Kentucky 41011) and the Embassy Suites Cincinnati RiverCenter (10 East Rivercenter Blvd., Covington, KY 41011).

We are able to offer discounted room rates because of our commitment to a contract for a minimum number of sleeping rooms at these two specific hotels. We encourage all attendees to support the ACA and reserve a room in the conference block. With your support, the ACA can continue to provide discounted room rates to attendees in the future.

The Northern Kentucky Convention Center is centrally located across the street from each of these hotels and is less than a minute walk away.

Travel:

The Cincinnati/Northern Kentucky International Airport (CVG) is consistently ranked as one of the best airports in the world. Northern Kentucky is within a two-hour flight from 60 percent of the nation's population. Cincinnati/Northern Kentucky is also within only a two-hour drive of the Port Columbus International Airport (CMH), Dayton International Airport (DAY), Louisville International Airport (SDF) and Lexington's Blue Grass Airport (LEX).

Foreign Travelers:

Obtaining a VISA: Advanced planning by foreign travelers is critical. Obtaining a VISA is the sole responsibility of the attendee. Meeting attendees should first determine whether a VISA is needed and if so, applications should be made at least ninety (90) days in advance of the travel date.

Helpful information regarding traveling to the US can be found on the US Department of State: Bureau of Consular Affairs (<https://travel.state.gov/content/travel.html>) and through the International Visitors Office (<http://sites.nationalacademies.org/PGA/biso/visas/index.htm>).

If you require a participation letter to the conference to submit with your application, please e-mail your request to: aca@hwi.buffalo.edu. Please include

your name, passport #, birth date, mailing address, e-mail address and the title(s) of any abstract(s) that you have submitted for the conference. A copy of the letter will be e-mailed to you.

Financial Support:

Members and attendees are important to the ACA and as such there are a number of opportunities for financial support to attend the meeting:

- Become a member! Discounted Meeting registration fees are available to members.
- ACA Travel support will be available for young scientists from the ACA. Applications for travel support will be available on the ACA's website and should be submitted to the ACA by March 31, 2019.
- More opportunities for travel support from ACA partners will be posted on the 2019 Annual Meeting website as they become available. The 2018 meeting provided over \$10,000 of travel support from our partners and we hope to continue to provide the same level of support in the future.
- Become a session room volunteer! Registered students and post-docs attending the 2019 ACA Annual Meeting can apply to be session room monitors. Session room monitors operate audiovisual equipment, and room lighting, photograph the speakers (cameras provided), track and record attendance, and perform other tasks requested by the session chairs. Applications to be a session room volunteer will be available on the ACA's website and should be submitted to the ACA by May 1, 2019.
- Volunteer at the front desk! Registered students and post-docs attending the 2019 ACA Annual Meeting can help hand out registration packets and assist attendees with general questions and inquiries. Volunteer for one (1) full-day (7:00 a.m.–4:00 p.m.) and receive half-off regular student/post-doc registration.

• Share a room! This is an option facilitated by the ACA to help those looking to save money on their hotel accommodations by sharing the cost of a hotel room. The ACA only assists in facilitating contact between roommates and does not guarantee room availability. Further, attendees/roommates are responsible for making their own hotel reservations. Check out the ACA's website for information on sharing a room and to find a list of attendees looking for roommates.

Program Information: All attendees will receive a hard copy of the program book, but the full set of abstracts will only be available online.

Workshop No. 1: Cryo-EM - A Guide to High Resolution Structure Determination



Marcus Brubaker discussing 3D reconstruction methods in WK.01. Photo by Richard H. Bromund.

A very informative and well attended one-day tutorial on cryoEM – from cryo-specimen preparation to data collection, image reconstruction and modelling – was organized by Lori Passmore, Wah Chiu and John Rubinstein. **Lori Passmore** and **Chris Russo** (MRC LMB) provided many up-to-date tips in preparing cryo-specimens with more random orientations and less specimen charging to improve data collection. **John Rubinstein**, **Marcus Brubaker** and **Ali Punjani** (Toronto Hospital for Sick Children) showed the audience the best practices in processing single particles with high efficiency and accuracy yielding high resolution single particle structures. **Matt Baker** and **Corey Hryc** (Baylor College of Medicine) and **Tom Terwilliger** (Los Alamos National Lab) discussed how to build models constrained by cryoEM maps and how to validate them properly.

Cathy Lawson

Workshop No. 2: Molecular Art & Animation in 3D



Group photo of WK.02 participants and speakers. Photo courtesy of Chelsy Chesterman.

Beautiful figures and animations have become synonymous with the publication of structural data in top research journals. Demonstrating molecular concepts and structural data using these strategies is also highly effective in scientific presentations or outreach activities. Many crystallographers enter the field with a background in chemistry or biology and are unfamiliar with creating such artwork. This year in Toronto we held the first Molecular Art and Animation workshop at an ACA annual meeting. This workshop was sponsored and organized by

the Young Scientists Interest Group in response to specific requests from graduate students. We had an amazing turn out with 43 participants and instructors including students, postdoctoral fellows, principal investigators, and industrial scientists.

The goal of this workshop was to expose structural biologists to a wide variety of software options for presenting their work including PyMOL, Chimera, Blender 3D, and Maya. The workshop aimed to provide enough information so that participants could make an informed choice about the correct platform for their needs. We discussed strategies for producing images and animations in these different programs and provided detailed tutorials to help participants get started with their own projects.

The morning presentation was given by **Maria Voight** (Protein Data Bank), who provided an exceptional introduction to the principals of visual communication. The morning session also included hands-on tutorials for the visualization of protein structures in PyMOL by **Krystle McLaughlin** (Vassar College) and the visualization of cryo-electron microscopy density in Chimera by **Chelsy Chesterman** (Rutgers University).



Participants in WK.02 receiving hands-on training in molecular art and animation. Photo by Richard H. Bromund.

The afternoon session focused on the production of molecular animations and began with a presentation on storytelling by **Travis Eisemann** (Princeton University). Travis and Maria also provided tutorials in the afternoon session on the general animation platforms Blender 3D and Maya with plug-ins for the inclusion of molecular coordinates.

Overall, it was a jam-packed day and we wish all the participants happy modelling! I would also like to extend a big thank you to all the presenters for taking the time to participate and providing detailed step-by-step guides for their favorite software package.

Chelsy Chesterman

Workshop No. 4: Application of Small Angle Scattering to Structural Biology: An Introduction

As the number of high-resolution molecular structures obtained from frozen and crystalline samples continues to grow, solution-based structural methods will continue to yield important insights into how those structures actually behave and interact under more physiologically realistic conditions. The great versatility of SAS enables studies under a wide range of experimental conditions. This, in combination with its ability to analyze flexible and disordered systems, has made SAS a popular technique with a steadily growing base of users. Wk.04 was organized with new users in mind.



Angela Criswell (Rigaku) introduces WK.04 students to the foundations of small angle scattering.

Photo courtesy of Richard Gillilan.

Since the tutorials in this workshop required that students install software on their laptops, the day opened with an informal help session for anyone who needed assistance getting started. **Richard Gillilan** (CHESS) began the morning with a talk entitled “Why Small Angle Scattering?” This talk was a sweeping overview of the many ways SAXS can be applied to problems in structural biology and biophysics. Richard finished by examining two literature examples in detail: one in which simple “entry-level” SAXS techniques were used as part of a larger study, and another in which advanced SAXS techniques were used to construct a complex pseudo-atomic homology model. **Angela Criswell** (Rigaku) followed with an introduction to the basics of SAXS data analysis: Guinier analysis, how to check for monodispersity and concentration effects, and other essentials. The first tutorial run by **Jesse Hopkins** (BioCAT, APS), introduced students to the BioXTAS RAW software, a now widely-used open-source package for processing SAS data. RAW was started by **Soren Skou** (SAXSLAB/Xenocs) during his time at the Technical University of Denmark, then brought to the Cornell High Energy Synchrotron Source where it has been used and refined for nearly a decade. After the morning break, **Richard Gillilan** continued with a lecture

on simple model-independent methods for data analysis. The second tutorial run by **Jesse Hopkins** covered molecular weight estimation and how to calculate pair-distance distribution functions ($P(r)$'s).

During lunch, representatives from Rigaku (**Angela Criswell**), Anton Paar (**Heiner Satner**), and SAXSLAB (**Soren Skou**) shared experience on doing SAXS with laboratory sources and discussed some of the latest technology including the possibility of doing size-exclusion-coupled SAXS (SEC-SAXS) on a laboratory source. SEC-SAXS has emerged as a powerful and highly-requested technique that is now available at all BioSAXS facilities and has even been performed on neutron sources. **Srinivas Chakravarthy** (BioCAT, APS) offered a detailed lecture on SEC-SAXS methods after lunch followed by the closely-related and very important topic of sample preparation, including multi-angle light scattering covered by **Kushol Gupta** (Perelman School of Medicine, UPENN).

We were very fortunate to have **Maxim Petoukhov** (EMBL Hamburg) lecture on bead modeling, rigid body docking, and other valuable tools that are part of the ATSAS package. Maxim also gave a hands-on tutorial in ab initio shape reconstruction. After the afternoon coffee break, **Thomas Grant** (University of Buffalo/Hauptman-Woodward Medical Research Institute), gave a guest research lecture on his new DENSS algorithm for electron density reconstruction. DENSS is now part of the BioXTAS RAW software and a tutorial was distributed to students with the course materials.

Both X-rays and neutrons can utilize differences in contrast to help identify components in complexes. **Kushol Gupta** spoke about both techniques giving several examples. The final talk of the day by **Richard Gillilan** focused on good practice for publishing data, including deposition of scattering curves into international databases.

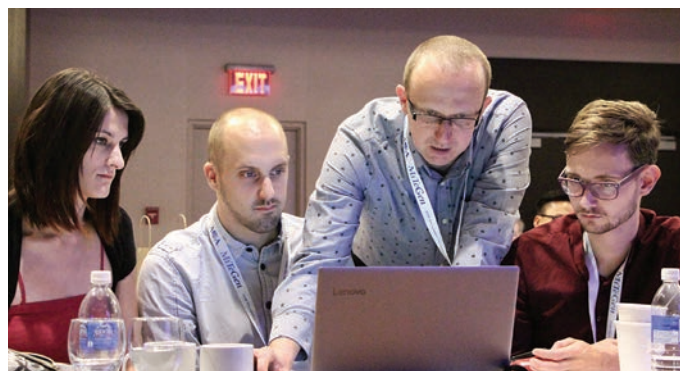
Wk.04 was supported by Anton-Paar, Rigaku Corporation, SAXSLAB, and Wyatt Technology.

Kushol Gupta, Richard Gillilan

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Workshop No. 5: Rietveld Refinement and Pair Distribution Analysis of In Situ X-ray Scattering Data Within GSAS-II



Olaf Borkiewicz assisting workshop participants in the use of GSAS-II.
Photo by Richard H. Bromund

The workshop on Rietveld refinement and pair distribution function analyses held during the 2018 ACA meeting in Toronto, Canada was focused on structural analysis of powder X-ray scattering data – one of the most comprehensive and powerful tools for evaluating crystal structures. The primary focus of the workshop was the discussion and explanation of all typical steps involved in structural analysis of X-ray scattering data with emphasis on data collected at modern users’ facilities using large-area detectors and data processing within General Structure Analysis System (GSAS-II).

The morning session began with a presentation by **Robert von Dreele**, one of the co-authors of GSAS-II software, on the development and features of GSAS-II program and its application to solving a variety of crystallographic and structural problems. This was an excellent opportunity for the participant to learn directly from the author on how to take full advantage of this powerful program for the reduction and analyses of data acquired with both X-ray and neutron probes.

The opening talk was followed by a series of hands-on exercises dealing with processing of X-ray scattering data collected at synchrotron X-ray sources. In the first part of the morning session, led by **Olaf Borkiewicz**, participants focused on the first steps of data minimization – the calibration and integration of powder X-ray diffraction data. Multiple examples of data collected at various experimental conditions at a number of beamlines were used during the exercise to ensure that participants get an opportunity to process “real-world” data and tackle challenges experienced by users during beamline measurements. Both single-pattern integration as well as integration of large data sets were discussed, to showcase the most commonly employed strategies for data processing within GSAS-II. Data generated during integration exercises were then used in the next module focusing on Rietveld refinement of powder diffraction data, led by **Wenqian Xu**.

Refinement of a single pattern was the last activity of the morning session.

After a short lunch break, the workshop resumed with the focus shifting to sequential Rietveld refinements of large data sets and subsequent structural analyses, led again by **Wenqian Xu**. This session, offered great insights into the advanced capabilities of the GSAS-II software package for structural analyses of diffraction data. The second part of the afternoon session was dedicated to structural analyses of nanoscale and disordered materials via pair distribution function (PDF). The session led by **Olaf Borkiewicz** began with an introduction to PDF analyses and was followed by exercises on processing total X-ray scattering data, extraction of PDFs and initial data analyses using sequential peak fitting algorithms within GSAS-II.

The workshop was very well attended and all participants seemed to have enjoyed the opportunity to learn directly from the author of the GSAS-II program and experienced beamline scientists of the APS.

Olaf Borkiewicz

Annual Statement of Ownership, Management, and Circulation

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16. Publication of Statement of Ownership will be printed in the Winter 2018 issue.
17. I certify that all information furnished on this form is true and complete.
(signed) Kristin Stevens for American Crystallographic Association, Inc.

ACA Election Results

Council Officers

Vice President

Brian Toby

Treasurer

Ilia Guzei

Standing Committees

Communications

Louise Dawe

Education

Allen Oliver

Data, Standards & Computing

Eric Reinheimer

Proposed Bylaws Amendment

Passed

Canadian Division

Secretary/Treasurer

Matthew McLeod

Canadian Proposed
Bylaws Amendment
Passed

Scientific Interest Groups

Best Practices for Data Analysis
& Archiving

Chair-elect: John Westbrook

Biological Macromolecules

Chair-elect: Andrew Howard

Secretary: Charles Stewart

Cryo-EM

Chair-elect: Gabriel Lander

Fiber Diffraction

Chair-elect: Joseph Orgel

Secretary: Thomas Irving

General Interest

Chair-elect: Brandon Mercado

Industrial

Chair-elect: Laura Silvian

Light Sources

Chair-elect: Arron Finke

Materials Science

Chair-elect: Efrain Rodriguez

Neutron Scattering

Chair-elect: Adam Aczel

Powder Diffraction

Chair-elect: Pavol Juhas

Service Crystallography

Chair-elect: Richard Staples

Small Angle Scattering

Chair-elect: Jesse Hopkins

Small Molecules

Chair-elect: Brandon Mercado

Young Scientist's

Chair-elect: Nichole Valdez

Secretary: Kenneth Childers

Vice President - Brian Toby:



Senior Physicist; Group Leader for Computational X-ray Science; APS Chief Computational Scientist; Advanced Photon Source, Argonne National Lab, Argonne, IL USA

Statement: I am running for vice president of the American Crystallographic Association because I am very concerned about the future of crystallography. Yes, scientists will continue to perform the structural analyses that are the *raison d'être* of the ACA – for as far in the future as my crystal ball is calibrated. The results will remain critical to scientific research. However, I wonder if the scientists doing this work will call themselves crystallographers? As in-depth study of crystallographic analysis disappears from our curricula, how will scientists be educated to perform this work? Will the quality of results suffer; will crystallography remain the gold standard? We can flail over the injustice in this, but like it or not, increasingly crystallography is just one of many techniques that domain scientists employ for their research, be it structural genomics, solid-state chemistry or condensed-matter physics. However, since my own crystallographic software generates >500 citations/year, I

know there is no shortage of people using crystallography. That will not change.

If elected, I want to lead the ACA in a discussion on how to best improve crystallographic education. The ACA needs to ensure that there will be a next generation of expert crystallographers in North America, best done I believe by advocating to the organizations that establish scientific policies on the importance of this crystallographic expertise. Likewise, I would also like to see the ACA take a greater role in educating younger scientists in crystallographic techniques. I have taught at the ACA Summer School for most years in the past ~15 and recently became a co-director of the Oak Ridge-Argonne Neutron/X-ray School. In that role, I cannot tell you how many young scientists (or their advisors) have written that they need external instruction because they can't learn enough about diffraction and crystallography at their home institutions. Nonetheless, I can vouch that as valuable as these summer schools are, they can only *introduce* students to crystallography. Anyone working in the field needs to know so much more. Educational outreach can bring new people to the ACA and perhaps even a small revenue stream.

For those who do not know me, an introduction is due. I started in crystallography at Rutgers in 1977 after my freshman year, when crystallographer Joseph Potenza offered me a summer job in single-crystal structure determination. I learned skills there that have served me well: to solving structures with MULTAN, Patterson and difference maps; I taught myself how to find burned-out chips in the CAD-3 that Nonius would no longer service, as well as how to reprogram data collection (in a PDP-8 with 4K of memory!) Building wooden-stick

crystallographic models, perhaps not. Based on Joe's advice about the decline in crystallography (even back then), I moved to another field for my graduate work, but was lucky enough to be Dick Marsh's teaching assistant. I was able to move back to my first love — crystallography — when Union Carbide (rest in pieces) hired me to run their corporate powder diffraction lab and sent me to Brookhaven, where I helped Dave Cox get the first dedicated synchrotron powder diffractometer running. Two years later I escaped Carbide to work for Takeshi Egami at UPenn, where I helped pioneer pair distribution analysis for structural analysis, demonstrating the accuracy of the technique and writing the first PDF fitting program for local-structure in crystalline materials. Also while in Philadelphia, I found the other love of my life, psychologist Diane Pies Toby. We then moved to Allentown, for a much happier industrial work experience with Air Products and Chemicals. There I did zeolite crystallography and would have set a record for the most complex structure to be determined from powder diffraction, had APCI then allowed me to publish it. I was later very lucky to be invited to lead the crystallography team at the NIST Center for Neutron Research, where my goal was to make neutron diffraction much more accessible to the community. At NIST, I created the EXPGUI program, which I believe is one of the most cited single-author papers in crystallography. Finally, I moved to Argonne about a dozen years ago, to lead construction of the 11-BM powder diffractometer, personally designing and implementing the mail-in access system that has allowed 11-BM to be the most productive instrument at the APS (likely the world) and has helped synchrotron powder diffraction to become so very widely used.

My most recent project has been to help Bob Von Dreele develop GSAS-II, which is the only general-purpose crystallographic software package initiated in the current century. GSAS-II is used for solving and fitting all scale of structures, from perovskites to proteins, from both single crystal and powder diffraction measurements, and using data from lab instruments, synchrotrons, reactors and TOF neutrons, potentially in combination. There, that covers 40 years and ~140 papers (www.researcherid.com/rid/F-3176-2013) in 1 paragraph. It has been quite a ride and a lot of fun!

As a member of the ACA for nearly 30 years, I have the chance to be involved in many ways, serving on a number of committees, organizing sessions, etc. I also served as vice-chair and chair of the U.S. National Committee for Crystallography. For the IUCr, I spent nearly a decade to extend CIF to powder diffraction by creating the pdCIF dictionary. I enticed the journal Powder Diffraction to add a section for educational articles, which I now co-edit. I have gotten a Bronze Medal from the U.S. Dept. of Commerce, the Barrett Award from Denver X-ray Conference and been named a Fellow of the ACA and the International Centre for Diffraction Data.

In closing, while this statement is already too long, I want to end by saying how proud I am to be associated with so many others I admire who also called themselves crystallographers. I think of the Braggs, who welcomed women into their groups in a time when many institutions would not admit them; Von Laue, who risked his career if not life, to speak up to Nazis for Jewish scientists such as Haber and Einstein. I will not go on, but my list of crystallographers/heros is extensive. I am very proud of the ACA's history with diverse leader-

ship from its start, long before this became fashionable.

Without knowing who else is running, from experience I can be sure that the nomination committee has provided another fine candidate; I am confident the ACA will be in good hands. Nonetheless, I see this as a pivotal time for the ACA to look forward to the future of our field and for us to plan to increase our organization's value to the next generation of scientists.

Brian Toby

Treasurer - Iliia Guzei:



Distinguished Scientist
Chemistry Department
University of Wisconsin, Madison
1101 University Ave
Madison, WI 53706, USA.

Statement: I thank the nominating committee for choosing me as a candidate for the three-year Treasurer position. Over the last decade I have been actively involved with the ACA, including serving on the USNC/Cr and co-chairing the New Orleans ACA meeting. In particular, serving as the Poster Chair for five years allowed me to meet a lot of the members from different scien-

tific backgrounds and to collaborate with the ACA leadership.

The current CFO and Treasurer have been successful in implementing their vision of getting our organization toward fiscal viability. I intend to sustain this momentum to ensure that the ACA makes wise investment choices, maximizes income, and controls expenses. I believe that the current upward trend on the ACA balance sheet will allow the organization to expand its programs and attract new members, which in turn will strengthen our association. The decline in the membership must be reversed, and Treasurer plays a critical role at this junction.

Whereas I do not have formal financial education, I have been the Treasurer of the WI ACS Local Section since 2017 and in that short time substantially improved its record-keeping, collaborated with the section's executive committee, reviewed financial and tax statements, and established a well-funded outreach grant program. Since 2014 I have been organizing the WI Crystal Growing Contest that requires a commitment to fund-raising and communication with a large number of sponsors and potential donors. I am happy to say the contest has always run at no cost to the participants.

I understand the financial challenges our organization faces and am looking forward to serving as Treasurer in a way that benefits the entire membership.

Iliia Guzei

Communications-Louise Dawe:



Associate Professor, Chemistry and Biochemistry Department
Wilfrid Laurier University
ON, Canada.

Statement: I am honored to have been considered by the nominating committee for membership in the ACA Communications Committee. I attended my first ACA meeting in 2008, where I found my professional "home". The colleagues and friends that I have made through the ACA have contributed enormously to my growth as a scientist. In particular, the "Would You Publish This?" session, held regularly at our annual meetings, has taught me that my colleagues in the ACA want to share their experiences to help others tackle challenging problems.

In turn, I have tried to give back to our association, and the wider crystallographic community. In addition to the official positions that I have held as part of my professional activities, I have been involved in several other ACA and IUCr initiatives, targeted at communicating crystallography to a wider audience. I was a member of the local organizing committee for the 23rd Congress and Assembly of the International Union of Crystallography (Aug. 2014, Montreal, Canada), where I coordinated

outreach activities for the United Nations International Year of Crystallography 2014 (IYCr2014). These activities included organizing public lectures by three international high impact scientists at McGill University, which were attended by over 300 members of the general public. I organized a public display of Jean-Louis Hodeau's panels, Journey into the Crystal at the metro stop of the Montreal Convention Centre. Foot traffic is very high in this area, and over the course of the eight day congress, it is estimated that several thousand people saw this display. I also organized lunchtime screenings of documentaries for the families and guests of Congress attendees, in collaboration with Prof. Juan-Manuel Garcia-Ruiz (producer and host of The Mystery of the Giant Crystals), and with the British Crystallographic Association (for the production Hidden Glory: Dorothy Hodgkin In Her Own Words.) I was a member of the ACA's task force for IYCr2014. In this capacity I worked with a sub-group of crystallographers on outreach to youth, and organized with Dr. Amy Sarjeant and Dr. Christine Beavers, a North American Video Contest on crystallography. In my capacity as the program co-chair for the 2015 ACA meeting, I again teamed with Prof. Garcia-Ruiz to organize two additional outreach activities for delegates and their families: 1) We displayed the poster exhibit CRIS-TALES; and 2) We held a lunchtime screening of The Mystery of the Giant Crystals, with a question-and-answer session which I chaired, and hosted by Prof. Garcia-Ruiz.

On International Women's Day 2018 (March 8) I had the unique and exciting opportunity to remotely connect with a high school class to discuss crystallography, science, and post-secondary expectations. This plays into my vision to make a contribution as a member of the

Communications Committee, by building off some of the outreach initiatives started by the ACA IYCr2014 taskforce, and some of my more recent experiences. If elected, I hope to include a notable outreach component to my activities with the Communication Committee.

Louise Dawe

Data, Standards & Computing - Eric Reinheimer:



Western Regional Account Manager
Rigaku Oxford Diffraction
The Woodlands, TX 77381, USA

Statement: First and foremost, I wish to thank the nomination committee for putting my name forward to serve as a member of the ACA Data, Standards and Computing Committee. This is a position in which I would be very honored to serve.

Ever since I solved my first structure almost twenty years ago, I've been fascinated by X-ray Crystallography. To this very day, I remain excited whenever I see a new structural model reveal itself on my computer screen. Having been blessed by various mentors over the years who've taught me the value structure determination has in garnering a fundamental understanding of the analyzed materials, I've come to appreciate the importance of data standardization in all aspects related to the

process of structure determination and reporting. While ultimately resolving a new structural model is the most exciting, strict attention to detail and how those underlying details are disseminated are the cornerstones upon which structural science can continue to make an impact in the understanding of fundamental processes across various scientific disciplines.

With the daily proliferation of new structures being reported, rigorous adherence to standards whereby the data and the context of that data can be understood is critical. From a pedagogical standpoint, at least within the context of peer-reviewed publications, how the structural data are reported and the context of that data is just as important as how a student may have synthesized their compound, purified their protein or above all grew that crystal to produce that seminal result. With so many students learning how crystallography can benefit their scientific understanding, new crystallographers should also learn that developing good practices on how that data is reported and catalogued is essential to crystallography as a whole. The data formats are there thanks to the continued efforts of the database organizations, software groups and instrument manufacturers; however the oratory the crystallographic community has with each of these entities must continue to not only maintain high data standards, but to also teach the next generation of crystallographers what those standards are and should continue to be.

It is truly a wonderful time to be a structural scientist! With the advent of new technologies related to Cryo-EM, SAXS, sources, detectors and computing, the science of structure elucidation is poised to continue making a strong scientific

impact for a long time to come. With the advent of these technologies and the discoveries being made by them, it is essential that high data and computing standards be upheld. As it has always done, the ACA has maintained a critical role in establishing those standards and will most assuredly continue doing so for many years to come.

Eric Reinheimer

Education - Allen Oliver:

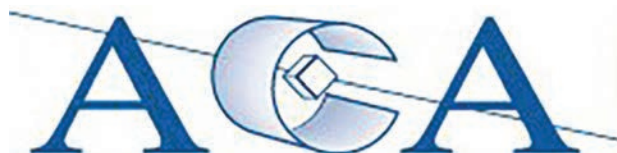


Research Professor
Dept. of Chemistry &
Biochemistry
University of Notre Dame
Notre Dame, IN 46556

Statement: It is an honor and privilege to be nominated for a position on the Continuing Education Committee. My interest in serving on the Continuing Education Committee stems from my participation as a crystallographic educator. I currently serve as one of the co-organizers of the ACA Summer Course in Chemical Crystallography. The primary mandates of the Education Committee are: selecting awardees for travel scholarships to the ACA conference; vetting proposed workshops that take place at the ACA Conference and expanding professional development within the community. I believe that with my experience in similar matters associated with the summer course I have a solid understanding of the needs of the committee. For the ACA Summer Course, I am directly involved with selection of scholarship awardees, planning the curriculum that includes a number of workshops, and developing networking opportunities for the course attendees. These are directly translatable skills to the mission of the Continu-

ing Education Committee. I have previously served on the Communications Committee, as Chair and Secretary for several SIG's within the ACA and as a program chair for the ACA annual conference. I feel that with this prior knowledge I have a broad insight into the needs of the community and have worked with committee members at all levels and will bring that knowledge and expertise to the position.

Allen Oliver

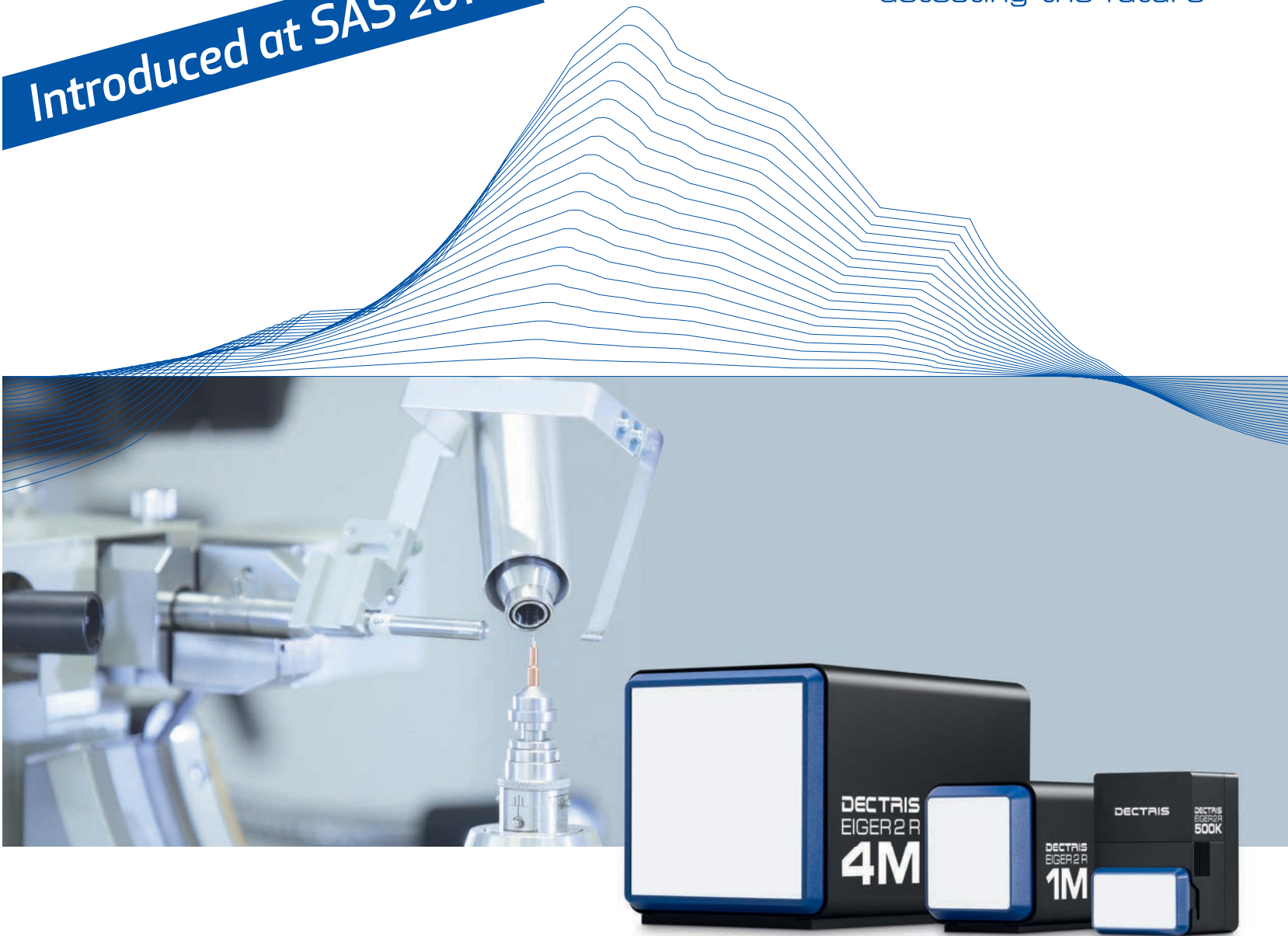


Contributors to this Issue

Olaf Borkiewicz, Chelsy Chesterman, Louise Dawe, Joseph Ferrara, Frank Fronczek, Richard Gillilan, Stephan Ginell, Kushol Gupta, Ilia Guzei, Cathy Lawson, Allen Oliver, Kay Onan, Virginia Pett, Daniel Rabinovich, Connie Rajnak, Eric Reinheimer, Ed Stevens, Kristin Stevens, Brian Toby, Diana Tomchick, Kristina Vitale

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Bryan Chakoumakos
Bau Award



Robert Von Dreele
Trueblood Award



Brian Toby
Trueblood Award

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Call for Nominations- 2020 Awards

2020 Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. Scientists involved in crystallographic research in the broadest sense will be eligible for the award. At the time of the closing date for nominations, nominees must be no more than 12 years beyond the awarding of their Ph.D. degree, not including career breaks, and must have begun their first independent (not postdoctoral) position within the past 10 years. Established in 2002 as an annual award, it consists of a \$1,000 honorarium and a plaque. The winner is also expected to present a lecture at the ACA annual meeting.

2020 A. L. Patterson Award: To recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information. Established in 1980, it consists of a monetary award of \$1,500 and up to \$1,500 travel expenses to accept the award and present a lecture at the Annual ACA Meeting, and a certificate. Awarded every three years. (Selection committee: Zbigniew Dauter (Chair), Steven Sheriff, and Nichole Valdez.)

2020 David G. Rognlie Award: To recognize exceptional discovery or technical development of particularly high impact in any area of structural science, to be awarded at any stage of a scientist's career without prejudice based on age, gender, ethnicity or race. Awarded every third year. May be given to more than one person but winner(s) will receive an honorarium of \$3000 and up to \$1500 expenses to attend the ACA meeting to present a lecture covering the discovery or development that led to their selection. (Selection committee: Helen Berman (Chair), Cathy Lawson and Aina Cohen.)

2020 Elizabeth A. Wood Science Writing Award: The award is to recognize individuals who have written books or articles that bring science to the attention of a wider audience. Successful nominees need not be crystallographers or scientists and 'writing' could include artistic efforts, museum displays, etc. Nominations should include the titles of books, copies of articles, or other documentation.

Selection of the winner will be made by ACA Council and presented at the Annual Meeting. A gift of glassware, \$1,500 cash and up to \$1,500 travel expenses to attend the Annual Meeting to accept the award. Awarded every three years. Established in 1997.

More information for all ACA Awards and nomination forms are available on the ACA website: www.amercrystalassn.org/awards. Nominations for 2020 are due April 1, 2019.

2020 ACA Fellows: The ACA Fellows program serves to recognize 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. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government.

More information on ACA Fellows, the nomination procedure, and the 2020 nomination form can be found at www.amercrystalassn.org/fellows. Nominations are due by April 1, 2019.

2020 ACA Offices and Committees: In the Fall of 2019 we will elect a Vice-President, Secretary, Canadian Representative, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 15, 2019.

Send all nomination suggestions to:
kstevens@hwi.buffalo.edu

2019 Dues are Due

Please renew your membership promptly and remember to support your favorite ACA Funds. It is now possible to renew online at:

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Please note: In an effort to reduce costs, you will now have the option of receiving ACA RefleXions in different formats. Select 'digital' to be sent a link to a PDF of the current issue or select 'hard copy' to continue receiving a hard copy by snail mail.

The Dame of the Rings

The hexagonal structure of benzene, first proposed by the German chemist August Kekulé in 1865, is certainly a milestone in the history of modern organic chemistry. Whether the story of his famous dream of a snake biting its own tail (i.e., a vision of the mythical ouroboros) is true or not, most chemists in the ensuing decades took for granted his suggestion. However, there was no concrete evidence to ascertain the exact configuration of the benzene ring (i.e., whether it was planar or not) or any experimental data to explain the purported presence of alternating single and double bonds. The advent of X-ray crystallography in the 1910's, and particularly the realization in the early 1920's that organic molecules were susceptible to single-crystal X-ray diffraction studies, finally validated Kekulé's venerable suggestion.



Almost exactly 90 years ago, in the November 24, 1928, issue of *Nature*, Kathleen Lonsdale, a renowned Irish crystallographer (1903-1971), outlined the crystal and molecular structure of hexamethylbenzene, a seminal piece of work that provided unequivocal proof of the symmetry and flat hexagonal shape of the benzene ring. In addition, the observation of very similar carbon-carbon bond distances (ca. 1.42 Å) had a profound effect on the subsequent development of fundamental concepts such as electron delocalization and aromaticity.

Kathleen Lonsdale (néé Yardley) was born in Newbridge, a small town southwest of Dublin, Ireland, and received her B.Sc. degree in physics from Bedford College in London at age 19. Her innate intelligence and excellent grades attracted right away the attention of the legendary William H. Bragg, who invited to join his laboratory and study for a Master's degree and at University College London (UCL). In 1923 Professor Bragg moved his research group to the Royal Institution, where Lonsdale did research in crystallography for more than two decades, except for a brief but fruitful stint at the University of Leeds (1927-1930). In December 1946 she returned to UCL, where she stayed until her retirement in 1968. In addition to her pioneering research on crystallography, she and the biologist Marjorie Stephenson were the first women admitted as Fellows of the Royal Society (1945) and she was appointed Dame Commander of the Order of the British Empire in 1956. Always a trailblazer, Lonsdale was also the first woman to be elected president of the International Union of Crystallography (1966) and the first female president of the British Association for the Advancement of Science (1968). Last but not least, she was a dedicated wife and mother of three children, an active participant in several international movements to promote world peace, and an advocate for prison reform and the education of women in science.



Although no postage stamps have regrettably been issued (yet) to honor Kathleen Lonsdale, the personalized Austrian stamp illustrated here, which shows the painting "Benzene Ring" by the artist Black Sura, represents my modest tribute to her life and work.

Daniel Rabinovich



ACA Summer Course in Chemical Crystallography

www.acasummercourse.net

June 23 – June 30, 2019

Northwestern University, Evanston IL

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Allen Oliver and Amy Sarjeant*

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Acceptance Notifications – March 2019

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Puzzle Corner



New Crystoquote, DISORDERED and Crystal Connections puzzles are provided, along with answers to the previous ones as well as mention of those who provided the solutions. Send me the solutions to these:

DISORDERED

Go directly from the observed letters to the solution

CREDIT	○ □ □ ○ □ □
OHMSTED	□ ○ □ □ □ ○ □
KALLIADO	○ □ ○ □ □ □ □ □
SLOWELF	○ □ □ □ □ ○ □
PHATUNAM	□ □ ○ □ □ □ □ ○



When Jerome Karfunkle shortened his name to Karle, his original name...

Answer:

□ □ □ " □ □ - □ □ □ □ □ □ "

Crystoquote #2

Letter substitution reveals a quote by a well-known crystallographer

**U CA JSCHYPIM PGS HNY GEEGSHIFUHT HG JUDY
QGAYHNUFJ KCLR HG HNY LGAAIFUHT XNULN NCQ
JUDYF AY QG AILN. VIOUHN PMUEEYF-CFOYSQGF**

Crystal Connections #15

- 1) The 1875 painting *Otoño* by Frederic E. Church celebrates this season
- 2) The symmetry of a wallpaper _____ is one of the 7 frieze groups
- 3) We are stardust, we are golden, we are billion year old _____
- 4) Buck, greenback, piastre, 8 bits.
- 5) Receptacle for unwanted delivery of canned meat? Spam _____
- 6) South of Toms River, near Double Trouble State Park in the Pine Barrens: _____ River
- 7) Take a stare at this spicy dancer: _____ Rogers
- 8) Statler is a _____; Waldorf too
- 9) The Kalpha wavelenth of _____ is about 0.56 Angstroms
- 10) His comedy routines included Phonetic Punctuation and Inflationary Language: _____ Borge

Solution to Crystoquote #1:

**I do the physical applications, he works on the theoretical. It makes a good team.
Science requires both types. Isabella Karle**

Joel Harp (Vanderbilt U. Center of Structural Biology) provided the solutions to both the soccer DISORDERED puzzle and Crystoquote #1.

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Guest Puzzlers are especially welcome! I thank **Greg McCandless** (Chemistry, U. Texas Dallas) for his hilarious suggestions for this month's column.

Frank Fronczek – ffroncz@lsu.edu

DISORDERED

From the database of jumbled words, make it your goal to find the hits.

GRENTFAM	CRAGMENT
GLUMO	MOGOL
NAWGRID	ORAWTINING
QUOSNECT	CONQUEST
CERASH	SEARCH



Cambridge futbol fans secretly communicated with the officials

Answer:

U S I N G R E F - C O D E S

APRIL 2019

22-26 **Materials Research Society Spring Meeting**, Phoenix, AZ
<https://www.mrs.org/Spring2019>



MAY 2019

19-21 **2nd IBA Conference**. La Jolla, CA
<http://industrialbiostructures.org>



JUNE 2019

23-28 **11th International Conference on Inelastic X-ray Scattering**.
Stony Brook University, NY
<http://www.bnl.gov/ixs2019/>



JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
<http://www.AmerCrystalAssn.org>



28-2 Aug **19th International Conference on Crystal Growth and Epitaxy**,
Keystone, Colorado
<http://www.crystalgrowth.org>



AUGUST 2019

22-26 **European Crystallographic Meeting**, Vienna, Austria
<https://www.ecm2019.org/home/>



DECEMBER 2019

1 - 6 **Materials Research Society Fall Meeting**, Boston, MA
<https://www.mrs.org/Fall2019>

JULY 2020

31-7 Aug **ACA 2020 Annual Meeting**. San Diego, CA
<http://www.AmerCrystalAssn.org>



AUGUST 2020

22-30 Aug **IUCr 25th General Assembly**. Prague, Czech Republic
<http://www.iucr25.org>



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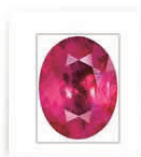
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