

**A History of Excellence in Neutron Diffraction**

Bryan Chakoumakos  
2019 Robert Bau Award

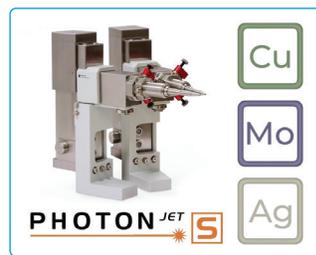
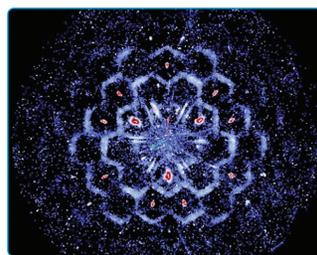
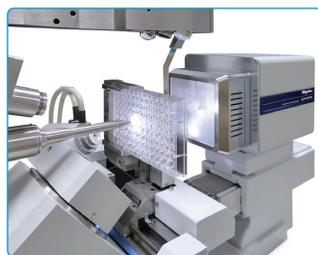
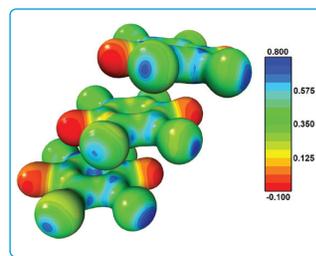
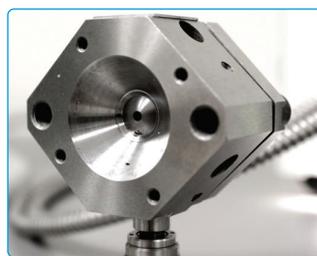
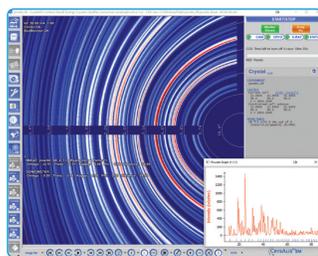
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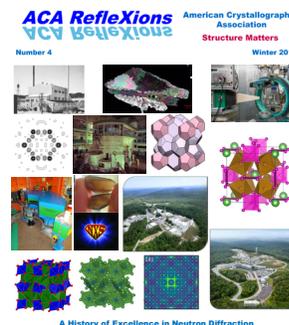


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**Brian Toby**  
2020 ACA President



Bryan Chakoumakos received the Bau Award for 2019. The cover images are described in the 'What's on the cover' page 6.

Bryan Chakoumakos  
2019 Robert Bau Award

## 2020 Award Winners



**Nozomi Ando**  
Margaret C. Etter  
Early Career Award



**James M. Holton**  
David J. Rognlie Award



**Vaclav Petricek**  
A. L. Patterson Award



**Winnie Wong-Ng**  
Distinguished Life Membership of American Ceramic Society

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**President's Column**



*Brian Toby*

After not even a full year to understudy from ACA Past-President Lisa Keefe and President Joe Ferrara, I find myself not ready to write my first President's Column for RefleXions and even less ready to follow in their very impressive footsteps. For those of you who are not part of Council or involved in our meeting planning or otherwise seen them in action, I want to let you know that Lisa and Joe have taken on ACA needs with an effort-level comparable to their day jobs and a daunting (at least to me) level of wisdom. Far from being burned out, Lisa has volunteered to be acting-CEO of the ACA for 2020, while we figure out how to restructure that role. If you get the chance, please thank them for all they have done and continue to do. I will aim to measure up to their level, but it will be quite a challenge. While at it, please also thank our administrative staff, Kristin Stevens and Kristina Vitale and the meeting co-chairs, Steve Ginell and Vivien Yee, for their excellent work in organizing and running our 2019 Annual Meeting in Covington KY so very well.

First some good news: the Covington meeting was a definite success and the ACA is expected to break even or perhaps have a small budget surplus after several years of running significantly in the red in 2019. No credit on this to me, but again thanks to our staff and Council members, past and present, for getting us back on track. Having said that, 2020 presents a significant challenge to the ACA. Our next meeting in San Diego had to be scheduled close to the Prague IUCr meeting due to a lack of better options. We anticipate this will cut into registration from more senior scientists and are orienting a program towards students and younger scientists, but that will cut into our meeting income in a site which is, well, not cheap. Our program chairs, Nozomi Ando and Carla Slebodnick along with our SIGs, have created an inspiring program that I am very excited about. They will be writing more about that elsewhere in this RefleXions issue. Council is pulling out all the stops to bring people to this meeting and we will offer a number of incentives.

Despite the extra costs projected for the 2020 annual meeting, we want to make sure that our most loyal

members will not be priced out. If you register by March 31, you will be able to register for the same fee as for the 2019 meeting. You will also have the option to bundle your 2020 ACA dues with your meeting registration, which can be advantageous for those who are lucky enough to be reimbursed for registration. We will also accept abstract submissions for post-deadline posters until we run out of poster space, perhaps even at the meeting, so we encourage you to present your hot new results in a last-minute poster! Another bit of good news is that we will not have abstract fees. However, due to the number of no-show presentation submissions (which create real costs for the ACA), abstracts will be accepted only from registered attendees.

The YSIG leadership has agreed to reinvigorate the early-career roommate program and the ACA President will donate his comp'ed room, so that the first five pairs of roommates matched through the process will get one night hosted by the ACA. Volunteers to help set this up in a social networking site would be much appreciated, I am sure. We will also have a centralized travel assistance program to help scientists of all ages based on need with some of their expenses. For this meeting we very much want to help those early in their careers to attend as best we are able. Applications will be reviewed on a revolving basis, so apply early before all funds are allocated. We do encourage those who are able to "pay it forward" (since we can never pay back the people who have helped us the most) to consider making donations to the ACA General Fund to help us assist more people. Note that the ACA Award funds are fully endowed, but our General Fund and Student Travel funds are very much in need of further donations.

Another challenge to the ACA will be to transition over the next year to an all-volunteer based leadership. Our CEO, Bill Duax, who has done so much for the ACA and IUCr for so many years, will have retired from that role by the time you read this. Our CFO, Narasinga Rao, will retire at the end of 2020. We expect, and in fact insist, that they continue to provide us with their sagacious advice for many decades to come, but the ACA must reorganize to fit our current membership profile and this will be one of the painful changes that must happen as we evolve. I have had the benefit to have worked with Bill over many years and to have seen the behind the scenes financial work done by Rao (as he prefers to be called). The ACA owes them truly eternal gratitude.

Please put a reminder on your calendar now for the March 31, 2020 San Diego early-bird registration deadline, as well as the meeting, August 2-6, 2020. You might also want to note the subsequent meetings:

Baltimore MD, July 31-August 3, 2021 and Portland OR, July 30-August 2, 2022. A lot of work goes into selecting a meeting site, and our Meeting Site Selection Committee (Treasurer Ilia Guzei, CFO Rao and Director of Administrative Services Kristin Stevens) are now working on the 2023-2025 meetings. For either 2024 or 2025, we hope to return to Canada. Noting that we occasionally hear from members who would like to recommend locations, the needs for a facility to host an ACA annual meeting are now outlined on our web pages (see Annual Meetings/ Technical Information or <https://acas.memberclicks.net/technical-information>), so you can see if your idea can meet our meeting needs. Note that a formal RFP is available on request. If you have a suggestion for a location you would like to be considered, please contact the ACA Office or me\*.

Finally, while mentioning deadlines, please also think about colleagues, mentors and perhaps respected competitors who are worthy of the honor of an ACA award, particularly scientists who are too busy promoting the careers of others to promote themselves. Nomination packets will be due April 1, 2020 for the Etter Award (early career), the Warren Award (physics of diffraction) and the Buerger Award (exceptional distinction). The same deadline also applies to nominating members to be an ACA Fellow. Awards are one of the few ways that we do get to pay something back; if you don't take the initiative to start the process, the deserving person you are thinking about right now may never be considered. Something else new, of which I am very proud, is that Lisa has formed a Nominations Oversight Committee with members\* Charlie Carter, Angela Criswell, Peter Khalifah and Amy Sarjeant. This committee is charged to seek out worthy individuals for our nominations pools. If you are unsure about how to put together a nomination, any of them can help advise.

*Brian Toby*

\*N.B.: contact information for all ACA members is found in our membership directory, see the home page of our website, <https://www.amercrystalassn.org/>, after logging in.

## **Highlights from the 2019 Summer and Fall ACA Council Meetings**



*Diana Tomchick*

The 2019 Summer Council Meeting was held in the Northern Kentucky Convention Center in Covington KY on July 20, 2019. Voting members in attendance were President Joseph Ferrara, Vice President Brian Toby, Treasurer Ilia Guzei, Past President Lisa Keefe, 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, Chief Executive Officer William Duax and Chief Financial Officer S.N. Rao.

ACA Treasurer Ilia Guzei reported that there are 519 meeting attendees to date, so a profit will be made for the meeting. Final statistics on the amount of money collected from the meeting exhibition will be gathered in December, these numbers will affect whether the ACA breaks even for 2019. Guzei expressed some concern about attendance numbers due to the cost of travel and registration for the 2020 San Diego meeting and suggested an examination of the registration fees and categories for the meeting. He reported that the ACA Finance Committee wants to re-establish a meeting site selection and hotel negotiation committee for the years of 2023-2025. Guzei is investigating alternative investment vehicles that may provide higher yields for the ACA restricted funds used for awards. As the transition of ACA financial accounting to QuickBooks is ongoing, Council endorsed Guzei and CFO Rao to open negotiations with an outside bookkeeper to provide backup support and training in accounting for Director of Administrative Services Kristin Stevens. This support will be on an hourly basis, as needed.

Every year the IUCr Executive Council (EC) has at least one meeting in the same location and just prior to an annual IUCr affiliate society meeting. This meeting rotates amongst the affiliate societies, and this year the meeting was in Covington for the ACA meeting. The ACA Executive Council (comprised of President, Vice President, Past President, Treasurer and Secre-

tary) met with the IUCr Executive Council, and ACA President Joseph Ferrara briefed the full ACA Council on that meeting. The Latin American Crystallographic Association (LACA) and IUCr are discussing a bid for Mexico to host the 2026 IUCr Congress and LACA and IUCr have suggested a joint meeting with the ACA for that year. The IUCr EC would also like the ACA to identify a community of crystallographers that are interested in supporting the nascent Pan African Crystallographic Association as well as the African Light Source initiative, LAAMP.

Vice President Brian Toby discussed the results of the membership questionnaire that was sent via email earlier in the month. At the General Business Meeting later in the week he planned to encourage more people, especially younger members, to respond the questionnaire.

Past President Lisa Keefe Keefe provided Council with a description of an ad-hoc Award Oversight Committee that would look for diversity in gender and discipline when putting forth potential candidates for awards.

Tomislav Frišćić, the Canadian Representative, provided a review of past Canadian meetings, including the 12th Canadian Powder Diffraction Workshop in Trois-Rivières, Québec, May 8 - 11, 2019; the 6th Crystal Engineering and Emerging Materials Workshop of Ontario & Québec (CEMWOQ-6) in Montreal, May 30 - June 1, 2019; the 102nd Annual Meeting of the Canadian Society of Chemistry, Québec City, June 3 - 7, 2019; and the 9th Annual Canadian Light Source Mx Data Collection School, June 25-30, 2019. The Canadian National Committee for Crystallography has awarded the first set of Larry Calvert Travel Awards for 2019, which assist Canadian students, postdocs and researchers to attend crystallography-related conferences; the results of the second round of applications will be announced on July 31, 2019. Frišćić stated that he had informed the Canadian National Committee that they needed to identify a new Canadian Representative to the ACA as his tenure ends at the end of the calendar year.

IUCr Representative Hanna Dabkowska presented highlights of IUCr activities, including the provision of \$9,000 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 IUPAP-IUCr project "Utilisation of Light Source and Crystallographic Sciences to Facilitate the Enhancement of Knowledge and Improve the Economic and Social Condition in Targeted Regions of the World" is funded under the 2-16-2019 ICSU Grants Program; the support of the IUCr Outreach and Education Fund of initiatives in Africa, the IUCr-UNESCO OpenLabs and crystallographic schools around the world; an African

Crystallographic Association (AfCA) Steering Committee is in the process of creation; a new IUCr award, named after W.H. and W.L. Bragg, was approved at the Hyderabad Congress in 2017 and a Bragg Prize Committee has been formed, nominations for this prize are now welcome; and Prague, Czech Republic will host the 25th IUCr Congress from August 22-30, 2020. Highlights of the report from George Lountos, the Young Scientists Interest Group (YSIG) representative, included a summary of the YSIG sponsored events at this meeting, including the Career Development workshop, the First Time Attendee meeting, the Three Minute Thesis Competition, the "Structure without Structure" Session as the inaugural Structural Dynamics session, the YSIG Mixer and co-sponsorship of several scientific sessions.

Director of Administrative Services Kristin Stevens reported that the new ACA History Portal, as part of the new ACA web site, launched last Monday. She reported that there will be a new abstract system for the 2020 ACA annual meeting, and she is looking into childcare options for San Diego.

Highlights of the August and September teleconferences included an update on the annual meeting from Kristin Stevens. The total attendance was 567 and more than 100 people responded to the meeting survey. Preliminary numbers for the annual meeting aren't available yet, but the expectation is that the ACA will have a profit by the end of the year. Council decided to raise the exhibitor booth rates for non-profits to the full non-member meeting registration fee (note: the non-profit booth rate already included a registration for one individual, but the rate was lower than a standard registration fee). ACA CFO Rao is searching for future meeting sites, including a suitable 2024 site in Canada.

The 2019 Fall Council meeting was held as a teleconference on October 10, 2019. Voting members in attendance were President Joseph Ferrara, Vice President Brian Toby, Treasurer Ilia Guzei, Past President Lisa Keefe, 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 and Chief Executive Officer William Duax.

The National Science Foundation (NSF) recently defunded the US National Committee on Crystallography (USNC/Cr), and after August 2020, they might no longer be under the National Academy of Sciences. This is problematic, as the USNC/Cr provides US representation to the IUCr, but the IUCr rules requires that a national committee must be created by an adhering body (i.e., the national committee can't exist as an

isolated entity). As the USNC/Cr is currently investigating several options with various organizations, they have contacted the ACA to see if it could become an umbrella organization for the committee. The ACA Council decided that it will invite the USNC/Cr to submit bylaws to become a US National Division of the ACA, with the stipulation that the officers of the US National Division and the officers of the USNC/Cr shall be the same.

ACA Treasurer Ilia Guzei proposed a solution to the high cost of meeting registration for Canadian members (note: Canadians must pay in US dollars, and the exchange rate is not favorable for them). Canadian members that sign up by the early registration date will receive a coupon code emailed to them so they can use the registration rate for 2019. Tentative deadlines for the 2020 meeting were set as follows: March 31, early registration; April 1, regular registration; April 20, oral abstract submission deadline; June 15, late registration; no final deadline for poster abstract submission. All abstracts will be published in *Acta Crystallographica C*. To streamline the number of registration categories, there will be one non-member meeting registration fee for 2020.

ACA CFO Rao submitted a draft 2020 budget for the ACA, but as he was not present at the meeting and there were numerous questions, approval of the 2020 budget was tabled until the ACA Finance Committee could review the budget.

President Joseph Ferrara announced that the American Institute of Physics (AIP) has offered to provide the funds for a consultant to perform a comprehensive review of the ACA that will take place this fall. Results will be provided to the ACA Council in January 2020. IUCr Representative Hanna Dabkowska presented highlights that included the new *Volume H* of the *International Tables for Crystallography, Powder Diffraction* that has been online since late 2018 and the print version is now available in July 2019; 34 meetings have been supported in 2019, and another 17 have been confirmed for 2020; there are currently 10 nominations for the new IUCr Bragg prize; the winners of the 2019 IUCr Crystal Growing Competition for school children will be announced soon; and the organization of the program for the 25th IUCr Congress in Prague in August 2020 is well underway.

Canadian representative Tomislav Frišćić reviewed upcoming meetings, including the Buffalo-Hamilton-Toronto Regional Meeting, on November 1, 2019; the 11th Canadian Chemical Crystallography Workshop at the University of Winnipeg, May 19-22, 2020; and the 13th Canadian Powder Diffraction Workshop at the Canadian Light Source, Saskatoon, May 19-22, 2020.

George Lountos, the Young Scientists Interest Group (YSIG) representative, provided highlights of the YSIG activities during the annual meeting. The Career Development Workshop, the YSIG Mixer and the scientific sessions co-chaired by the YSIG were successful, but the Three-Minute thesis session had a drop in attendance, perhaps due to holding it during the lunch break. Next year, the YSIG would like to hold it during the coffee breaks. For next year's meeting, a lunch panel session on Industrial Careers will be co-sponsored with the Industrial SIG. As Lountos has been on the ACA Council for three years, he will be stepping down and Chelsy Chesterman will become the YSIG Council representative. Council thanked YSIG representative Lountos for his excellent service.

Director of Administrative Services Kristin Stevens reported that as of 10/7/2019, there are 1,058 ACA members. During the annual meeting, session attendance was recorded and the two times where the greatest number of people attended sessions were the Monday morning (276 people) and Wednesday morning (242 people) periods, when there were six simultaneous scientific sessions. The Transactions Symposium for the 2020 meeting will be "Training the Next Generation"; the program and abstracts will be online only; and Stevens is still evaluating companies for providing abstracting services.

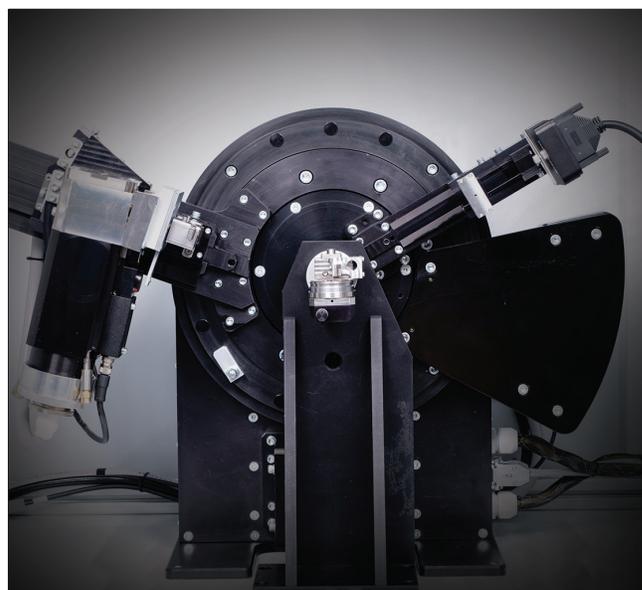
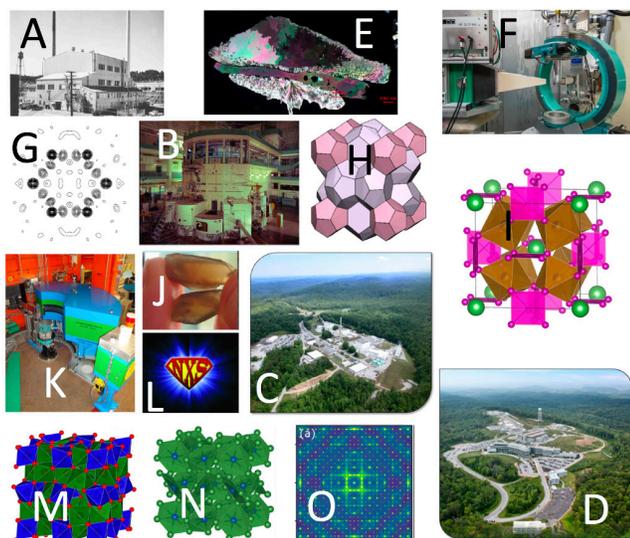
Highlights of the November teleconference included a revised draft ACA 2020 budget that had been reviewed by the Finance Committee. Approval of the budget was postponed to the December teleconference. Council approved the proposal of the company Core-apps for the 2020 abstracting and app services. Kristin Stevens provided preliminary information about a daycare service that would be provided by the Sheraton hotel in San Diego, and a survey will be sent to members to gauge how many people would be likely to take advantage of the service.

Abstract deadlines for the 2020 meeting were set as follows: March 31, travel grant deadline (applicants must attach an abstract); April 20, oral abstract submission deadline; June 10, poster deadline, although the abstract window technically never closes and will stay open accepting posters until the meeting begins.

Diana Tomchick

**What's on the Cover**

Evolution of neutron sources for neutron scattering at Oak Ridge A) Graphite Reactor (1943-1963), B) Oak Ridge Research Reactor (1958-1987), C) High Flux Isotope Reactor (1965-present), D) Spallation Neutron Source (2006-present). E) Polarized light micrograph of a fish otolith from a Chinook salmon with a heterogeneous microstructure of calcite, vaterite and aragonite, studied by neutron diffraction. F) Neutron four-circle single-crystal diffractometer at ORNL High Flux Isotope Reactor (HFIR). G) Nuclear scattering length density map of a 6-membered ring in deuterated CO<sub>2</sub>-hydrate (structure I) showing the disordered water molecules (large peaks are oxygen and the smaller peaks are deuterium). H) Clathrate Structure I of various gas hydrates and semiconductor silicide and germanide thermoelectrics. I) Filled skutterudite structure type, an important thermoelectric. J) Natural crystals of triphylite-lithiophilite. K) Neutron powder diffractometer at ORNL HFIR. L) National School of Neutron and X-ray Scattering is now in its 22nd year. Disordered antiferromagnetic bixbyite, (Mn<sup>+3</sup>,Fe<sup>+3</sup>)<sub>2</sub>O<sub>3</sub>, M) polyhedral structure drawing, N) Magnetic ions in bixbyite form nearly perfect edge-sharing hexagons, and O) neutron diffuse scattering in bixbyite at low temperature.



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## Nozomi Ando Selected to Receive the 2020 Margaret C. Etter Early Career Award



**Nozomi Ando** is the recipient of the 2020 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.” Nozomi is often referred to as fearless, unafraid of tackling difficult biophysical problems that are well out of the mainstream if they have the potential to provide insight about protein function and stability. She is currently an Assistant Professor of Chemistry and Chemical Biology at Cornell University where her laboratory works at the interface of chemical biology, structural biology and physical chemistry, studying enzymes using non-conventional x-ray techniques. For instance, her current studies are on using diffuse scatter to study protein allostery. Nozomi earned a B.S in Physics at MIT and a PhD in Physics at Cornell University. Her goal was to answer fundamental questions about protein stability using new tools and technologies and her work focused on the design of instrumentation for use in high-pressure biological studies using small-angle x-ray scattering (SAXS).

With a solid background in physics, Nozomi sought to learn more about chemistry and biochemistry to gain a broader understanding of protein structure/function relationships. To do so, she joined Catherine Drennan’s laboratory at MIT for her post-doctoral studies. Here Nozomi’s main emphasis was on ribonucleotide reductases (RNRs) and the relationship between oligomeric state structure and enzymatic activity. It was in this large and collaborative project that her leadership skills shone.

It was in the Drennan laboratory that Nozomi carried out the mentored phase of her prestigious NIH K99 Pathway to Independence Award; her independent career - developing a comprehensive program to study the structural basis of protein allostery - started at Princeton University. She was then awarded a highly-respected five-year Maximizing Investigators’ Research Award from NIGMS. Last year Cornell University was able to attract her.

Nozomi’s group is one of the first to successfully analyze diffuse x-ray scattering on protein crystals and provide information on not just average structure but also on correlated molecular motions. Nozomi is also applying other types of novel x-ray scattering experiments to understand protein conformational change

and dynamics. In this latter work, she has developed novel computational tools to analyze SAXS data from complex systems.

Nozomi is highly regarded in the field. Indeed, as a junior faculty member she was solicited to write a Chemical Reviews article on the future of biophysics and it was heralded by Chemical Reviews as the best review of the year. She is a visionary and her efforts represent the future of crystallography and x-ray diffraction.

## James M. Holton Selected to Receive the David J. Rognlie Award



**James Holton**, Scientist at the Molecular Biophysics and Bioimaging division at Lawrence Berkeley National Laboratories (LBNL) and Full Adjunct Professor Biochemistry and Biophysics at the University of California, San Francisco, is the 2020 recipient of the

ACA’s David J. Rognlie Award. This award is awarded “to recognize an exceptional discovery of technical development of particularly high impact in ... structural science.” James is being honored to recognize his work in the development of the beamline 8.3.1 at the advanced light source (ALS) in the LBNL, one of the most productive beamlines, in terms of both publication number and impact, in the world. He is one of the most insightful proponents, designers and visionaries of synchrotron beamline development. The innovations that James has designed, built and installed have always been carried out with the goal of optimizing the process of data collection.

James’ doctoral dissertation reported the first-ever, fully-automated solution of a previously unsolved protein structure. In order to carry out this structure determination, James single-handedly wrote a computer program called ELVES which has continued to be the core structure-solving program at the 8.3.1 beamline. He has optimized the process of data collection by incorporating a robot to mount pins, a touch screen for centering crystals, automated data backup, seamless data processing interfaces and a highly intuitive control system. His interests have grown to addressing the question: Why do so many structure determinations at the beamline fail? He has revealed the bottlenecks in x-ray crystallography by archiving, curating and analyzing all the data collected at his beamline. This has resulted in a number of key practical insights, one of them being the predictability of radiation damage to macromolecular crystals. James’ vision, now realized, is for users to find answers to critical questions during data collection when there is time to revise plans to make the best use of beam-time rather than after lesser quality

data have been collected.

James has made numerous pioneering contributions to the synchrotron experience, starting with a vision for optimizing all aspects of data collection to structure determination and developing and implementing novel hardware and software solutions. His software developments allow users to solve problems concurrent with data collection, not after leaving the beamline. James is a generous colleague who has done much to educate beamline users.

### **Vaclav Petricek Selected to Receive the A. L. Patterson Award**



**Vaclav Petricek**, Senior Scientist at the Institute of Physics of the Academy of Sciences of the Czech Republic, is the recipient of the ACA's 2020 A. L. Patterson Award. This award is given "to recognize and encourage outstanding research in the structure of matter by diffraction methods, including the methodology of structure determination ..." Over the course of his career, Vaclav's research has made him the leader in the field of analysis of incommensurately modulated crystals. Through his work a good percentage of aperiodic crystals, the so-called incommensurately modulated structures, can now be determined with accuracy comparable to what one can achieve for ordinary periodic structures.

Vaclav has spent essentially his whole career at the Czechoslovak Academy of Sciences as a researcher. A post-doctoral position with Philip Coppens at the State University of New York, Buffalo, helped shape the direction of his research. Until the seventies the existence of aperiodic crystals was considered rare but now it is known that incommensurate crystals occur in all kinds of materials. One of the breakthroughs that made the quantitative characterization of incommensurately modulated structure accessible to the wider community of crystallographers was the development of computational tools for the practical application of the theoretical superspace formalism to the analysis and determinations of incommensurate structures. It was Vaclav who developed the necessary tool that made a good theory work in practice, and this tool is the program JANA. Over 25 years he has continued to introduce many options which have made this computing system useful in solving periodic and aperiodic crystals. The latest version of JANA also supports powder diffraction data, simultaneous refinement against various data sets (powders, single crystals) and radiation sources (x-rays, neutrons, electrons), Time-of-Flight neutron diffraction data and refinement of symmetry deformation modes.

Vaclav's contribution is not restricted to a user-friendly, all-purpose computer program for structural analysis; he also proposed new scientific methods - such as saw-tooth functions and the refinement of magnetic structures against neutron powder diffraction data - and added them into JANA2006.

The pioneering practical approach to the superspace formalism and Vaclav's development of appropriate computation tools for its application has been fundamental for the development of the field of aperiodic crystals. Indeed, the mature stage that the crystallography of aperiodic crystals has reached would be unthinkable without the existence of Vaclav's program JANA.

### **2019 Distinguished Life Membership of American Ceramic Society**



**Winnie Wong-Ng** was awarded the 2019 Distinguished Life Membership of American Ceramic Society in recognition of her contributions to the development of crystallographic structures and phase equilibria diagrams for complex ceramic compositions and for her volunteer service to the American Ceramic Society. Distinguished Life Membership is the highest honor accorded to members of the scientific and technical organization and recognizes eminent contribution to the ceramic and glass profession.

### **2019 Elizabeth A. Wood Science Writing Award**

The 2020 ACA Elizabeth A. Wood Science Writing Award is being given to Alan Alda and the Alan Alda Center for Communicating Science. This Center empowers scientists and health professionals to communicate complex topics in clear, vivid, and engaging ways, leading to improved understanding by the public, media, patients, elected officials, and others outside of their own discipline.

Alan Alda, an actor and writer, has, over the past 2 decades, become a crusader for science communication. A life-long interest in science led to his hosting *Scientific American Frontiers*, a PBS series in which he interviewed hundreds of scientists, helping them make their research clear to the public. These interviews showed scientists presenting their work spontaneously and vividly. Alda decided that this was something that could be taught and thus was born the idea of a center to train scientists in STEM and medical communication. Using improvisational techniques he had learned in his years as an actor, he devised *The Alda Method*<sup>®</sup> to help scientists "tap into

innate connections that come alive naturally when people recall a passion for their work.”

The Alda Center for Communicating Science was established in 2009 with support from Stony Brook University, Stony Brook School of Journalism, Brookhaven National Laboratory and Cold Spring Harbor Laboratory. This Center incorporates three entities: the Alda Center, the Alda Communication Training Company, and the Alda-Kavli Learning Center. The Alda Center conducts research on and offers programs and workshops for science and medical communication. The Alda Communication Training Company provides operational support so the Alda Center can devote more of its resources to research and development and does the administrative work for clearing and processing contracts for clients and trainers. The Alda-Kavli Learning Center is a place for scientists, researchers, healthcare professionals and others to continue to learn about and improve their communication style. The Center’s signature program is the Alda Science Communication Experience workshop.

The on-line learning experiences, workshops and other trainings offered by the Alda Center for Communicating Science have been valuable in bringing tools to 19,000 researchers to aid them in presenting their research findings in ways that inform economic and policy decisions, increase support for research, and help individuals make informed decisions. Beyond this, AlanAlda has helped to create a sense of wonder and joy in the natural world around us.

*Kay Onan*

## 2019 Election Results

<i>Position</i>	<i>Candidate</i>
<i>Vice-President</i>	<i>David Rose</i>
<i>Can Rep</i>	<i>Gerald Audette</i>
<i>Com Committee</i>	<i>Rajni Bhardwaj</i>
<i>Continuing Ed.</i>	<i>Christine Zardecki</i>
<i>DS&amp;C Committee</i>	<i>John Bollinger</i>
<i>Meetings</i>	<i>Brandon Mercado</i>
<i>Best Practices SIG: Chair Elect 2020</i>	<i>Herbert Bernstein</i>
<i>Best Practices SIG Sec/T 2020-2021</i>	<i>Raquel Bromberg</i>
<i>BioMac SIG Chair Elect 2020</i>	<i>Jane Richardson</i>
<i>Canadian Division Chair 2020</i>	<i>Louise Dawe</i>
<i>Cryo-EM SIG Chair Elect 2020</i>	<i>Jose Rodriguez</i>
<i>Cryo-EM SIG Sec/T 2020-2021</i>	<i>Dominika Borek</i>
<i>General Interest SIG Chair Elect 2020</i>	<i>Marc Giulanotti</i>
<i>General Interest SIG Sec/T 2020-2021</i>	<i>Joseph Tanski</i>
<i>Industrial SIG Chair Elect 2020</i>	<i>Joshua Carter</i>
<i>Industrial SIG Sec/T 2020-2021</i>	<i>Ardian Soca Wibowo</i>
<i>Light Sources SIG Chair Elect 2020</i>	<i>Ana Gonzalez</i>
<i>Materials Science SIG Chair Elect 2020</i>	<i>Vicky Doan-Nguyen</i>
<i>Neutron SIG Chair Elect 2020</i>	<i>Benjamin Frandsen</i>
<i>Powder SIG Chair Elect 2020</i>	<i>Cheng Li</i>
<i>Service SIG Chair Elect 2020</i>	<i>Matthias Zeller</i>
<i>Service SIG Sec/T 2020-21</i>	<i>Matthias Zeller</i>
<i>SAS SIG Chair Elect 2020</i>	<i>Steve Meisburger</i>
<i>SAS SIG Sec/T 2020-2021</i>	<i>Sai Venkatesh Pingali</i>
<i>Small Molecule SIG Chair Elect 2020</i>	<i>Xiaoping Wang</i>
<i>YSIG Chair Elect 2020</i>	<i>Daniel Decato</i>

### **Consider the ACA in Your Estate Planning**

You can’t take it with you, and it is likely not possible to do anything for the people who helped you build your successful career, but you can have a positive impact on the next generation of crystallographers by gifting to the ACA. There are many ways you can support the ACA, such as putting the ACA in your will or donating an IRA distribution. The AIP has a great set of web pages that describe some of the tax advantages (see <http://aipgift.org/?pageID=10>), but please donate to us. We would love to hear ([aca@hwi.buffalo.edu](mailto:aca@hwi.buffalo.edu) or 716-898-8690) if you do.

## May 2019 ACA Self-Identification Survey Summary

I should preface these results with the statement that I am not a professional survey writer nor experienced in their analysis, but my goal here was to see if early-career ACA members saw themselves differently with regards to crystallography, compared to old timers, such as myself. For this we constructed a survey, which was distributed as a web link to ACA members in May of 2019. (See <http://bit.ly/2NKjvga> for a copy of the survey questions.) The first survey question probed self-identity by asking respondents how they label themselves professionally. Figure 1 and Table 1 shows most of the responses to that. Note that early career scientists are much more likely to label themselves with respect to a larger field such as chemistry or structural biology. In addition to the five labels shown here, 12 of 146 respondents used other labels. Four people, all late career, labeled themselves as biophysicists, and labels of engineer, biologist DNA nanotechnologist, educator, beamline scientist and physical chemist were selected by one person each, and a few individuals responded with two-part labels such as Chemistry/Crystallography, Crystallographer/Structural Biologist, Mathematician/Computer Scientist.

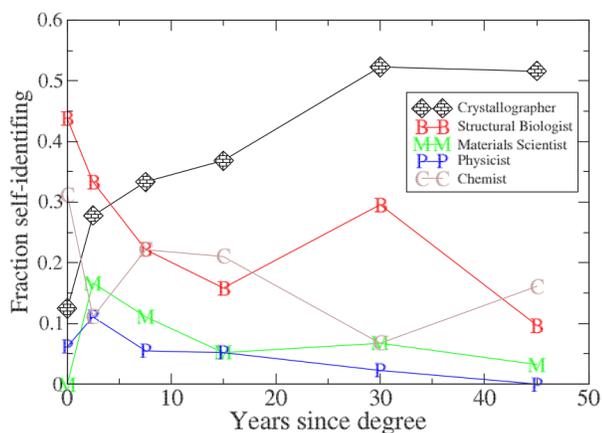


Figure 1: fraction of responding ACA members who labeled themselves as a crystallographer (black diamonds), structural biologist (red B), materials scientist (green M), physicist (blue P) or chemist (brown C).

In contrast, when asked a yes/no question, if the respondent was a crystallographer, the vast majority answered yes, regardless of level of professional experience, shown in Figure 2 and Table 2. Likewise, the vast majority of respondents said that they are

performing crystallographic analyses. The “5-10 years since degree” group was anomalous and I can only think this somehow might be related to the tenure process.

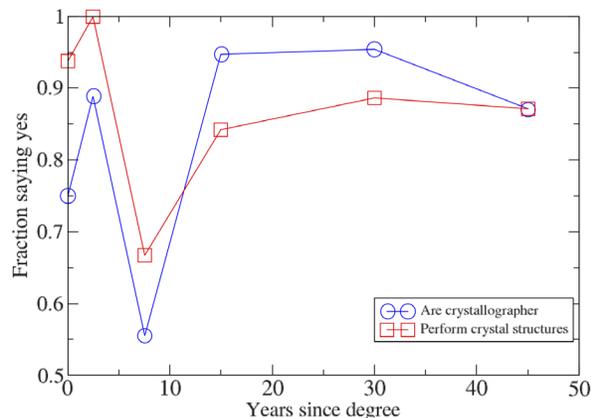


Figure 2: fraction of respondents saying yes to “are you a crystallographer” (blue circles) and “do you perform crystallographic analyses” (red squares).

Respondents were also asked how they would identify themselves to a high-school audience. This was to see how respondents saw themselves as part of a larger community. The responses showed a larger fraction of people affiliating to a more broad category such as chemist or structural biologist. Later-career people were more likely to still call themselves crystallographers. Stubbornness or lack of experience with explaining their work to general audiences? I was surprised that fraction of chemists was so high, at least in comparison to structural biologists. Perhaps chemists like surveys.

Finally, respondents were asked about the ACA’s name. All comments and suggestions are tabulated online (see <http://bit.ly/375c22K>). The majority of respondents are happy with the American Crystallographic Association, but many people are looking for a title that connects more to structural analysis.

### My Analysis

These results only represent on the order of one quarter of members of the ACA and those individuals who chose to answer a survey may not be representative of the majority. Nonetheless, I tend to think that these results are still quite important as they represent some of the most motivated of our members. Based on this I conclude that there is indeed a difference between the attitude for

members earlier in their careers with regard to how they view their professional connection with crystallography. This could be a developmental process and these younger scientists will come to the same views as their older peers with time, but I rather think this reflects how the practice of crystallography has changed. Our early career members are doing plenty of crystallography; crystallographer is a clear part of their professional identity but only one part. They label themselves by the scientific field where they work and likely use crystallography only as one aspect of their work. Older members see crystallography as their main focus and are more likely to see that is their primary identification. If there is an action item here, it is that the ACA needs to orient itself to people who are working in or with crystallography and not just people who would label themselves as crystallographer.

Many respondents, though a minority overall, would like to see the ACA have a name that connects to a wider range of techniques, since cryoEM, bioSAS, NMR, PDF, etc. have long been part of the ACA. A more comprehensive name would make clear that they are as much under our umbrella as traditional crystallography. There are some comments I will make with regard to our naming. We are primarily a US and Canadian organization that has plenty of members from other countries. For this reason, I'd suggest that North American would be a better choice than American in our name. Using biology in our name alienates a large fraction of our membership (including me). Calling ourselves a Structural Society will leave the general public wondering if we build bridges and tunnels. Atomic structure is what particle physicists do – worrying about how atoms are put together. Using molecular structure in the name annoys the solid-state chemists amongst us, as their entire crystal is a single giant molecule. Branton Campbell recently told me that he coined the term atomostructure to describe arrangements of atoms; a great idea but we will need to see if that catches on. The comments from the survey make good reading (see <http://bit.ly/375c22K> for the full set).

The ACA is our name and our history; it reflects my personal professional identity. I would be reluctant to see us lose that, but I'd like to see us adopt a two part name that retains our connection

to crystallography but also spells out that our ultimate interest as a professional society is in the determination of how structure of molecules and materials allows us to understand their properties. Naming of our society is going to be a long-term discussion topic for all of us.

Brian Toby

**Table 1. Self-identification as percentages of survey respondents**

Description to professionals	Years since last degree						overall
	students	0-5 years	5-10 years	10-20 years	20-40 years	40+ years	
Crystallographer	12.5%	27.8%	33.3%	36.8%	52.3%	51.6%	40.4%
Structural Biologist	43.8%	33.3%	22.2%	15.8%	29.5%	9.7%	24.7%
Materials Scientist	0.0%	16.7%	11.1%	5.3%	6.8%	3.2%	6.8%
Physicist	6.3%	11.1%	5.6%	5.3%	2.3%	0.0%	4.1%
Chemist	31.3%	11.1%	22.2%	21.1%	6.8%	16.1%	15.8%
(crystallographer or Structural Biologist)	56.3%	61.1%	55.6%	52.6%	81.8%	61.3%	65.1%
(total responses)	16	18	18	19	44	31	146

**Table 2. Self-identification as percentages of survey respondents to yes/no questions**

Yes/No questions	Years since last degree						overall
	students	0-5 years	5-10 years	10-20 years	20-40 years	40+ years	
Are you a crystallographer	75.0%	88.9%	55.6%	94.7%	95.5%	87.1%	85.6%
do you perform crystallographic analysis?	93.8%	100.0%	66.7%	84.2%	88.6%	87.1%	87.0%
American Crystallographic Association adequately describes our organization	75.0%	88.9%	55.6%	68.4%	72.7%	77.4%	73.3%

**Table 3. Self-identification as percentages of survey respondents when asked how they would identify to a high-school audience.**

Description to high schoolers	Years since last degree						overall
	students	0-5 years	5-10 years	10-20 years	20-40 years	40+ years	
Crystallographer	0.0%	14.3%	16.7%	43.8%	21.4%	33.3%	25.2%
Structural Biologist	25.0%	28.6%	16.7%	25.0%	21.4%	13.3%	22.7%
Materials Scientist	0.0%	21.4%	8.3%	6.3%	9.5%	6.7%	9.2%
Physicist	6.3%	14.3%	8.3%	6.3%	2.4%	0.0%	5.0%
Chemist	43.8%	42.9%	58.3%	25.0%	23.8%	30.0%	36.1%

Survey Questions: <http://bit.ly/2NKjvga>

Survey Comments: <http://bit.ly/375c22K>

## Workshop No. 1: Advanced Structural Characterization of Nanomaterials



*Katharine Page demonstrating the program PDFGui at the workshop*

Modern diffraction instruments allow the collection of scattering data containing a complete structural finger print of nano particles including atom-atom pair information from every aspect, e.g. the core, shell and possible ligand contributions. The analysis and modeling of total scattering data is becoming a growing area of interest and need in the crystallographic community. The workshop “Advanced Structural Characterization of Nanomaterials” introduced participants to the principles of modeling from using a simple unit cell based model with a shape function all the way to modeling a complete disordered nanoparticle with refinable model parameters. The workshop was organized and held by Thomas Proffen and Katharine Page from Oak Ridge National Laboratory. The program included lectures highlighting science examples as well an overview of the different modeling techniques for total scattering analysis of nanomaterials. The majority of the time during this full day workshop, participants got face-to-face with the modeling programs PDFGui and DISCUS running through hands-on exercises creating nano-particle models of increasing complexity.

*Thomas Proffen and Katharine Page*

## Workshop No. 2: Accelerating your Career Development

This free half day workshop was organized by the Young Scientist Interest Group to provide an opportunity for our peers to learn about career development. We covered many topics in the workshop including academic vs industry jobs, conducting a job search,

networking, and provided ample time for open questions from the participants. We had 3 primary activities this year; a broad presentation by Patrick J. Mulvey (American Institute of Physics), a panel discussion, and a hands-on networking activity. We would like to extend our gratitude to our panelists; Corie Ralston (Lawrence Berkley National Laboratory), Bruce Noll (Bruker), Michael Thompson (University of California, San Francisco), and Louise Dawe (Wilfrid Laurier University). We would also like to thank all of the mentors who joined our participants for the speed-networking activity. It was a very interactive workshop and we look forward to return of speed-networking at the 2020 meeting in San Diego.

Workshop 2 was generously supported by the American Institute of Physics, Rigaku, and Constellation Pharmaceuticals.

*Chelsy Chesterman, Korey Carter, Kenneth Childers*

## Workshop No. 3: Introduction to PHENIX for electron Cryo-Microscopists

With cryoEM becoming more popular, this workshop provided an overview of the tools available in Phenix for working with cryoEM models. The morning was filled with lectures from Phenix developers: Paul Adams, Pavel Afonine, and Jane Richardson. Paul Adams described the tools from Tom Terwilliger that can be used to improve maps and to automatically build models into those maps. Pavel Afonine talked about the refinement program in Phenix that works directly with real-space maps. And Jane Richardson talked about some new approaches toward model validation and importance of validation for cryoEM structures.

During the morning break and lunch period, the participants installed Phenix onto their computers so that they can do the hands-on tutorials in the afternoon session. Similar to the format of the morning lectures, there were tutorials for map improvement and model building, model refinement, and validation. The tutorials were a great way to familiarize the participants with the tools described in the morning and the general workflow within Phenix for structure solution using cryoEM maps.

The workshop was well attended and it was a wonderful opportunity for the Phenix developers to interact with the participants. There were insightful questions and discussions, especially during the breaks

and over lunch, where we could help solve some of the issues the participants were experiencing with their models.

## Workshop No. 4: Saturday Morning Serial Crystallography: Obtaining Protein Structure from Many Crystals

The Saturday morning crystallography workshops would not have been complete without a bowlful of serial crystallography (SX)! Although contemporary SX techniques were originally developed for the XFEL, there is growing interest in pursuing SX at synchrotron sources where beamtime availability is not as scarce. Serial methods can provide vital insight into challenging areas such as room temperature studies, protein dynamics and overcoming problems from radiation damage. During a SX experiment, diffraction images are taken from tens to thousands of crystal samples. The difficulty then is to merge data from a large enough number of crystals in order to determine the protein structure. With generous funding from MiTeGen and BioXFEL, organizers from SLAC National Laboratory (Jennifer Wierman, Aina Cohen, and Art Lyubimov), Cornell High Energy Synchrotron Source (Aaron Finke), Lawrence Berkeley National Laboratory (Nick Sauter) and Diamond Light Source (Graeme Winter) teamed up to introduce participants to SX, from sample preparation and data collection to structure solution. Speakers from multiple institutions across the US and the UK offered valuable insight into designing SX experiments and how these powerful methods can benefit the structural study of biomolecules.



Group photo of the Workshop No. 4 speakers and organizers.

L to R: Aaron Finke, Benjamin Stauch, Aaron Brewster, Jennifer Wierman, Art Lyubimov, Nick Devenish, Aina Cohen, Graeme Winter and Guillermo Calero.

Photo by Richard H. Bromund

Throughout the one-day workshop, 35 attendees were given not only a comprehensive overview of cutting-edge technologies for SX experiments, but also hands-on experience with handling the (often gigantic) SX datasets. The workshop was divided into three parts, beginning with a series of lectures on various

modes of experimental design specifically aimed at the complexities of these sorts of setups. Guillermo Calero (U. Pittsburgh) offered tips and tricks for optimizing sub-micron sized crystals using transmission electron microscopy (TEM) and crystal seeding methods. Following in the next step in the data collection pipeline - sample delivery to the beam - Benjamin Stauch (U. Southern California) used compelling examples of GPCR structures to demonstrate the utility of viscous liquid sample injectors. Jennifer Wierman (SLAC) continued the unbiased exploration of delivery methods showcasing the various fixed target platforms developed across many facilities. Next, in a clear example of cross-oceanic collaboration, Graeme Winter (DLS) introduced a user program for the study of protein dynamics with fixed-target serial synchrotron crystallography at Diamond Light Source in the UK. The morning lectures were then rounded out by Aina Cohen (SLAC), illustrating how to best make use of the standard goniometer setup for serial diffraction studies at both an XFEL (LCLS-MFX) and a synchrotron source (SSRL BL12).

After a quick break for food, participants gathered for an exciting live demonstration of serial data collection via a remote desktop connection to beamline 12-2 at the Stanford Synchrotron Radiation Lightsource (SSRL). Methods for automated positioning and exposure of multiple crystals on fixed-target mounts were demonstrated including helical data collection modes for larger crystals and the use of UV-tryptophan fluorescence microscopy for randomly orientated micro-crystals.

Diving straight into the challenge of gigantic SX datasets, Aaron Brewster (Lawrence Berkeley National Lab) paid special attention to injector-based “stills” data and introduced new capabilities of cctbx.xfel in data handling and processing. Art Lyubimov (SLAC National Lab) added to the stills processing landscape by describing a user-friendly interface for serial data processing with IOTA/cctbx.xfel. In addition, and as current beamline facilities are now enabling serial oscillation data collection, Nick Devenish (speaker, Diamond Light Source) and Aaron Finke (organizer, CHESS) revealed promising improvements with serial oscillation data with DIALS and XDS/nXDS, respectively.

The last part of the workshop highlighted a “Data Frames to PDB” session for offline data reduction and processing, where participants were given sample data sets (had they not their own) and worked through diffraction image processing, with assistance from Aaron Brewster (cctbx.xfel), Aaron Finke (XDS/nXDS), Nick Devenish (DIALS) and Art Lyubimov (IOTA).



Art Lyubimov (middle, SLAC) assisting participants with hands-on training of IOTA/cctbx.xfel. Photo by Richard H. Bromund.

As serial macromolecular crystallography matures, techniques will open the doors to a wide variety of exciting new time resolved experiments, providing new ways to study protein dynamics. We hope to see more workshops continue to make these techniques more routine.

*Jeney Wierman*

### **Workshop No. 5: Fundamentals of Single Particle Cryo-EM**

Cryo-EM is rapidly becoming the method of choice for structure determination of proteins larger than ~100 kDa, including membrane proteins, large assemblies and multi-protein complexes. Cryo-EM instrumentation is being installed in many universities, and is also available at large multiuser facilities both in the U.S. and worldwide. The 2019 ACA Workshop on Biological Structure Determination using Cryo-EM was intended to benefit those who want to use cryo-EM in the future, or who have recently transitioned into it, with up-to-date discussions of cutting-edge methods and technology. The workshop was co-organized by Cathy Lawson (Rutgers U), Wen Jiang (Purdue U), and Michael Cianfrocco (U Michigan) and sponsored by ThermoFisher Scientific, Electron Microscopy Sciences, MiTeGen, and Amazon Web Services. The two-afternoon workshop was held on two consecutive afternoons during the ACA 2019 main meeting (Mon. and Tues.) and had over 80 registered attendees.

This workshop introduced scientists with crystallographic backgrounds to procedures used by cryo-EM. The new Cryo-EM National Service Centers

were introduced by Ed Eng (New York Structural Biology Center). Lectures by Wen Jiang and Leifu Chang (Purdue U) focused on the steps involved in producing a cryo-EM map, from specimen preparation and data collection through to image processing and reconstruction. Aspects of workshop were hands-on: state-the-art programs were used by the students to process several sample datasets including the T20S proteasome, aldolase, TrpV5, spliceosome, and HIV trimer. Particle picking and reconstruction tutorials were designed and guided by Michael Cianfrocco, with additional one-on-one assistance provided by Brenda Gonzalez (Purdue U) and Jennifer Cash (U Michigan). Each student was given access to their own GPU computing node on the AWS cloud, as well as a temporary CryoSparc license, and was requested to install UCSF Chimera in advance of the workshop. Participants were also introduced by Brenda Gonzalez, Ziwei Huang, and Jiahui Dong (Purdue U) to virtual reality training for specimen preparation.



Top row: Wen Jiang, Brenda Gonzalez, Leifu Chang, CryoVR equipment, Michael Cianfrocco, Ziwei Huang, Jiahui Dong.  
Bottom row: Jennifer Cash, Cathy Lawson, Ed Eng.

### **Workshop No. 6: Phase Identification and Materials Characterization Using Powder X-ray Diffraction**

*no report submitted*



## μS DIAMOND – Simply Brilliant

### **'Diamonds are a crystallographer's best friend'**

The extreme hardness of diamonds has allowed crystallographers to study materials at pressures greater than the core of the Earth. Now, the extreme heat conductivity of diamond gives crystallography a new X-ray source without equal: the μS DIAMOND source. Diamond conducts heat five times more efficiently than any other known material, making it perfect to cool the intense heat loads in a modern microfocus source.

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Crystallography



# ACA 2020

American Crystallographic Association

August 2 - 7, 2020 • San Diego, CA

*TRAINING THE NEXT GENERATION*

**www.acameeting.com**  
**70th Annual ACA Meeting “Training the Next Generation”**  
**Sheraton San Diego Hotel & Marina**  
**Sunday, August 2, 2020 – Friday, August 7, 2020**

Scientists interested in molecular and materials structure with specialties in biology, chemistry, geosciences, materials science and much more will converge on the San Diego waterfront in August 2020 for exchange of scientific research and technique know-how for the 70th Annual Meeting of the ACA. For 2020, the meeting has the overall theme of “Training the Next Generation.” Session topics will expand well beyond traditional single-crystal and powder X-ray diffraction techniques to include next-generation methods and facilities such as cryo-EM, micro-electron diffraction, and advanced capabilities at national synchrotron and neutron sources. The conference also seeks to empower the next generation with session content balanced between new scientific results and education on how to perform similar work.

## 2020 PROGRAM COORDINATORS

<b>Nozomi Ando</b>	2020 Meeting Committee Member & 2020 Program Chair
<b>Carla Slebodnick</b>	2020 Meeting Committee Member & 2020 Program Chair
<b>Stephan Ginell</b>	2020 Meeting Committee Member & 2019 Program Chair
<b>Vivien Yee</b>	2020 Meeting Committee Member & 2019 Program Chair
<b>Louise Dawe</b>	2020 Poster Co-Chair
<b>Tiffany Kinnibrugh</b>	2020 Poster Co-Chair

## Important Dates!

Jan 2020: Call for Papers  
 Website Launch  
 Travel Grant Window Opens

Feb 2020: Registration Opens  
 Abstract Window Opens

Mar 2020: Early Registration Closes 3/31/20  
 Travel Grant Deadline 3/31/20

April 2020: Oral Abstract Submission Deadline  
 4/20/20

May 2020: Oral Talk Speakers Notified of  
 Acceptance, Date/Time of Talk

June 2020: Regular Registration Closes 6/15/20  
 Hotel Block Closes 6/30/20  
 Poster Presenters Notified of  
 Acceptance, Date/Time of Poster

## KEYNOTE - AWARDS

**Keynote**  
 Prof. Venki Ramakrishnan

**David G. Rognlie Award**  
 Dr. James Holton

**A.L. Patterson Award**  
 Dr. Václav Petříček

**Margaret C. Etter Early Career Award**  
 Prof. Nozomi Ando

**Elizabeth A. Wood Science Writing Award**  
 The Alan Alda Center for Communicating Science  
 at Stony Brook University’s School of Journalism

## EVENTS

Opening Reception  
 Three Minute Thesis Contest  
 YSIG Mixer  
 Exhibit Show  
 Poster Sessions  
 Banquet

**Workshops**

- Applications of Small Angle Scattering to Structural Biology: An Introduction
- Crystallographic and Cryo-EM Structure Solution with Phenix
- Introduction to Hydroxyl Radical Foot-printing Methods for Structural Analysis of Proteins and Complexes
- Introduction to Diffuse Scattering Analysis from Single Crystal Neutron Diffraction
- Protein crystal crystallization for neutron macromolecular crystallography: Practicum and overview.
- Fundamentals of Single Particle Cryo-EM

**Transactions Symposium**

- Innovating Structural Science Education Inside and Outside the Classroom

**Sessions of Broad Interest (Sponsoring Scientific Interest Groups)**

- Communicating Science to the Public (Communications, Canadian, General Interest)
- General Interest I and II (General Interest)
- Open Exchanges in Crystallographic Education (General Interest, Small Molecule)
- Meeting the Challenges of Raw Data Deposition (Industry, CryoEM, Light Sources)

**Macromolecule Sessions (Sponsoring Scientific Interest Groups)**

- Molecular Structure in K-12 Education (BioMac)
- Ion Channels (BioMac, CryoEM, Industrial)
- MicroED of Biomolecules (BioMac, CryoEM)
- Ion Channels (BioMac, CryoEM, Industrial)
- MicroED of Biomolecules (BioMac, CryoEM)
- Metalloproteins (BioMac, Light Sources)
- Hot Structures (BioMac, Canadian, YSIG)
- Macromolecules Involved in Mental Health (BioMac, Industrial)
- Structural Dynamics I. Conformational Heterogeneity (Cryo-EM, SAS Scattering)
- Structural Dynamics II. Biological Dynamics: Collective Motion of Macromolecules (SAS, BioMac)
- Protein Sample Preparation for Crystallography and Cryo-EM (Cryo-EM, Industrial, BioMac)
- Advances in Fiber Diffraction (Fiber)
- CryoEM in Industry (Industrial, CryoEM)
- Facilities for the Next Generation of Structural Biologist (Light Source, YSIG)
- Frontiers in SAS (SAS, Light Sources)
- Self-Assembly in Soft Matter Systems (SAS, Neutron)

**Materials/Neutron/Powder Sessions (Sponsoring Scientific Interest Groups)**

- Structural Analysis of Thin Films (Materials, Neutron, Powder, Small Angle Scattering)
- Materials for Sustainability and Energy (Co-Sponsoring SIG: Small Molecule)
- Geological Crystallography
- Extreme Environments of Pressure, Temperature, and Field
- In situ / operando: From Synthesis to Devices
- Short-Range Order and Local Structure
- PXRD with Multimodal & Multidisciplinary Approaches
- Magnetic, Quantum, & Exotic Phenomena in Condensed Matter
- Facilities for the Next Generation of Material Scientist (Light Source, General Interest, Materials, Neutron, Powder)

**Small Molecule Sessions (Sponsoring Scientific Interest Groups)**

- MicroED of Small Molecules (Small Molecule, CryoEM, YSIG)
- Cool Structures (Small Molecule, YSIG)
- Solid State Supramolecular Chemistry and Crystal Engineering (Small Molecule, YSIG, Neutron, Materials, Powder, General Interest)
- Materials and Processes in Drug Development and Formulation (Industrial, Small Molecule)
- My First Crystal Structures (Service, Small Molecule, GIG)
- Crystallography on the International Space Station (Service, Small Molecule, GIG)
- Would You Publish This? (Service, Small Molecule, Canadian)

## GENERAL MEETING INFORMATION

### Abstracts:

Over 40% of oral presentations are drawn from the general submission pool, offering opportunities for young and less well-established scientists to give talks and network with top researchers. There is also extensive opportunity for scientific discourse through multiple poster sessions. Each registrant may submit one abstract for free.

### Registration & Financial Opportunities:

The ACA is committed to assisting students and young scientists cover the cost of attendance through our travel grant program and the session room monitor program.

### Travel Grants:

Through a combination of ACA contributions and generous donations from individual members and businesses, the ACA awarded over \$15,000 in travel grants to offset expenses associated with attending the 2019 meeting. Check out the meeting homepage for details and information on how to apply.

### Session Room Monitors:

Registered students and postdocs attending the meeting can assist the ACA by working as a session room monitor. See the meeting homepage for details and information on how to apply.

### Registration:

Registered participants receive a name badge securing admission to the opening reception, exhibit show and scientific sessions. Fees for workshops and certain social events are additional and the cost will be specified on the registration site.

Registration as a Non-Member includes all items listed for member registration, above, and membership in

	"Early Bird"	Regular	"Belated"
Deadline	March 31, 2020	June 15, 2020	After June 15, 2020
<b>ACA MEMBERS</b>			
Regular	\$595	\$795	\$895
Retired	\$325	\$390	\$425
Canadian	\$500	\$795	\$895
PostDoc	\$325	\$390	\$425
Graduate/Undergrad	\$275	\$340	\$375
<b>NON-MEMBERS</b>			
Non-Member (ALL)	\$795	\$1,085	\$1,185
Guest	\$150	\$150	\$150
Children under 12	\$75	\$75	\$75

the ACA for the remainder 2020.

"Guest" and "Child" registrants receive a badge granting them access to the general meeting areas, the Opening Reception, the YSIG Mixer (when attending with a qualifying attendee) and the Closing Banquet. Guests may not attend meeting sessions. Registration for a "Guest" or "Child" is a fixed price, regardless of event participation.

### Venue/Hotel:

All scientific sessions, workshops and poster exhibits will take place at the Sheraton San Diego Hotel & Marina, 1380 Harbor Island Drive, San Diego, CA 92101.

The 2020 nightly rates, not including customary taxes, services charges or gratuity:

The ACA offers discounted room rates as part of a contract commitment to fill a minimum number of

Rooms	Single	Double	Triple	Quad
Regular	\$219	\$219	\$239	\$259
Student	\$189	\$189	\$209	\$229

rooms at this hotel. We encourage all attendees to support the ACA by reserving a room in the conference block. With your support, the ACA can continue to provide discounted room rates to attendees in the future.

Consider sharing a room! The ACA will help facilitate contact between attendees looking to save money by sharing the cost of a room. The ACA does not guarantee room availability and attendees/roommates are responsible for making their own hotel reservations. See the meeting website for information on room sharing.

### Foreign Travelers:

Obtaining a VISA: Advanced planning by foreign travelers is critical. Obtaining a VISA is the sole responsibility of the attendee. If a VISA is needed, 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:

The US Department of State: Bureau of Consular Affairs <https://travel.state.gov/content/travel.html>

The National Academies of Sciences Engineering Medicine <https://travel.state.gov/content/travel.html>

US.GOV: How to Enter the US <https://www.usa.gov/enter-us>

If you are required to submit a Letter of Participation in the Conference with your application, e-mail your request to: [aca@hwi.buffalo.edu](mailto: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.

## Call for Nominations to the 2021 Awards

	<i>Deadline to Submit</i>	<i>Decision</i>	<i>Presentation</i>
Bertram Eugene Warren Diffraction Physics Award	April 1, 2020	July 2020	ACA 2021
M.J. Buerger Award	April 1, 2020	July 2020	ACA 2021
Margaret C. Etter Early Career Award	April 1, 2020	July 2020	ACA 2021
Fellows	April 1, 2020	June 2020	ACA 2020

### Bertram Eugene Warren Diffraction Physics Award



To recognize an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. Works published within a six-year period ending June 30 of the year preceding the Award may be nominated. A monetary award of \$1,500, and up to \$1,500 travel expenses to accept award at Annual Meeting, and a certificate are awarded every third year. Established in 1970 by students and friends of Professor B.E. Warren on the occasion of his retirement from the Massachusetts Institute of Technology.

### M.J. Buerger Award



To recognize mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. There are no restrictions as to nationality, race, sex, religion, or membership in the ACA. Awarded triennially in memory of Martin J. Buerger, Institute Professor Emeritus of M.I.T. and University Professor Emeritus of the University of Connecticut, a mineralogist who made major contributions to many areas of crystallography. Established in 1983. The first award was made in 1985. A monetary award of \$1,500, and up to \$1,500 in travel expenses to accept award at Annual Meeting.

### 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. The award is established to honor the memory of Professor Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. She had a love for people, for science, and especially for people who do science, that we honor. Established in 2002 as an annual award, it consists of a monetary award of \$1,000 and plaque. The winner will present a lecture at the American Crystallographic Association Annual Meeting. 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. Nominees employed in tenure-track academic positions must not yet have received tenure. Nominations must include as a minimum a nomination letter clearly indicating the accomplishments of the individual since beginning their independent career and assessing the future potential of the nominee. Three supporting letters and a c.v. for the nominee may be provided but are not requirements. Self-nominations are permitted. Nominees may be employed in regular academic positions, as service crystallographers, in industrial positions or in government laboratory positions.

## **Call for Nominations to the 2021 Awards**

### **Fellows**

In 2011 the ACA Council established a Fellows program to recognize a high level of excellence within our membership in scientific research, teaching, and professional duties, or in service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. The ACA Fellows program celebrates the excellence of our society's members and promotes their recognition world-wide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. ACA Fellows serve as scientific ambassadors to the broader scientific community and the general public to advance science education, research, knowledge, interaction, and collaboration. It allows us to significantly recognize and honor a broader cross-section of the membership than is currently possible. It is envisioned that eventually about 5% of the membership will be recognized as ACA Fellows, and the ACA will announce new inductees and honor all ACA Fellows at the Awards Banquet each year at our national meeting.

### **Guidelines for Selecting ACA Fellows**

The ACA Council has established a Fellows program. It 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. 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 us to significantly recognize and honor a broader cross-section of the membership than was previously possible with other, more specific awards. We envision that eventually about 5% of the membership will be recognized as Fellows, and the ACA will announce new inductees and honor all ACA Fellows at the annual Awards Banquet.

### **Criteria**

A Fellow is defined as "a Member whose efforts on behalf of the advancement of crystallography or its applications that are scientifically or socially distinguished." Examples of areas in which nominees may have made significant contributions are research; teaching; technology; services to professional societies; administration in academe, industry, and government; and communicating and interpreting science to the public. Fellows are elected annually by the current group of Fellows.

### **Procedure**

The procedure for nominating and selecting Fellows is as follows:

- Candidates for ACA Fellow must be a current ACA member, meaning that the candidate must have paid ACA dues for the year they are nominated.
- A nomination package must be completed by the nominator, who must also be an current ACA member. In a cover letter, a case should be made for how the proposed Fellow meets the above criteria. A brief CV must also be provided, as well as two letters from at least other current ACA members supporting the nomination.
- Nominations are due each year by April 1st . All nominations will be collected at ACA Headquarters and distributed to the current Fellows for review. A score sheet shall be provided.
- Nominations for ACA Fellows shall roll over twice, without any additional submissions from the nominator (i.e., candidates for Fellow who are nominated but not elected in one year will be automatically reviewed during each of the following two years), provided that the candidate remains as current ACA.
- Current Fellows shall provide a yes/no/abstain vote on each nominee. Fellows will submit their recommendations to ACA Headquarters within 3 weeks of receipt of the nomination packet. For a candidate to be approved as a Fellow, greater than 50% of the votes actually cast for that candidate must be "yes," AND the number of yes votes must be greater than or equal to 25% of the total number of current Fellows. An abstention does not count as a vote.

# ACA HISTORY

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION



## ACA History Project Update



Robin Payne

We gratefully acknowledge the work of Vanessa Reitz as Webmaster, especially during the recent transition to the new web host; Vanessa will continue as design consultant. We welcome Robin Payne, the new Webmaster, who began uploading material to the ACA

website on October 1. Robin has been part of the Western North Carolina nonprofit community for twenty years, serving in a variety of roles from volunteer to Board Chair to Executive Director. After receiving her MBA from Western Carolina University she launched her company, Auxilium, which specializes in operations and back-office support for nonprofits. Robin and her husband and two children live in Asheville, North Carolina, where she loves to hike, garden, and dance.

## Michael Rossmann Memorial Session



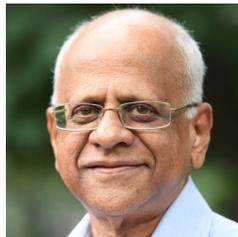
Michael Rossmann

The late Michael Rossmann was a giant in macromolecular crystallography. He discovered the Rossmann fold, a common motif that he recognized in nucleotide binding proteins. He and his research group determined the structure of the human rhinovirus (common

cold virus). Using a combination of crystallography and cryo-electron microscopy, the group published the structures of the dengue virus and the zika virus. He pioneered new methods, such as high-performance computing, molecular replacement techniques, and non-crystallographic symmetry averaging. At the Covington, KY meeting, five speakers described their experience in Michael's laboratory, beginning in 1972 with Jack Johnson, then Eddy Arnold, Hao Wu, Rui Zhao, and S. Saif Hassan – a beautiful summary of ground-breaking research. The [video](#) of the session is now online at ACA History online.

## Gautam Desiraju's Living History Now Online

[Gautam Desiraju](#), past president of IUCr, contributed formative concepts in crystal engineering and investigated weak hydrogen bonds. Desiraju grew up in India and traveled to the University of Illinois for his Ph.D. Soon thereafter he returned to India and took



Gautam Desiraju

how these two features may be largely unconnected.

a position at the University of Hyderabad. Since he lacked a diffractometer in Hyderabad for the first 20 years, he collaborated internationally and made extensive use of the CSD. In his memoir he illustrates how a work may be conceived—and how it may be received—and

## Mike Glazer's Living History and 2017 Bragg Lecture



Mike Glazer

notes that both William Henry and Lawrence Bragg were “quite competent artists”; he believes that their interest in both art and science may have led to their crystallographic discoveries.

[A. Michael Glazer](#), former vice-president of the IUCr, is one of the founders of Oxford Cryosystems. Mike obtained his Ph.D. with Kathleen Lonsdale followed by a post-doc in Helen Megaw's laboratory. In his [2017 Bragg Lecture](#) he discusses structure-property relationships in perovskites. He

## Benno Schoenborn's Bau Diffraction Award Lecture

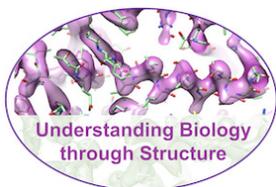


Benno Schoenborn

video and the accompanying [slides](#) describe his later work on xenon binding to myoglobin and neutron scattering studies of membranes and membrane proteins.

The video of Benno Schoenborn's 2016 ACA [Bau Neutron Diffraction Award lecture](#) is now online. He has been aptly called the “father of neutron protein crystallography,” since he was the first to determine a protein structure (myoglobin) by neutron diffraction. The

## ACA members to speak at Understanding Biology through Structure 2020



Seven ACA members will be giving lectures at the second "Understanding Biology through Structure" conference, to be held in Santa Fe, NM March 16-20, 2020 (see <https://cvent.me/4kq9P>). This conference series is intended to bring together junior and senior structural biology researchers as well as to showcase developments in structural biology. The first Understanding Biology through Structure meeting was in May of 2017 and attracted researchers from around the world, including 10 National Academy and Royal Society members (many of the talks are available on line at <https://bit.ly/2Gg39rm>). Some 30 of the students and postdocs at the first meeting were given full travel fellowships to attend, a first for many of them that helped to make them feel that they were an essential part of the meeting.



Hao Wu



Wayne Hendrickson



David Eisenberg

The second Understanding Biology through Structure conference will feature talks on both new methods in structural biology and recent results in protein-nucleic acid complexes, viral pathogenesis and vaccine design, cell signaling, design and discovery of drugs, and structure, dynamics, and function of membrane proteins. This second Understanding Biology through Structure meeting will be giving partial support to students and postdocs for attending the meeting and these students and postdocs will be giving poster presentations during the meeting.



Chris Hill



Marie Pancera



Peijun Zhang



Thomas C Terwilliger

ACA members who will be giving lectures include **Hao Wu** of Harvard University, **Wayne Hendrickson** of Columbia University, **David Eisenberg** of UCLA, **Chris Hill** of the University of Utah, **Marie Pancera** of the Fred Hutchinson Cancer Research Center, **Peijun Zhang** of the electron Bio-Imaging Centre at Diamond, and myself of the New Mexico Consortium.

Three ACA members will give Keynote lectures at the meeting. Hao Wu will be giving a Keynote lecture about supramolecular complexes in innate immunity (see [http://wulab.tch.harvard.edu/PDF/Humayun\\_Nature\\_2019.pdf](http://wulab.tch.harvard.edu/PDF/Humayun_Nature_2019.pdf)). Wayne Hendrickson (<https://biology.columbia.edu/people/hendrickson>) will give a Keynote lecture on allosteric control of protein disaggregation by Hsp70 molecular chaperones, and David Eisenberg will give a Keynote lecture on the differences between pathogenic and functional amyloid proteins (see <https://www.nature.com/articles/s41594-018-0064-2>). Chris Hill will talk in a session on nanomachines, lecturing on AAA Unfoldases (<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5716660/>) and Marie Pancera will talk in a session on developing therapies, speaking on antibody/antigen complexes for vaccine design (<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5557343/>). Peijun Zhang and I will be in a session devoted to cryo-EM technology. Peijun Zhang will speak on cryo-electron tomography and sub-tomogram averaging for in situ structural biology (<https://www.sciencedirect.com/science/article/pii/S0959440X18300927>) and I will talk about density modification and model-building for cryo-EM (<https://www.biorxiv.org/content/10.1101/845032v1>).

Following the main Understanding Biology through Structure conference there will be a workshop where students and postdocs can learn about using the Phenix software to determine structures by X-ray crystallography and cryo-EM (<https://cvent.me/4kq9P>). Phenix developers including **Paul Adams**, **Randy Read**, **Massimo Sammito**, **Dorothee Liebschner**, **Billy Poon**, **Pavel Afonine**, **Nigel Moriarty**, and **Jane Richardson** will be giving lectures and hands-on instruction on recent developments in macromolecular structure determination.



## ACA Summer Course in Chemical Crystallography

May 31<sup>st</sup> – June 6<sup>st</sup>, 2020

Purdue University  
West Lafayette, IN

**Applications will be accepted starting January, 2020**

[www.acasummercourse.net](http://www.acasummercourse.net)

Sponsored by:

The American Crystallographic Association

Bruker AXS, Rigaku Americas, The Cambridge Crystallographic Data Centre, The Pittsburgh Diffraction Society, The International Centre for Diffraction Data, MiTeGen, Triclinic Labs, Inc, Anton Paar Instruments



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UNIVERSITY

Northwestern  
University

**The ACA gratefully acknowledges the following contributors  
to the various award funds**

**African Award**

Christine M. Beavers  
Alexander Buhse Brady  
Prabal Dasgupta  
Anna D. Gudmundsdottir  
John Richard Helliwell  
Andreas Kreusch  
James W. Pflugrath  
James Christopher Phillips  
Gerold Rosenbaum  
Amy Sarjeant  
Cynthia Vianne Stauffacher  
Rik Wierenga

**Etter Early Career**

Helen Berman  
Norma Duke  
Jane Griffin  
Anna D. Gudmundsdottir  
Cheryl Klein Stevens  
Mariusz Krawiec  
James Loehlin  
James W. Pflugrath  
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William Stallings  
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**Warren Diffraction**

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John Edward Warren  
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Pavol Juhas  
James W. Pflugrath  
Marc Lee Pusey  
Amy Sarjeant  
Stephen Robert Sprang  
Robert M. Sweet  
Crissy Tarver  
Bi-Cheng Wang  
Mark A. Whitener  
Winne Wong-Ng

**Outreach Education**

Alexander Buhse Brady  
Diane A. Dickie  
Frank R. Fronczek  
Wilfred Fullagar  
Anna D. Gudmundsdottir  
Andrew Jay Howard  
Andreas Kreusch  
Nicholas Noinaj  
Katharine Page  
James W. Pflugrath  
Gerold Rosenbaum  
Amy Sarjeant  
Cynthia Vianne Stauffacher  
Martha M. Teeter  
Bi-Cheng Wang  
Winne Wong-Ng

**History Program**

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Charles Bugg  
Frank R. Fronczek  
Wilfred Fullagar  
Professor Glazer  
John Richard Helliwell  
Daniel R. Knighton  
Virginia Pett  
James W. Pflugrath  
James Christopher Phillips  
William Stallings  
Dale Tronrud

**Student Travel Program**

Roger Burnett  
Helen Berman  
Paul Butler  
Charles Williams Carter  
Bryan Chakoumakos  
David Ernest Cox  
Drake Eggleston  
Andrew Fisher  
Frank R. Fronczek  
Millie M. Georgiadis  
Anna D. Gudmundsdottir  
Pavol Juhas  
Paval Karen  
Clara Louise Kielkopf  
Tiffany L. Kinnibrugh  
Daniel R. Knighton  
Andreas Kreusch  
Nicholas Noinaj  
Katharine Page  
James W. Pflugrath  
James Christopher Phillips  
Marc Lee Pusey  
Jane S. Richardson  
Maria Mercedes Silvia  
William Stallings  
Cynthia Vianne Stauffacher  
Robert Michael Stroud  
Dale Tronrud  
Mark A. Whitener  
Carrie Mary Wilmot

**Pauling Poster Prize**

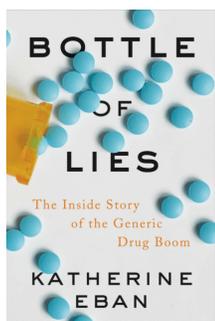
Helen Berman  
Charles Williams Carter  
David Ernest Cox  
Sylvie Doublee  
Anna D. Gudmundsdottir  
Andrew Jay Howard  
Paval Karen  
Clara Louise Kielkopf  
James W. Pflugrath  
James Christopher Phillips  
Marc Lee Pusey  
Frank Rotella  
Michal Sabat  
Toshiya Senda  
Cynthia Vianne Stauffacher  
John Tainer  
Thomas Webb  
Mark A. Whitener  
Winne Wong-Ng

# Opening Mixer Covington ACA Meeting



**The ACA wishes to thank the vendors who participated in the Covington ACA Meeting**

# Book Reviews



## **Bottle of Lies: The Inside Story of the Generic Drug Boom**

Katherine Eban

ISBN 978-0-06-233878-5

Katherine Eban's *Bottle of Lies* is a remarkable piece of investigative journalism, one that she has been working on for over a decade, though the story she tells is one with roots digging even decades deeper. The focus of her narrative is the Indian pharmaceutical company Ranbaxy Laboratories. Founded in 1961, Ranbaxy was operated by the Singhs, its founding family, for the majority of its years of operation. Despite being worth billions of dollars, the Singhs chose to run Ranbaxy like the family-owned-and-operated corporation that it was. The company, as many of our readers may know, essentially folded in 2014 when it was absorbed by Sun Pharma in the wake of enormous controversy, including recalls and reports of glass fragments in prescription capsules.

But, as Eban herself admits in her opening Author's Note, her interest in generic prescription drugs did not start with Ranbaxy. In 2008, the host of an NPR radio show called *The People's Pharmacy* reached out to Eban with concerns expressed by his listeners that their generic drug replacements for brand-name pharmaceuticals were not working. Patients with an established brand name drug regimen found themselves relapsing when their prescriptions switched to the cheaper, more affordable generic version. Eban did what investigative reporters do best--she investigated. Her first piece on generic drugs was published in *Self* in 2009. It was her reporting for that first article that inspired *Bottle of Lies*.

Ranbaxy was the focus of an investigative follow-up

piece Eban wrote for *Fortune* in 2013. It was in May of that year that the corporation's corrupt manufacturing and management practices became the center of media attention. Felony charges were brought against the company in the United States as the result of more than half a decade of FDA investigations, sparked by the actions of a single whistleblower: Dinesh Thakur. The company pleaded guilty, to the tune of a \$500 million dollar settlement.

Ranbaxy's fall from grace--it went from winning awards for brand trust to publicly pleading guilty of multiple felony drug fraud counts--consumes the majority of Eban's narrative. Her key protagonist, Dinesh Thakur, is the former employee turned whistleblower who brought evidence of the company's malpractice to the FDA. Thakur's journey, from a respected employee at Bristol Meyers-Squibb, one of America's prestige brand-name pharmaceutical companies, to one who resigned amidst a cloud of controversy at a generic drug company in India, provides a lens through which Eban encourages her readers to view the web of lies and deceit that dominate generic drug industry.

The Ranbaxy news is already over half a decade old at this point. There is some semblance of justice, as one reads, knowing the bad guys got caught, so to speak. Reading *Bottle of Lies* is like watching *The Untouchables*--you know Elliot Ness got Al Capone in the end, because Capone died in jail. But you still watch the movie because you want to know how--and that's why you need to read *Bottle of Lies*.

Though Thakur dominates much of the narrative, other crusaders of pharmaceutical justice make noteworthy and repeated appearances, such as FDA inspector Peter Baker. Baker uncovered the unsettling reality that generic drug companies not only manufacture and distribute defective drugs to American consumers, they do so around the world. Often, the generics shipped to third-world countries in Africa are those that did not pass muster to be sent to the United States. We are not getting the good stuff, but Americans are also not the ones getting the worst stuff.

At the heart of the generic drug controversy is

the very definition upon which they are based: bioequivalence. As long as a generic drug has the same amount of active ingredient (give or take) as the name-brand drug for which it is being substituted, it is considered an equal substitution. But there is a lot more to prescription medication than active ingredients. And not all generics are created equal. At the end of the day, do generics cost less money to purchase at the pharmacy than name-brand prescriptions? Oftentimes, insurance covers the full cost of the generic, rendering it seemingly free to the average consumer. But the real cost of generic prescription medication is often that of patient health.

If you have ever taken a generic prescription medication, you need to read this book, especially if you take a generic prescription medication on a regular basis.

\*Disclosure: Katherine Eban spoke to a class I attended as a journalism student at NYU about her reporting on Ranbaxy, and the process by which she conducted her investigative reporting.

Jeanette S. Ferrara, MA

### How To: Absurd Scientific Advice for Common Real-World Problems

By Randall Munroe

ISBN: 978-0525537090

How To: Absurd Scientific Advice for Common Real-World Problems, is the latest work from the mind of Randall Munroe, perhaps

best known for his hysterical online comic strip xkcd. If you are a fan of Munroe's comics, you will certainly enjoy this book. It combines Munroe's iconic comic style with very scientific pseudo self-help advice.

Mostly, Munroe takes real-world problems and

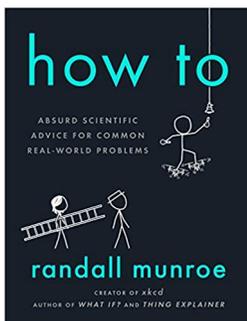
scenarios, and performs a reverse *reductio ad absurdum*, presenting the reader with the most absurd yet scientifically sound solutions to some terribly banal inquiries. Would they work in actuality? Possibly not, but they work in theory—and make for wildly entertaining hypothetical scenarios bolstered by delightfully sarcastic comic illustrations.

Some of the highlights include “How to Throw a Pool Party,” “How to Move,” “How to Play Tag,” and “How to Build a Lava Moat.” If you are thinking “one of these is not like the others,” you are correct. “How to Build a Lava Moat” is an example of one of the chapters that answered a question I don't imagine most readers would have even thought to ask, although the resulting response is highly entertaining. “How to Throw a Pool Party” was quite hilarious as well, as it operated under the initial assumption that one does not necessarily have a pool and needs to build one before hosting a party in it.

However, the absolute best chapter was “How to Make an Emergency Landing.” For this section, Munroe conducted a question and answer series with test pilot and astronaut Chris Hadfield. The contrast between Munroe's increasingly absurd queries, which include among others, “How to Land on a Farm,” “How to Land on an Aircraft Carrier,” “How to Land on a Hostile Aircraft Carrier,” and “How to Land a Space Shuttle in Downtown LA,” and Hadfield's serious and scientifically sound expert responses, makes for a wildly entertaining departure from the typical format Munroe follows in his other chapters.

All in all, the book is a wonderfully comedic approach to everyday self-help grounded in very real but very absurd scientific solutions.

Jeanette S. Ferrara, MA





**Making Black Scientists: A Call to Action**

By Marybeth Gasman and Thai-Huy Nguyen

ISBN: 978-0674916586

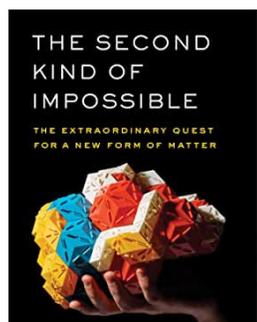
Making Black Scientists: A Call to Action is just that—a call to action for educators both at the collegiate and pre-collegiate level to cultivate black scientists. The book’s structure mirrors that of a typical graduate dissertation but an incredibly well-written and well-researched one at that.

Gasman and Nguyen investigate the education system, and where it fails in encouraging black students to pursue coursework in the sciences. But, and perhaps most importantly, they also investigate instances of the education system’s successes. In particular, they take a deep dive into 10 Historic Black Colleges and Universities, also known as HBCUs.

These colleges and universities at one point were the only institutions of higher knowledge that sought to admit and educate black students. By following their exceptional examples for educating and cultivating all black students, especially those interested in the sciences, other non-HBCUs can hopefully increase the number of black scientists who pass through their gates.

Science, like politics, literature, or any other field, benefits from diversity. Making more black scientists can only broaden the potential for achievement in the field.

*Jeanette S. Ferrara, MA*



**The Second Kind of Impossible: The Extraordinary Quest for a New Form of Matter**

Paul J. Steinhardt

ISBN 978-1-4767-2992-3

The Second Kind of Impossible starts with Paul J. Steinhardt’s 2011 expedition to the Kamchatka Peninsula in Russia.

Being swarmed by mosquitoes and traipsing through muck while conducting research out in the field sounds like a typical day in the life of a wildlife biologist—not a renowned Princeton physics professor such as Steinhardt. Already, by page 2, he has the reader hooked—what on Earth was he doing there, and what was he looking for?

Steinhardt then hits rewind, taking his reader back 35 years to a presentation he gave at his alma mater, Caltech. He and his colleague, Dov Levine, had theoretically invented a new type of matter. Richard Feynman, one of Steinhardt’s former professors and a member of the audience, boomed that the theory was “impossible.”

Here, Steinhardt takes another step back, explaining his personal history with Feynman as a professor, and his realization “that “impossible,” when used by Feynman, did not necessarily mean “unachievable” or “ridiculous”—sometimes it just meant “wow!” (Steinhardt 12). All this to say, Steinhardt’s presentation of “quasicrystals” violated the very laws of physics Feynman taught in his famous lectures—and Feynman was duly impressed.

Before moving forward with his quest to solve the quasicrystal mystery, Steinhardt takes another slightly larger step back, to France in the late 1700s. He lays the foundation for his story, introducing his readers to René Just Haüy, a French priest whose studies of various minerals and their physical structures earned him the moniker “The Father of Modern Crystallography.”

Steinhardt also includes some helpful illustrations and detailed but digestible explanations of the fundamentals and history of crystallography in these early pages. Any crystallographer could skim over these parts, but for someone less familiar with the field, Steinhardt’s clear tone and helpful descriptions early on make the narrative easy to keep up with later in the book.

One of the interesting early segues in Steinhardt’s book involves Dan Shechtman, who won the Nobel Prize in 2011 for the experimental proof of quasicrystals. Shechtman was working in a Maryland laboratory in the early 1980s when he discovered five-fold symmetry in a synthetic aluminum alloy—

around the same time that Steinhardt was working on his theoretical explanation. But the two men were unaware of each other's research at the time. Shechtman's discovery was determined "impossible" and his paper was rejected by The Journal of Applied Physics. Steinhardt laments "if there had ever been any exchange between our two teams there is a good chance we would have joined forces and presented the theory and experiment together" (Steinhardt 79). However, if that had been the case, this would be a very different story.

The rest of the book follows Steinhardt's research into naturally-occurring quasicrystals, spanning more than three decades. Quasicrystals, whether natural or man-made, break those fundamental laws Steinhardt laid out so eloquently in his first 25 pages.

The Second Kind of Impossible is a must read. Even if you have no interest in quasicrystals or five-fold crystalline structures, Steinhardt's book is a delight. The 364-page book reads like a novel--and a past-faced, well-written one at that. Steinhardt manages to maintain a quick and thrilling pace without skimping on the science behind the story.

Jeanette S. Ferrara, MA

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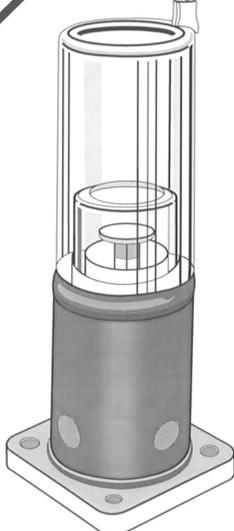
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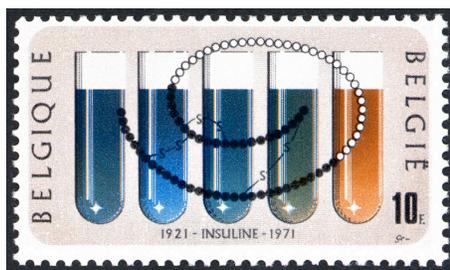

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## Dorothy Hodgkin's Magnum Opus

As far as science anniversaries go, there's plenty to celebrate in 2019. It is Alexander von Humboldt's 250<sup>th</sup> birthday and the 50<sup>th</sup> anniversary of the Nobel Prize in Physics awarded to Murray Gell-Mann (who passed away a few months ago) "for his contributions and discoveries concerning the classification of elementary particles and their interactions". Chemistry milestones include the discovery of phosphorus by Hennig Brand 350 years ago, the 150<sup>th</sup> anniversary of the introduction of the periodic system by Dmitri Mendeleev, and the birth centennial of Primo Levi, author of *The Periodic Table*, a collection of short stories inspired by various episodes of his life, including nearly a year as a prisoner in Auschwitz.

Readers of *RefleXions* may recognize 1969 as the year when the legendary Dorothy Crowfoot Hodgkin (1910-1994) published her seminal paper describing the crystal structure of insulin, the hormone that regulates the absorption of glucose into liver, fat, and skeletal muscle cells (M.J. Adams *et al.*, *Nature* **1969**, 224, 491-495). This was the successful conclusion to an effort that started almost 35 years earlier, shortly after the beginning of her independent career at the University of Oxford in 1934. In the intervening years, Hodgkin solved the molecular structures of several important biomolecules, including penicillin (1945) and vitamin B<sub>12</sub> (1955), and was honored with the 1964 Nobel Prize in Chemistry "for her determinations by X-ray techniques of the structures of important biochemical substances".



But let's go back to the insulin story. Discovered by Frederick Banting, Charles Best, and colleagues at the University of Toronto in 1921, and first crystallized by John Abel in 1926, insulin was a molecule of unprecedented complexity in 1934. In fact, the primary structure of insulin, which consisted of two amino acid chains linked by two disulfide bonds, was only established in the early 1950's by the British biochemist Frederick Sanger (1918-2013) who, incidentally, is the only recipient of two Nobel Prizes in Chemistry (in 1958 and 1980). In any event, the development of the isomorphous replacement method by Max Perutz and John Kendrew in the 1960's provided much-needed impetus to the project and Hodgkin finally put all the pieces of the puzzle together 50 years ago.

*Daniel Rabinovich*

## PUZZLE CORNER



For this issue, we have a new DISORDERED puzzle and a Crystoquote, along with the solutions to the previous puzzles.

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

Frank Fronczek  
ffroncz@lsu.edu

### ***Crystoquote #6:***

*Letter substitution reveals a quote by a well-known crystallographer*

***XEYDO Y ZYZ FGV HFGX ZYJH BRUCE XODD, Y JRF VOCVYKM***

***VERV EO BOFVGUOZ BM JRUOOU, KUGB RKRU, XYVE EYC***

***JRUOKLD XGUH GF VEO JGUUOJVYGF, RFZ CGBO RBRPYFADM***

***JRUOKLD CVULJVLURD XGUH, QOUM GKVOF XYVE R BOCCRAO***

***KGU DORUFYFA R FOX VEGLAEV GU VUYJH!***

***IULJO KGNBRF***

### ***Solution to Crystoquote #5:***

***There was always the possibility that Nature would provide a surprise to the investigator.***

Linus Pauling

***Martha Teeter and Diane Dickie provided the solution to the bad habit DISORDERED puzzle.***

***Diane Dickie also solved Crystoquote #5***

## Winter 2019 DISORDERED Puzzle

### DISORDERED

These words have drifted apart.  
Reassemble them to obtain high quality

TIVYRAG	○	○	□	□	□	□	
INEPTOR	○	○	○	□	□	□	
VECCTON	○	□	□	□	□	○	
CHOSKEN	○	○	□	□	□	○	
GRUBOPUS	□	□	□	□	○	○	○



Answer:

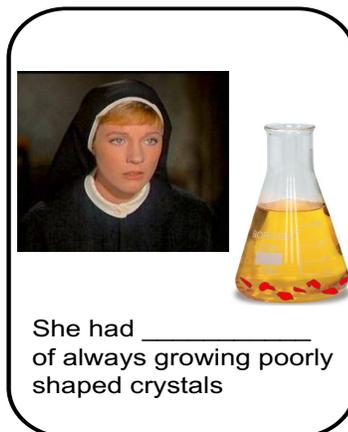
□	□	□	□	□	□	□	□	□	□	□	□	□	□
---	---	---	---	---	---	---	---	---	---	---	---	---	---

## Solution to Fall 2019 DISORDERED Puzzle

### DISORDERED

Recrystallize these distorted words into nicer forms

SIMPR	P	R	○	S	M				
HALTS	L	○	○	○	S				
BULODIAC	C	U	○	O	I	D	○	A	L
ELENDE	N	E	○	D	L	E			
KBOCL	○	L	○	C	K				
DELAB	B	L	○	D	E				



Answer:

A	B	A	D	H	A	B	I	T
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**January 2020**

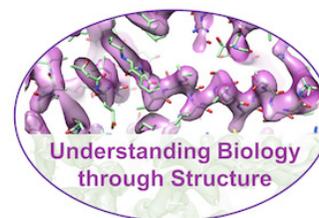
- 7-9 **CCP4 Study Weekend 2020, Nottingham, United Kingdom**  
<https://tinyurl.com/ccp4sw2020>
- 28-30 **7th BioXFEL International Conference, San Juan, Puerto Rico**  
<https://www.bioxfel.org/events/details/1218>

**February 2020**

- 15-19 **Biophysical Society Annual Meeting, San Diego, CA**  
<https://conference.sns.gov/event/78/>

**March 2019**

- 16 - 20 **Understanding Biology through Structure, Santa Fe, NM**  
<https://cvent.me/4kq9P>
- 30 - 4 Apr **2020 edition of RapiData at SSRL, Menlo Park, CA**  
<http://smb.slac.stanford.edu/news/rapidata/rapidata-2020/>

**April 2020**

- 13-17 **Materials Research Society Spring Meeting, Phoenix, AZ**  
<https://www.mrs.org/spring2020>

**May 2020**

- 26-30 **17th European Powder Diffraction Conference (EPDIC17), Šibenik, Croatia**  
<https://www.epdic17.org>

**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>



### Diamond Level: \$2,200

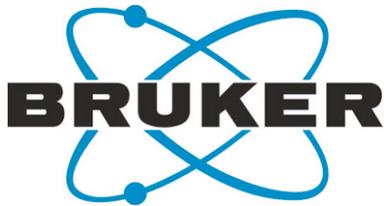


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