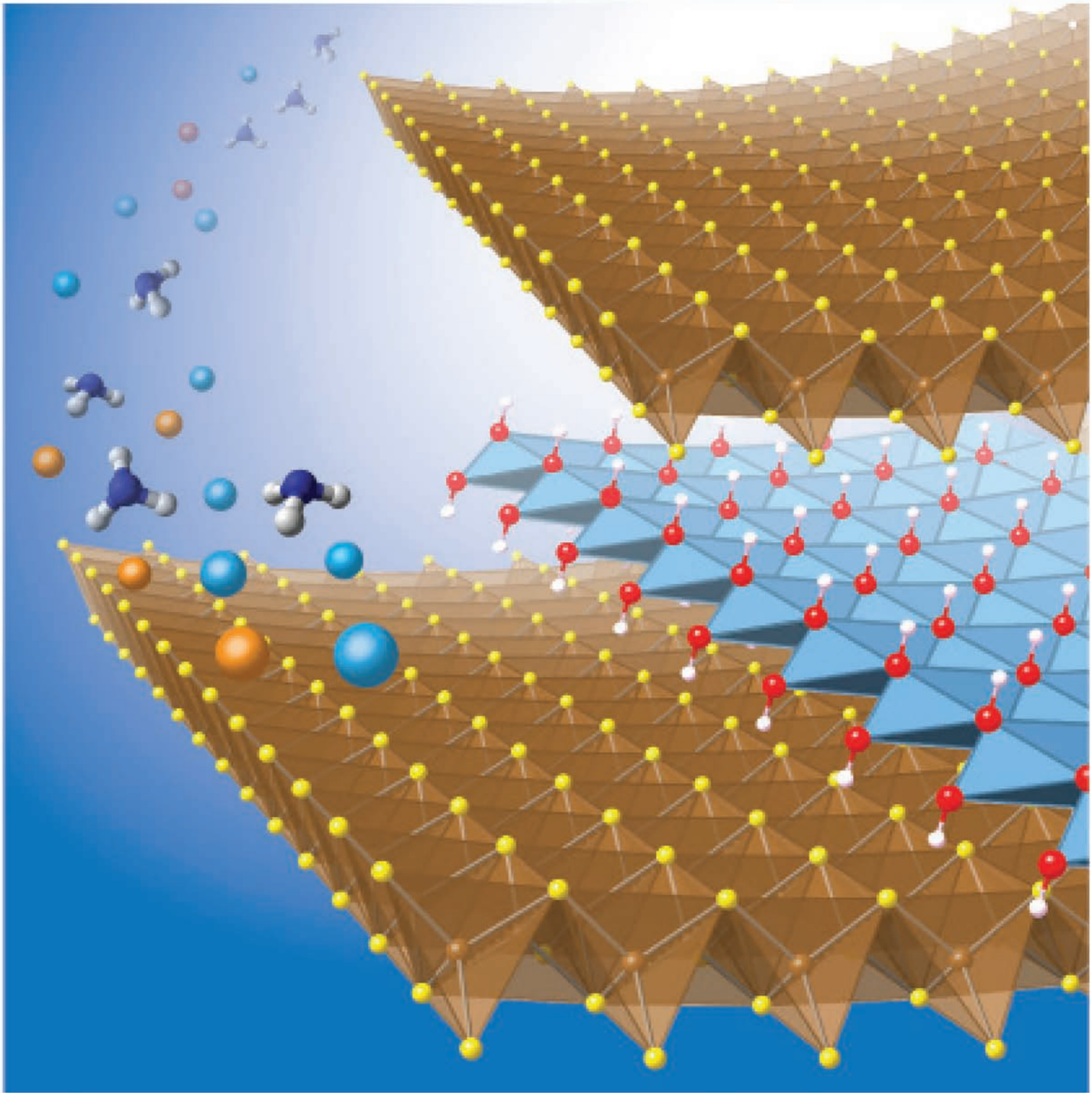
ACA RefleXions

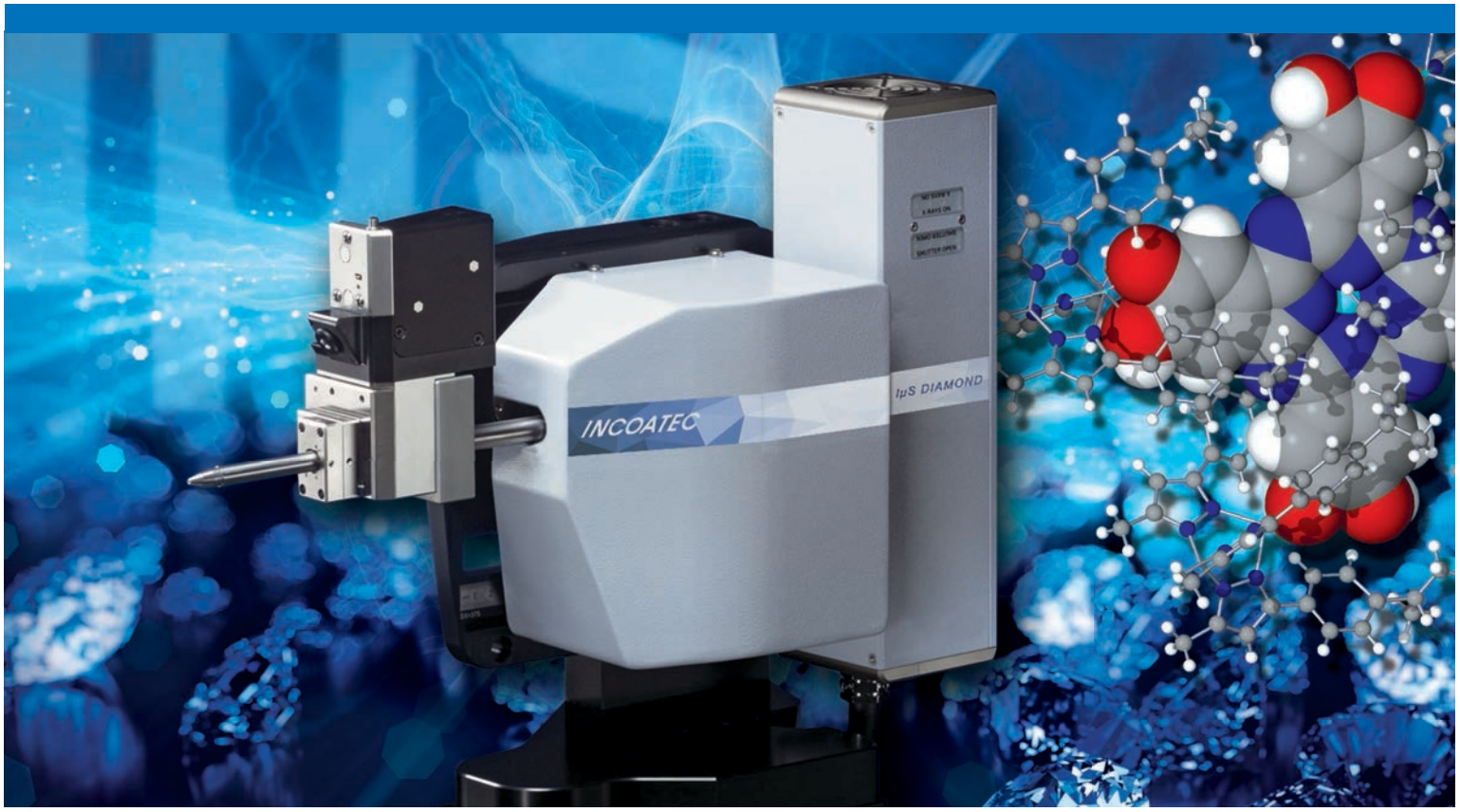
American Crystallographic Association
Structure Matters

Number 2

Summer 2019



Etter Early Career Award in Covington, KY



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ACA RefleXions

ACA - Structure Matters

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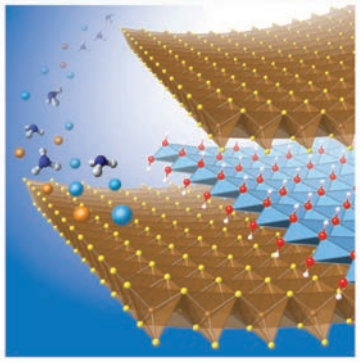
Joseph Ferrara
2019 ACA President

What's on the Cover?
The image at right is from Efrain Rodriguez, the 2019 Etter Early Career Award Winner. See page 6 for details.



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Bryan Chakoumakos
Bau Award

Efrain Rodriguez
Etter Award

Eaton Lattman
Frankuchen Award

Brian Toby
Trueblood Award

Robert Von Dreele
Trueblood Award

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Deadlines for contributions to *ACA RefleXions* are: February 1 (Spring), May 1 (Summer), August 1 (Fall), and November 1 (Winter)

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President's Column

Joseph Ferrara

By the time you read this, we'll be in the final weeks leading to the 2019 Annual Meeting in Covington. We have an excellent program planned and I encourage you to join. I can't remember the last time we had the banquet on a river boat; this year we will and I expect it will be a lot of fun. The band, Trailer Park Floosies, has a broad range of music in their repertoire. Above all, the Annual Meeting is an opportunity to network with colleagues and is one of the most important benefits the ACA provides.

I mentioned in my last column that we were exploring bystander training. Council has engaged Nancy Watt to provide this training before the start of the annual meeting and work with a group of about 40 people including: Council, staff, Meeting Committee, Poster Chairs, YSIG leaders and select vendors. This is just the first step to make our meetings a safe place for everyone. We realize that others may wish to participate but that is not possible at this time. We will explore ways to allow more members to participate in this type of exercise.

The ACA has also joined The Societies Consortium On Sexual Harassment In STEMM (Science, Technology, Engineering, Mathematics and Medicine) as a founding member. The consortium provides member societies a set of tools and resources to promote professional and ethical conduct, climate and culture. The tools and resources will take a year or so to be fully developed and Council looks forward to their availability.

At the April Council meeting we formed an *ad hoc* committee for Strategic Planning to be chaired by Lisa Keefe. The committee will formulate and execute strategic planning. One of the problems with strategic planning in the ACA has been a lack of continuity. In order to ensure continuity, our intent is that this committee will be reformed each year by the current ACA president and chaired by the current past president. So, VP nominees, bear in mind that you will be making a long-term commitment to the future of the ACA.

At the Council meeting we also took some time to engage in a 6-3-5 brainstorming. In this exercise groups of six people gather and everyone writes down three problem solving ideas in five minutes and passes the sheet to the next person. This is repeated a total of 6 times. The result can be up to 108 new ideas, or fewer ideas that build upon previous entries. However, everyone's first idea is equally weighted. This would be difficult to perform at the enterprise level but I may try to schedule this for some smaller groups. I want to capture everyone's input and we will have a suggestion box at the registration desk.

Later in the issue you will see that the first Judith Flippen Anderson Structural Dynamics Poster Prize was awarded at the British Crystallographic Association held in April in Nottingham. In other news about Structural Dynamics, George Phillips, John Helliwell, Majed Chergui and Council were successful in convincing American Institute of Physics Publishing (AIPP) to require PDB Validation Reports for structural work presented in Structural Dynamics. This brings our publication in line with other high profile publications.

From May 4 through May 7 Lisa, Brian and I participated in the Council of Scientific Society Presidents Spring Workshop. This group is made of a number of society presidents across a broad range of science at various stages in their tenure. CSSP provides a mechanism for support for society presidents and advocates for science in government. I find the sessions on Best Practices and Ethics to be most helpful. All of us were very motivated by the last session this year, which was titled "Changing the Framework of the Conversation: Gender inclusivity in a wide variety of sciences can and should be incorporated in both research and behavior". This session and the discussion afterwards reinforced the need to continue with our plan for bystander training and our participation in the Sciences Consortium in order to ensure that the ACA provides a safe space for all our members.

In this issue we have the statements for all the candidates running for office in the fall. Please take a few moments to peruse them and remember to vote in the fall.

Joe Ferrara

2018 Fall ACA Council Meeting Highlights

Diana Tomchick

Teleconference meetings were held in the months of November and December 2018, and January, February and March 2019. In order to fast track the new Council members for 2019 (Brian Toby as Vice President and Ilia Guzei as Treasurer), they were invited to join the November and December meetings along with the then current officers for 2018. The November teleconference focused primarily on a review of 2018 income and expenditures and an introduction of new accounting practices. Kristin Stevens will provide in-house accounting under the supervision of ACA Chief Financial Officer S.N. Rao, and a different accounting firm will be enlisted for filing taxes and performing audits. These changes are expected to save $10,000 – 15,000 per year. The December teleconference focused on approval of an update to the ACA Handbook (Secretary's note: this is the handbook that outlines the duties and responsibilities of Council members, SIG and Committee officers, requirements for Annual Meetings, and so much more.), approval of the ACA 2019 budget and online advertisement rates for the new ACA web site as well as approval of the preliminary program and workshops for the 2019 ACA Annual Meeting. At the January meeting, Council reviewed the accounting changes and updates on the progress of the ACA 2019 Annual Meeting. The February teleconference focused on inclusion and diversity issues, and it was decided that professional bystander training for intervention in harassment incidents would be conducted on-site in Covington prior to the 2019 Annual Meeting in July. The training would include members of ACA Council, the Annual Meeting Program Chairs, ACA staff, and as many people deemed responsible parties for the ACA Annual Meeting. President Joe Ferrara reported that he had met via teleconference with SIG and Committee officers in order to clarify expected duties and answer questions. Topics of discussion for the March Teleconference included the pros and cons of an early abstract deadline versus a hard deadline for future ACA Annual Meetings, ACA Summer School proposals and how to encourage ACA members to provide nominations for awards.

The 2019 Spring Council Meeting was held at Hauptmann-Woodward Institute (HWI) in Buffalo, NY on April 11. Voting members in attendance were President Joe Ferrara, Vice President Brian Toby, Treasurer Sue Byram, Past President Lisa Keefe, Canadian Representative Tomislav Friščić 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 CFO S.N. Rao. Visitors included Stephan Ginnell (2019 Annual Meeting Program Co-Chair) and John Haynes (American Institute of Physics Publishing CEO).

Stephan Ginnell reported that preparations for the annual meeting in 2019 in Cincinnati/northern Kentucky are well underway, and there was much discussion regarding how to handle abstract submission deadlines for future meetings. The relatively large gap of time between the deadline and the actual meeting has been dictated in the past by the requirement to format a meeting booklet. A decision was made that for future meetings (starting in 2020), instead of providing a printed meeting booklet a mobile meeting app as well as a PDF file of abstracts would be made available for download prior to the meeting. A discussion of methods for publicizing the meeting in various venues, including web sites, email list serves, social media, etc. and various Council members volunteered to assist the ACA Headquarters with this effort.

ACA Treasurer Ilia Guzei reported that the annual meeting will need 421 regular attendees to break even, and the current target is 450. He reported a 30% reduction in revenue from exhibitors, and Council members were tasked with providing a list of potential exhibitors to solicit for the meeting.

President Joe Ferrara announced that Thomas Koetzle has agreed to be the ACA Representative to the AIP Publishing (AIPP) board; John Rose has indicated that the first draft of submissions for the 2019 ACA Annual Meeting Transactions, "Data Best Practices: Current State and Future Needs" should be delivered for publication to *Structural Dynamics* at the end of the 2019 Annual Meeting; Ferrara has discussed with Majed Chergui, editor of *Structural Dynamics*, the possibility of special issues on the subjects of "XFELS and Material Science" and "Time-Resolved ED and EM"; Ferrara attended the AIP Assembly of Society Officers with Brian Toby and met with various AIP officials to discuss matters related to outreach, strategic planning, and membership increase. Ferrara, Toby and Keefe will attend the Council of Science Society Presidents Spring Leadership Workshop in May.

Vice President Brian Toby discussed his attendance along with President Joe Ferrara at the American Institute of Physics Annual Meeting on March 28, 2019. He observed that many of the other 9 member societies have a closer relationship with AIP, perhaps based on physical proximity to AIP headquarters and to exchange of staff. He suggested for the ACA to make the best use of AIP would be to establish a liaison that spans a 5-10 year time period with a plan for overlap of the successor to this position.

Past President Lisa Keefe presented a proposal to include a role description and list of responsibilities for the Past President in the ACA Handbook. The suggested responsibilities include working with an ad-hoc Strategic Planning, Oversight & Assessment Committee; working with an ad-hoc Awards Oversight Committee; and updating the ACA Handbook with issues pertaining to policy, roles and responsibilities. Keefe will draft a formal proposal on this matter to be submitted to Council for a vote at a later meeting. Keefe also reviewed the discussion over the past year of the ACA President, Vice President and Past President with the AIP to provide funding for the ACA's need for strategic planning. Potential mechanisms for funding of a strategic planning initiative include the AIP Venture Partnership Fund (VPF) or via cost-sharing with other AIP member societies. Keefe recommended that the Past President chair an ad hoc Strategic Planning Committee which would be tasked with drafting membership surveys, revising a VPF proposal and working with AIP to achieve a collaborative approach to strategic planning.

Tomislav Friščić, the Canadian Representative, provided a preview of future 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; and the 102nd Annual Meeting of the Canadian Society of Chemistry, Québec City, June 3 - 7, 2019. The Canadian National Committee for Crystallography has awarded the first set of Larry Calvert Travel Awards, which assist Canadian students, postdocs and researchers to attend crystallography-related conferences; the next application deadline is June 30, 2019.

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 and is getting excellent reviews; the support of the IUCr Outreach and Education Fund of initiatives in Africa, the IUCr-UNESCO OpenLabs and crystallographic schools around the world; the 2019 IUCr Crystal growing competition for schoolchildren is now open; and Prague, Czech Republic will host the 25th IUCr Congress from August 22-30, 2020. The next IUCr Executive Council (EC) meeting will be held prior to the ACA Meeting in Covington, Kentucky, July 2019. Members of the ACA Council will meet with the EC on Friday, July 19, and members of the EC will attend the ACA Summer Council meeting on Saturday, July 20.

Highlights of the report from George Lountos, the Young Scientists Interest Group (YSIG) representative, included a summary of the planned events the YSIG will sponsor during the 2019 meeting. These include a Saturday afternoon Career Development workshop, A First Time Attendee meeting, a Three Minute Thesis Competition, a "Structure without Structure" Session as the inaugural *Structural Dynamics* session, the YSIG Mixer and co-sponsorship of several scientific sessions.

The AIP Publishing CEO, John Haynes, spoke to Council about the challenges of transitioning from a purely "pay to read" to "pay to publish" for the AIPP. Currently 1/3 of journals published by AIPP are 100% open access, while 2/3 are hybrid, where some articles are pay to read and others are open access. The ACA's journal *Structural Dynamics* is 100% open access. The AIPP is looking for growth in an eBook program, with books written at the chapter level, being more tutorial or pedagogically focused, with a target audience of scientists looking to broaden into new fields. The books will be sold as an electronic only database, and users will be able to print on demand. The AIPP also organizes the ACA Annual Meeting exhibition, by providing a permanent staff member that functions as the head of technical exhibits. For many years this was Bob Finnegan, and he is undergoing a partial retirement, but will still be working with his replacement, Dan Cook. Kristen Stevens has been working with Dan Cook on ways to modernize relations with the vendors, corporate partnerships, etc. Haynes described a low or no-cost membership new/renewal campaign that could be conducted by including an advertisement on a PDF cover page that would be included on all downloaded article PDFs from Structural Dynamics.

After the meeting was adjourned, Council participated in a brainstorming session wherein they wrote down suggestions for two topics: Improving Member Renewal and Improving Meeting Attendance. These suggestions were forwarded to the Finance Committee for discussion at a later date, and Council will review these at the next teleconference meeting to be held on June 20, 2019.

Highlights of the May teleconference included a review of various items of Old Business from the Spring Council Meeting, a financial update from Treasurer Ilia Guzei, an update on the 2019 Annual Meeting and a discussion of a member survey created by Vice President Brian Toby, that will be distributed electronically prior to the 2019 Annual Meeting.

The next in-person Council meeting will occur in Covington, KY on Saturday, July 20, 2019 at the 2019 ACA Annual Meeting.

Diana Tomchick

Contributors to this Issue

Eddy Arnold, Gerald Audette, Jason Benedict, Rajni Bhardwaj, John Bollinger, Paul Boyle, Stephen Burley, Sue Byram, Indranil Chakraborty, Jeanette Ferrara, Joseph Ferrara, Frank Fronczek, Ilia Guzei, John Helliwell, Brandon Mercado, Virginia Pett, Vanessa Reitz, David Rose, John Rose, Connie Rajnak, Amy Sarjeant, Dmitriy Soldatov, Ed Stevens, Diana Tomchick, Nick Vukotic, Suzanna Ward, B. C. Wang, Christine Zardecki

American Crystallographic Association, Inc.

Statement of Financial Position
December 31, 2018 and 2017

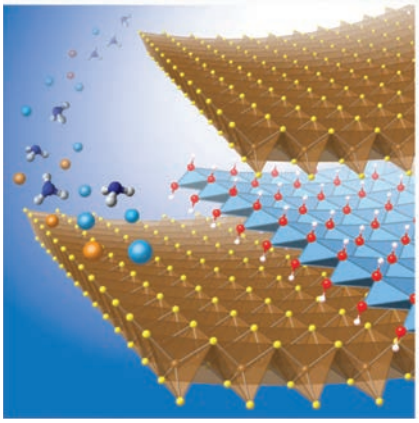
Assets	2018	2017
Cash and Cash Equivalents	$103,628	$120,057
Investments	$945,507	$1,035,465
Other Assets	$39,130	$0
Total Assets	**$1,194,220**	**$1,205,814**
Liabilities and Net Assets		
Unearned Revenues	$56,255	$57,730
Other Liabilities	$10	$2,491
Uncashed Checks	$9,926	$22,022
Total liabilities	**$66,191**	**$82,243**
Net assets- Unrestricted	$458,975	$508,502
Net Assets - Restricted	$563,153	$565,270
Total liabilities and net assets	**$1,088,319**	**$1,156,015**

Restricted Fund Balances

(as of December 31, 2018)

Bau award	$36,494
Buerger Award	$38,978
Rognlie Award	$60,000
Etter Award	$69,509
Fankuchen Award	$71,343
Patterson Award	$48,786
Pauling Award	$39,135
Student Travel Award	$23,006
Supper Award	$12,661
Trueblood Award	$40,459
Warren Award	$31,549
Wood Award	$54,211
TOTAL	$526,131

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0906. You may also request this information using the 'contact us' form on the ACA website, or email directly to kvitale@hwi.buffalo.edu.



On the Cover

The 2019 Margaret C. Etter Early Career Award will be presented by the ACA to Efrain E. Rodriguez, Associate Professor of Chemistry and Biochemistry at the University of Maryland, College Park. Efrain will present his lecture titled "Hydrogen Bonding and Symmetry Relationships in Quantum Materials" at 8:00 AM on Wednesday July 24 during the ACA Annual Meeting in Cincinnati/Northern Kentucky.

Efrain received his BS from the Massachusetts Institute of Technology and his PhD from the University of California, Santa Barbara. At UCSB Efrain worked with Anthony K. Cheetham, FRS, on the solid state chemistry of solids containing transition metals and their physical properties. His NSF CAREER Award centers on finding transition metal sulfides and understanding how their structures relate to their magnetic and super-conducting properties

At UMD Efrain has established a program in solid-state chemistry with a multidisciplinary approach for the preparation and study of functional inorganic materials. Efrain and his group study crystallography in order to establish structure-property relationships in materials, and his group heavily uses neutron and synchrotron X-ray diffraction techniques. A particular expertise of Efrain's group has been the use of neutrons to solve the magnetic structures of crystalline materials. Currently, Efrain is working on using crystallography and polararized neutron beams to study the phenomena of magnetoelectricity in metal phosphates with the olivine-type structure and metal silicates with the pyroxene-type structure. His group also uses in-situ synchrotron X-ray and neutron diffraction studies to understand the reactivity of extended solids under various chemical environments such as oxidizing and reducing environments and hydrothermal conditions

The cover image shows the intercalation chemistry of layered metal chalcogenides Efrain studies for the phenomenon of superconductivity. These layered materials consist of all edge-sharing FeS_4 or $FeSe_4$ tetrahedra, and since these layers are held together by van der Waals interactions, they can be intercalated by amines, metal amides, alkali and alkaline cations, and metal hydroxides. Efrain's hypothesis is that hydrogen bonding can assist in the intercalation chemistry of these materials. Many of these materials can be prepared by hydrothermal or solvothermal methods, and understanding their crystal growth remains an intense area of research for him. Furthermore, electron charge doping from the cationic intercalates into the FeS or FeSe layers can drastically affect the bonding and physical properties of these superconductors. A larger implication of having hydrogen bonding direct the stacking of these metals chalcogenides is that it suggests a way to pursue materials design for the stacking of 2D inorganic solids.

Beyond his academic interests, Efrain likes to read the history of chemistry, Western philosophy, art, and literature. He is particularly interested in the philosophy of matter and change in the pre-socratic philosophers of Greece. Efrain also works on his bonsai collection and enjoys listening to music with his wife Mercedes Castelo and daughter Alicia.

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Connie Rajnak

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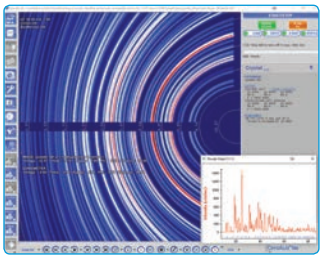

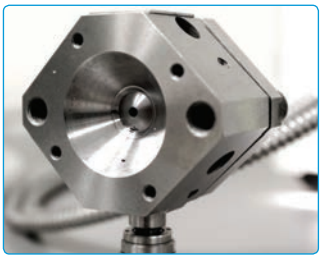

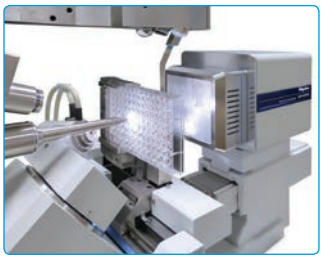

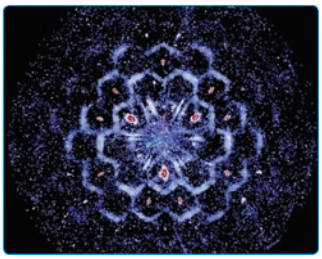

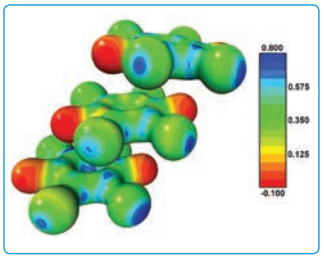

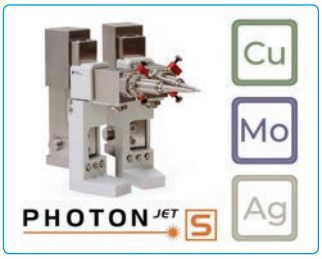

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ACA History Project Update

The new ACA History pages are live! Go to the ACA homepage and click on History in the main menu at the far right.

As readers of this column know, it's been a long process to complete the migration to the new web hosting provider. Kristin Stevens, ACA Director of Administrative Services, and Vanessa Reitz, the ACA History Webmaster, took the lead in negotiating with MemberClicks on pricing and style changes. A $400 upcharge gave the ACA History pages a separate menu structure similar to the previous History pages, and MemberClicks imported the rest of the previous History pages. The History pages now have a distinctive layout and menu structure, the missing pages have been restored, and broken links are being repaired as they are discovered. If you make use of the Donate button on the ACA History Home page, it will be greatly appreciated!

Helen Berman

When you visit the ACA History page, scroll down to the Latest Additions. You will see that we've added some new videos. Helen Berman's 2006 Buerger Award presentation, "A Personal Journey Through Structure Space" is now linked on the new ACA History Home page. Also, the two-part Symposium in Honor of Bill Duax at the 2017 IUCr Congress in Hyderabad is once again available.

Bill Duax

John Spence's 2012 Buerger Award lecture, "The Future of Diffraction Physics in Crystallography" is noteworthy for his discussion of XFEL, lensless imaging and serial femtosecond nanocrystallography. The quality of the sample and radiation damage are the two factors that limit the quality of the diffraction data, he said. If the radiation pulse is brief enough, diffraction data are not contaminated by sample degradation. "It's just a matter of how many photons you can pack into the pulse. That is the main point of my talk."

John Spence

The ACA has bought a MacBook Pro computer and Camtasia presentation software. The Camtasia software was suggested by Brian Toby and Amy Sarjeant as a convenient way to record Award and Plenary presentations at ACA Annual Meetings. The software records what is shown on the computer screen – typically a PowerPoint presentation – and the speaker's voice from the computer microphone. If the speaker chooses to stand in front of the computer camera the speaker's face is also captured. Just to be sure, Dick Bromund and I will also be videorecording the speaker and the projection screen with the two ACA video cameras at the Cincinnati meeting.

John Spence's lecture, described above, was not recorded with Camtasia, but with a single camera that recorded both speaker and projection screen. I tested the editing capabilities of the Camtasia software in producing the video. The new software is capable and user friendly, and I was able to edit the frame to juxtapose the speaker and the projection screen, omitting the unused lectern in the center of the frame.

Virginia Pett
pett@wooster.edu

Press release:

Big data leads the way for structural chemistry

The Cambridge Structural Database reaches one million structures, leading the way in structural data to inform drug discovery and materials development

Cambridge UK, 6 June 2019. CCDC (The Cambridge Crystallographic Data Centre), world-leading experts in structural chemistry data, software and knowledge for materials and life science research and application, today announced a huge milestone for structural chemistry with the addition of the millionth structure into the Cambridge Structural Database (CSD).

The CSD is the world's repository of highly curated experimentally determined organic and metal-organic crystal structures. It is used globally by scientists in over 70 countries to understand how molecules behave and interact in three dimensions in the solid form and ultimately how this affects physical properties.

As the interest in 'Big Data' continues to grow in a time where machine learning and automation are changing the way pharmaceutical, agrochemical and many other industries work, reaching such a significant milestone is a huge achievement for the CCDC and the wider scientific community that contribute to and rely on this resource.

Large volumes of data such as this enable scientists to generate more replete answers from a more complete and diverse volume of information, ensuring confidence in the insights being drawn from the data. Furthermore, CCDC's focus on ensuring the integrity of the data within the CSD through stringent quality assurance and control steps adds even more value and confidence that scientists are obtaining the highest quality information to inform their research.

This rich data resource, alongside advanced search, 3-D data mining, analysis and visualisation software from CCDC enables scientists from both industry and academia to further their research and predict new outcomes. In addition, knowledge derived from the CSD underpins computational chemistry and molecular modelling and is relied on by industry for the development and manufacturing of new drugs and within academia to teach chemistry.

Dr Jürgen Harter, CEO of CCDC commented, 'This is truly an important milestone not only for CCDC but also for the wider scientific community. In addition to the value that lies in large sets of data like this to help scientists inform their research and decision making, we also pride ourselves on the high quality of the data, a result of the hard work of our expert in-house database team. Maintaining a policy of strict data interrogation ensures the value of the plentiful insights that can be drawn from the CSD, avoiding misinformation that can lead to wasted time, resources and ultimately cost.'

CCDC have announced the 1,000,000th structure to be a N-heterocycle produced by a chalcogen bonding catalyst activating multiple reactions steps sequentially. In the paper the authors describe a class of extraordinary chalcogen-bonding catalysts which enable the assembly of discrete small molecules leading to the construction of N-heterocycles in a highly efficient manner. The structure was determined by Yao Wang and co-authors from Shandong University in China and published in the Journal of the American Chemical Society (JACS).

'We'd like to congratulate Yao Wang and all of his co-authors, for publishing the millionth structure and we are so grateful to the 350,000 plus scientists from around the world that have contributed their data, enabling us to reach this milestone and placing CSD as the go-to resource for structural information within the scientific community', **said Suzanna Ward, Head of the CSD.**

Dr Wang commented 'We are delighted to hear that our structure (1-(7,9-diacetyl-11-methyl-6H-azepino[1,2-a]indol-6-yl)propan-2-one; CSD Refcode XOPCAJ) is the millionth structure to enter the CSD! We have used the CSD for over ten years because it is an excellent platform to report new crystal structures and an outstanding database to find inspirable chemical structures. It is a valuable resource to us and to many other scientists around the world so we are very proud to be associated with this milestone for the community.'

Peter Stang, Editor-in-Chief, JACS, said "We are delighted to hear that the millionth structure in the CSD was published in JACS. We know our readers value the CSD as a trusted repository of structural data and some of our authors have demonstrated how this rich resource can accelerate scientific research. Our continued collaboration with the CCDC helps make this wealth of data more accessible to the community as well as helping us ensure the integrity of data published in our journals and we are proud to be associated with such a significant milestone in structural chemistry."

When asked what's next for the CSD, Dr Harter commented that although the use of the CSD in the pharmaceutical and agrochemical industries is already well-established, it is now fast becoming a fundamental resource for research into new materials such as batteries, paints, pigments and dyes, and in particular the development of gas storage frameworks and tailored catalysts. As environmental contamination and sustainability become increasingly important there is considerable potential on a global scale.

CCDC have noted a consistent rise in deposits from research taking place in China over recent years.

"It is an exciting time for life science and materials development research with markets such as China leading the way in scientific discovery. We are excited to see what insights we obtain from this market going forward" **Dr Harter commented.**

CCDC also have plans to further draw on insights and trends from the data to inform the direction of future research across different industries

For more information visit: https://www.ccdc.cam.ac.uk/csd-1-million, or contact: Lucy White at l.white@ccdc.cam.ac.uk.

About CCDC

CCDC are world-leading experts in structural chemistry data, software and knowledge for materials and life science research and application.

They are dedicated to the advancement of chemistry and crystallography for the public benefit. They specialise in the collation, preservation and application of scientific structural data for use in pharmaceutical discovery, materials development and research and education.

CCDC compile and distribute the Cambridge Structural Database (CSD), a certified trusted database of fully curated and enhanced organic and metal-organic structures, used by researchers across the globe.

Their cutting-edge software empowers scientists to extract invaluable insights from the vast dataset, informing and accelerating their research & development.

One million thanks to the ACA Community

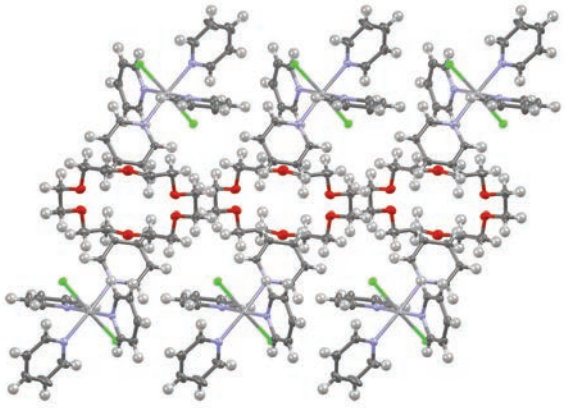
In June this year, the Cambridge Structural Database added its one millionth structure. Now that we have reached this impressive feat, we'd like to take the opportunity to thank the members of the ACA community who – in ways small and large – have contributed to this achievement. We would like to share with you some of the ways in which the many members of the ACA have helped us reach this milestone.

Frank Fronczek celebrating his 1000+ CSD Communications at the 2016 ACA meeting in Denver, CO.

The sharing of one million structures is a feat we could not have achieved on our own. Crystallographers from all around the globe have not only contributed data to the database but have also helped to shape the CSD into what it is today. Members of the ACA have had an incredible impact on this by depositing data, working for and with the CCDC, and by serving as leaders on our Board of Trustees. Of course, it would take over a million hours to list the very many people who have helped us on this journey, but we can reflect here on a few of the ways in which the ACA has supported the CSD.

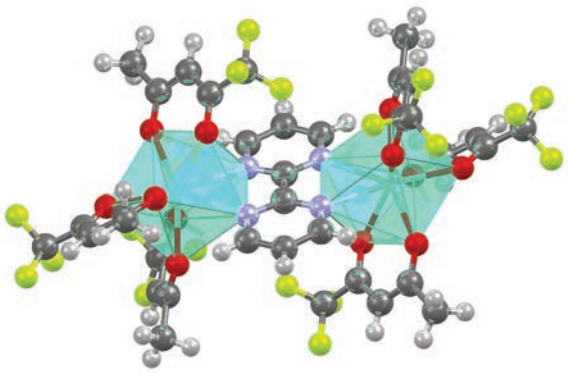
While the one millionth structure added to the CSD didn't come from North America, we are pleased to announce that it was Yao Wang and his team in China who deposited the milestone structure, XOPCAJ[1]. North Americans have contributed to other milestone structures over the years, including VAVFAZ (200,000th), EHUFUI (300,000th) and PATXEQ (900,000th). Over all this year, the US sits third in the list of countries publishing structures in 2019 to date with over 2,200 structures and Canada sits at eleventh, with around 500 structures. Combined, however, they sit at number two which is an impressive contribution from the ACA community as a whole.

One crystallographer from North America sits at number 3 in our all-time depositors list, Arnie Rheingold of UCSD. This year Arnie is leading the way in top authors publishing data in 2019, with a total of 169 structures at the time we sat down to write this. Another US crystallographer, Matt Zeller of Purdue cracked the top-ten author list for 2018 with 175. There's still time to get your name in the top 10 list for 2019! You can see these statistics and more on our website here: https://www.ccdc.cam.ac.uk/CCDCStats/Stats.



A packing diagram highlighting one of the beautiful structures (XOMKAO[2]) deposited by Peter Zavalij on CSD one million day.

On CSD one million day, we added over 550 other structures to the database. These included some from both the US (5th highest) and Canada (10th highest), which together accounted for over 65 structures deposited by 18 different individuals – who were all so close to being the millionth! A special mention goes to Peter Zavalij of the University of Maryland whose 18 CSD Communications added that day were just shy of being perfectly timed!



A structure (XOPLIA[3]) from Muralee Murugesu's group at the University of Ottawa, determined by Bulat Gabidullin and added to the database on CSD one million day.

We can't mention them all, but some other crystallographers from the ACA community who were tantalizingly close to CSD 1 million were Brandon Mercado, Charlotte Stern, Frank Fronczek, Joe Tanski, Bulat Gabidullin, Pat Carroll and Thierry Maris. All of these structures are special in their own unique ways and help contribute to the power and beauty of the CSD.

For those of you who are looking for more information on the structures added on CSD one million day, we will be publishing a series of blogs on our website in the coming. Check our website and social media posts to see which structures were in the mix and which other crystallographers were oh so close!

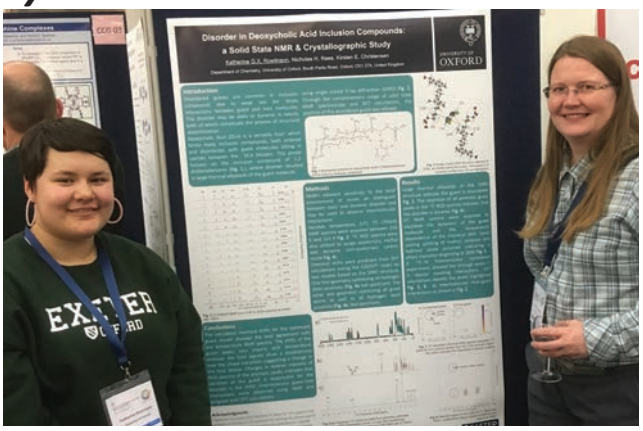
Suzanna Ward and Amy Sarjeant

1 Wei Wang, Haofu Zhu, ShuYa Liu, Zhiguo Zhao, Liang Zhang, Jingcheng Hao, Yao Wang, Journal of the American Chemical Society, 2019, 141, DOI: 10.1021/jacs.9b03806

2 Peter Y. Zavalij, Yi Wang, Bryan W. Eichhorn CCDC 1920997: Experimental Crystal Structure Determination, 2019, DOI: 10.5517/ccdc.csd.cc22gyn5

3 Dylan Errulat, Riccardo Marin, Diogo A. Gálico, Katie L. M. Harriman, Amélie Pialat, Bulat Gabidullin, Fernando Iikawa, Odilon D. D. Couto, Jani O. Moilanen, Eva Hemmer, Fernando A. Sigoli, Muralee Murugesu, ACS Central Science, 2019, 5, DOI: 10.1021/acscentsci.9b00288

Judith Flippen-Anderson Structural Dynamics Poster Prize at BCA 2019



The ACA Judith Flippen-Anderson journal of Structural Dynamics Poster Prize at BCA 2019 was awarded to Katherine Rowlinson (left) of the Chemistry Department, University of Oxford for her poster entitled "Disorder in deoxycholic acid inclusion compounds: a solid state NMR and crystallographic study". Along with DFT calculations, determination of the dynamics and binding position details of the guest in the host were achieved. Such a combination of methods was a frontier example of the study of chemical structure and dynamics, and carefully explained by Katherine in answers to questions from the judging panellists. The judges were John R Helliwell, UK as Chairman, Igor Levin, NIST, USA and Nori Yasuoka, Japan.

John R Helliwell

Michael G. Rossmann (1930-2019), pioneer in macromolecular and virus crystallograph: scientest and friend

Michael Rossmann with a virus model in 2018.

(photo courtesy of Roger Castells Graells)

Michael George Rossmann, who made monumental contributions to science, passed away peacefully in West Lafayette, Indiana, USA, on 14 May 2019 at the age of 88, following a courageous five-year battle with cancer. Michael was born in Frankfurt, Germany, on 30 July 1930. As a young boy, he emigrated to England with his mother just as World War II ignited. The eminent crystallographer Dame Kathleen Lonsdale helped him gain admittance to a Quaker School for his school studies (Sir John Meurig Thomas, personal communication) and also sparked his interest in crystallography. Michael was a highly innovative and energetic person, well known for his intensity, persistence and focus in pursuing his research goals. Michael was a towering figure in crystallography as a highly distinguished faculty member at Purdue University for 55 years. Michael made many seminal contributions to crystallography in a career that spanned the entirety of structural biology, beginning in the 1950s at Cambridge where the first protein structures were determined in the laboratories of Max Perutz (hemoglobin, 1960) and John Kendrew (myoglobin, 1958). Michael's work was central in establishing and defining the field of structural biology, which has described the structures of a amazing array of macromolecules and macromolecular assemblies, contributing to our understanding the basis of health and disease at the molecular level, and facilitating the discovery of many drugs.

1. Education in crystallography with J. Monteath Robertson and William N. Lipscomb

Michael had enormous impact on developing methodology for the determination of macromolecular crystal structures. His grasp of mathematics was always a strength, as he continually developed methods that would become part of the standard repertoire of macromolecular crystallographic tools. Michael obtained undergraduate degrees in mathematics and physics at the University of London. For his graduate work, he studied crystal structures of organic compounds with J. Monteath Robertson at the University of Glasgow. Following his graduate studies he was a postdoctoral fellow with William N. Lipscomb at the University of Minnesota, USA, pursuing structures of relatively complicated organic crystals. In his work at Minnesota, Michael wrote computer programs for crystal structure analysis, taking advantage of the new digital computers that would revolutionize the practice of crystallography. In a lecture by Dorothy Hodgkin at the Fourth IUCr Congress in Montreal in 1957, Michael learned about exciting work on the structure determination of hemoglobin by Max Perutz at Cambridge University. Michael wrote to Max and was given an offer to join the hemoglobin structure determination team.

2. First protein structures at Cambridge: hemoglobin with Max Perutz

Michael worked closely with Max Perutz and was instrumental in elucidating the hemoglobin structure by writing the computer programs required to solve and analyze these first structures, and by calculating the Fourier maps that gave rise to the hemoglobin structure. Max had been pursuing the crystal structure of hemoglobin since the late 1930s and was a protégé of Sir Lawrence Bragg, one of the giants of crystallography who had helped to create the field of X-ray crystallography with his father, Sir William Bragg. When Michael arrived at Cambridge he began to analyze the X-ray diffraction data that Max and Ann Cullis had collected for the native hemoglobin crystals and multiple heavy-atom derivatives.

He invented methods and created computer algorithms for reliable phasing using heavy-atom isomorphous replacement and the practical determination of protein structures. While processing and analyzing the existing heavy-atom derivative datasets, he developed the difference Patterson map using squared difference coefficients $(|F_{heavy}| - |F_{native}|)^2$ to assist in locating the relative positions of heavy atoms in the isomorphous datasets (Rossmann, 1960). Michael also applied similar considerations to locating heavy atoms using anomalous dispersion (Rossmann, 1961) and with David Blow developed the single isomorphous replacement method (Blow & Rossmann, 1961) and mathematical representations of combining phase information from multiple sources (Rossmann & Blow, 1961). By 1959, Michael had computed a 5.5 Å resolution electron-density map for hemoglobin that permitted a trace of the overall fold of this predominantly helical protein and revealed its three-dimensional relationship with myoglobin (Perutz et al., 1960).

3. Molecular replacement has become the most common method for solving macromolecular crystal structures

During his extraordinarily productive time at Cambridge, Michael also proposed and created

the foundations for the molecular replacement method, which became the predominant approach for solving three-dimensional structures of proteins and other large biological assemblies such as complex enzymes and viruses. Michael had been fascinated with what he learned from conversations with other scientists at Cambridge, often during afternoon tea. For example, Crick and Watson had hypothesized that viruses would contain many identical protein subunits based on considerations of their limited genomic capacity (Crick & Watson, 1956). Michael thought that the recurrence of biological structure in different environments, whether in a structure with multiple subunits (oligomeric enzymes, viruses *etc.*) or in different crystals, would provide information to help in phasing crystal structures. The monumental paper that Michael wrote together with David Blow (Rossmann & Blow, 1962) presented the rotation function as a method for demonstrating the presence of rotational non-crystallographic symmetry within a crystallographic asymmetric unit and determining relative orientations. Walter Hoppe (Hoppe, 1957) had also hinted at a convolution of a similar type to find the orientation of known molecular fragments and these ideas were implemented by Robert Huber (Huber, 1965). Michael developed the rotation function based on the realization that the Patterson function would produce multiple "peaks" where vector sets corresponding to the different orientations of the repeating units were coincident. He demonstrated its utility by detecting the relative orientation of the α and β chains in horse hemoglobin crystals. Later he and others would develop methods for locating the position of objects in crystals, so-called translation functions. He went on to champion these ideas, while along the way determining the structures of many crucial enzymes and viruses.

Currently, the molecular replacement method is the most common approach used for solving new macromolecular structures, accounting for some 85%+ of all new PDB structure depositions and the majority of all 150 000+ known structures. Molecular replacement is most frequently used to determine the orientation and location of related structures in new crystals. The search model can be the same as the new structure, or a homolog with significant three-dimensional similarity. The initial phases can then be refined using the actual sequence corresponding to the new structure using a wide variety of phasing approaches including isomorphous replacement, density modification and ultimately atomic model refinement. Non-crystallographic symmetry averaging is especially powerful in refining phases and producing electron-density maps with great clarity, particularly with systems that have a high degree of symmetry such as viruses. Modern computer program systems have facilitated use of these approaches by making the process more convenient.

4. Conserved nucleotide-binding fold in glycolytic enzymes: the Rossmann fold and revolutionary concepts in molecular evolution

Michael moved to Purdue University in 1964 to develop his own research program and apply his innovative methods to solve important biological structures. By 1971 he had determined the structure of the largest protein to date, the enzyme lactate dehydrogenase (Adams et al., 1970). Within a few years he solved another related glycolytic enzyme, lobster glyceraldehyde-3-phosphate dehydrogenase, and showed unexpectedly that the nucleotide cofactor-binging portion of the structures had highly similar folds. Based on these observations he suggested that the architecture of proteins evolved in the same way as the anatomy of animals (Buehner et al., 1973; Rossmann et al., 1974). This conserved part of protein anatomy is called the 'Rossmann fold' to recognize Michael's ingenious new idea. He had initially thought along these lines at Cambridge: when solving the structure of hemoglobin, a protein that carries oxygen in red blood cells, Michael saw that the two protein chains of hemoglobin had strong three-dimensional resemblance to each other despite having significant sequence differences, and also to myoglobin, which carries oxygen in muscle tissues. Although these concepts are very well accepted now, they were revolutionary when suggested, and were often greeted with resistance.

5. Passion for viruses: technology and a plant virus structure

A driving force behind Michael's interest in pursuing more and more complicated biological structures and in technology development was his passion to study virus structure. Michael subsequently pioneered the structure solution of entire viruses in atomic detail, requiring considerable advances in technology to handle the larger unit cells and massive amounts of crystallographic data. Following the publication of the tomato bushy stunt virus structure (Harrison et al., 1978) from Stephen Harrison's group in 1978, Michael reported the structure of Southern bean mosaic virus (Abad-Zapatero et al., 1980), and the surprising revelation that the coat protein structures of these two plant viruses shared a common protein fold, an eight-stranded β-barrel also known as a 'jelly roll' fold. This work required the development of oscillation photography for data collection, and processing and post-refinement of the intensity data measured on X-ray film (Rossmann et al., 1979; Winkler et al., 1979). Writing programs and developing efficient algorithms for location of heavy atoms in the presence of non-crystallographic symmetry and averaging of the electron density were also massive undertakings, especially given the more limited computing resources of that era.

6. The common cold virus structure: more innovations and amazing biology

Michael shifted attention to animal viruses in the early 1980s. His work gained wide attention when he reported the structure of a common cold virus in 1985, human rhinovirus 14, the first animal virus described in atomic detail (Rossmann et al., 1985). The rhinovirus structure was a landmark in terms of its biological significance, illuminating principles of viral assembly, and interactions with neutralizing antibodies, cellular receptors and antiviral drugs. Michael's career-long theme of making fundamental discoveries in molecular evolution struck once again – the coat protein structures of human rhinovirus 14 showed great similarity to the plant virus structures, in spite of having essentially no detectable sequence conservation!

The structure determination of rhinovirus itself was extraordinary, using a pioneering combination of high-intensity synchrotron radiation, high-speed supercomputing and the most convincing demonstration up to that time of phase extension using non-crystallographic symmetry averaging and reconstruction (Arnold et al., 1987). Heavy-atom phases were only available to 5 Å resolution from a single $Au(CN)_2$ derivative, and phase extension via 20-fold non-crystallographic symmetry averaging and reconstruction in gradual steps to 3.5 Å resolution led to a complete trace of the four chains of VP1, VP2, VP3 and VP4 in the protomeric unit. Within three weeks a complete model of the >800 amino acids in the icosahedral asymmetric unit had been built using a newly acquired Evans & Sutherland computer graphics system. The phase extension was carried out to 3.0 Å resolution, and the refined phases were subsequently used as observations in atomic model refinement because of their accuracy (Arnold & Rossmann, 1988). A great deal of programming was required to adapt the Rossmann laboratory software from earlier CDC6000 series computers (CDC6500 and CDC6600) to the Cyber 205 supercomputer.

7. Virus structures for all seasons and initial work using cryo-EM

Following the common cold virus structure work, Michael solved the crystallographic structures of many other RNA viruses from plants and animals including polio-, coxsackie-, and cardioviruses. He also determined the crystal structures of DNA viruses including human, canine, feline and porcine parvoviruses. In addition, Michael solved the detailed structures of both small and large bacteriophages. To further probe biological function, Michael pursued the structures of complexes of viruses with their cellular receptors, neutralizing antibodies and small-molecule drugs. To study some of the complexes with cellular receptors and antibodies, Michael began to use cryo-EM with Tim Baker, who had set up an experimental facility at Purdue University for the study of virus structure by cryo-EM. Michael and Baker used this approach to show that the ICAM-1 receptor for HRV14 bound in the canyon as predicted (Olson et al., 1993). Jack Johnson and Tom Smith also worked with Baker to study interactions of antibodies with plant viruses and HRV14, respectively.

8. Cryo-EM: large and enveloped viruses including the flavivirus structures

As many viruses cannot be crystallized easily, Michael also recognized, fairly early on, the importance of cryo-EM for structural virology. When cryo-EM investigations can be augmented by crystallographic determination of the component proteins, they produce 'pseudo atomic resolution' structures of the whole virus, a method dubbed hybrid technology that Michael helped to develop. Today, cryo-EM is capable of producing high-resolution structures providing atomic detail with suitable samples, but during the 1990s the cryo-EM technology yielded structures limited to the 10–20 Å resolution range. With Tim Baker, Michael was able to use the hybrid method to determine the structure of the lipid enveloped alphaviruses Ross River virus (Cheng et al., 2002) and Sindbis virus (Zhang et al., 2002). Together with virologist Richard Kuhn who had joined the Purdue structural biology group, Michael determined the structures of flaviviruses, e.g. dengue virus (Kuhn et al., 2002) and West Nile virus (Mukhopadhyay et al., 2003), and mapped their interactions with antibodies and conformational changes under acidic conditions. In the astonishing Zika virus work, he and collaborator Richard Kuhn obtained a sample of the virus in February 2016 and published the complete atomic structure in Science in April (Sirohi et al., 2016). Michael's laboratory was equipped by this time with state-of-the-art cryo-EM technology underlying the 'resolution revolution' in EM that permits high-resolution structure determination of complex macromolecular structures from averaging of many thousands of randomly oriented single particles or viruses. As was characteristic for him throughout his research career when working on new topics and technological areas, Michael wrote computer programs to perform EM analyses including obtaining optimal fits of atomic models into cryo-EM electron-density maps.

9. Awards, honors, recognitions, and honorary degrees

Michael's achievements, which have been recognized by many awards, are among the most impactful contributions to the chemical and life sciences: inventing crystallographic methodology used to solve most macromolecular structures; solving virus structures and developing the methods for doing so; and suggesting that proteins could evolve, with folded domains being the fundamental evolutionary unit. Michael was a Member of the US National Academy of Sciences (1984) and the American Academy of Arts and Sciences (1978), and the Royal Society (1996). Among his most notable awards were the Ewald Prize, Gregori Aminoff Prize, Fankuchen Award, Louisa Gross Horwitz Prize, Gairdner Foundation Award, Paul Ehrlich and Ludwig Darmstaedter Prize,

Sackler Prize in Biophysics, Stein and Moore Award from the Protein Society, and three consecutive NIH MERIT Awards. He held six honorary degrees from international universities and was a Member of the National Science Board (2000–2006).

10. Crystallographic awards and contributions to education in crystallography

Michael was especially proud that the Ewald Prize (1996), the highest award given by the IUCr only once every three years, recognized his inventions in crystallographic methodology, including the molecular replacement method. The Fankuchen Award from the American Crystallographic Association (1986) was also especially fitting because Isador Fankuchen published the first diffraction patterns from virus crystals. Michael created, with Eddy Arnold, Volume F of the *International Tables for Crystallography*, which was the first volume of the series that focused on macromolecular crystallography (Rossmann & Arnold, 2001). A second volume was published in 2012 (Arnold et al., 2012). A third, in preparation with the participation of Liang Tong, will be dedicated to Michael's memory.

Michael trained a legion of scientists, including postdoctoral and graduate students who themselves have established many vibrant and productive research programs worldwide. Michael developed many close life-long friendships with his students and co-workers. Michael also played a key role in the education of young scientists in crystallography and structural biology. In 1976, he organized the first macromolecular meeting of the International School for Crystallography in Erice, Italy, on the topic of macromolecular crystallography. In 2006, Michael again organized the school on the topic of biological macromolecules and their assemblies. The 2006 program included a strong representation of the field of cryo-EM, reflecting Michael's passion for that approach. The Erice school often has as many as 100 or more students at the graduate and postdoctoral level in attendance for a ten-day program that features a mix of talks on fundamental methodology and new results.

11. Michael's family life

Michael and his dear wife of 55 years, Audrey, had three children. In addition to son Martin, and daughters Alice and Heather, he is also survived by four grandchildren. Following Audrey's death, Michael met Karen Bogan. They were married a year ago and enjoyed great happiness together. At a Memorial Service in West Lafayette, following his death, many memories of him as a warm and influential family member, friend and mentor were shared, including his child-like curiosity about almost everything and diverse interests in exploring the natural world, both physically and intellectually.

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This is adapted from a recently published obituary (Arnold, E., Wu, H. & Johnson, J.E., *Acta Cryst.* (2019). D75, 523–527). A special session of the ACA 2019 Annual Meeting will include a presentation from Jack Johnson, Eddy Arnold, Hao Wu, Rui Zhao, and Saif Hasan, about various epochs of the Rossmann laboratory at Purdue University.

James C. Phillips (1952-2019)

James was born on 1952 in Bury, England, eventually emigrating to the United States and becoming a Naturalized Citizen in 1989. In 1973, James was awarded a B.A. degree in Natural Sciences from Trinity College, Cambridge (UK). Afterwards, he attended Stanford University on a Fulbright Scholarship, receiving an M.S. degree in 1975 and Ph.D. in January 1979. His thesis work on Crystallographic Applications of Synchrotron Radiation was advised by Professor K.O Hodgson at SSRL. There, he built a monochromator for his early work and he was instrumental in the first use of a light source for protein crystallography. After graduate school, James enjoyed a long and varied career in the field of x-ray crystallography.

(*Abstracted from Legacy.com*)

It was my pleasure to work with James from 1992 through 2003 at Siemens Analytical Instruments and then at Bruker AXS in Madison WI. He was a colleague who became a friend.

James (lower left) with Bruker CCD design team, circa 2000.

Our families spent time together and James and I often had long conversations over lunch at work. James was very intelligent and had many topics to discuss – it was never dull around James. We resumed those luncheon conversations after he retired, and I shall greatly miss him.

He was justifiably proud that he did the very first protein crystallography experiments at the Stanford Synchrotron, working as a graduate student with Professor Keith Hodgson and post docs Alex Wlodawer and Marguerite Yevitz Bernheim. He was first author on the 1976 publication describing these important results in the Proceedings of the National Academy of Sciences of the USA, *73*, 128-132. Thousands of protein crystal structures have since been deposited in the Protein Data Bank, leading to fundamental advances in knowledge and practical development of new drugs.

Figure 3
A hutch of the first macromolecular crystallography beamline 1–4 at Stanford that was supposed to prevent scientists from getting too close to the beam. From the left: Marguerite Yevitz Bernheim, Keith Hodgson, AW and James Phillips. Of course, the beam was closed when this picture was taken!

Photo circa 1975 courtesy of Dr. Alex Wlodawer, from the paper 'Impact of synchrotoron radiation on macromolecular crystallography: a personal view', by Z. Dauter, M. Jaskolski, and A. Wlodawer, J. Synchrotron Radiation, 2010, 17,433.

James and Bruker protein applications scientist colleagues with Sue Byram in 2015.

At Siemens in Madison, James worked extremely well with our R&D personnel, particularly in recognizing the potential of our novel multilayer X-ray optics, later called Goebel mirrors. He conducted the first prototype tests of these lab-source optics using protein crystals. James had outstanding scientific knowledge and decades of practical experience working with scientific X-ray instrumentation. He was the best person in our group for reporting on the results of his numerous experiments, resulting in many publications.

Sue Byram

I first met James Phillips in the early 90's when he participated in the ACA Summer Course for Crystallographers hosted by the University of Pittsburgh. He was working for Enraf-Nonius then and his contributions to the Course were key to the success of small molecule hands-on data collection using the Enraf-Nonius CAD4 diffractometer. He later moved to Siemens (now Bruker) where he was responsible for demonstrating Bruker's X-ray instrumentation for macromolecular crystallography including the large format lens-based synchrotron detector he demonstrated at SER-CAT. Later when Bruker scaled back their synchrotron applications group in 2003 James joined my group at the University of Georgia where he quickly became proficient in the use of Rigaku equipment for data collection and a variety of data processing programs.

August 2003 group photo of Wang lab with James Phillips in the far left of the picture.

James impressed me with his knowledge of X-ray instrumentation and synchrotron data collection techniques. He was an excellent teacher always ready to offer help from basic crystallography knowledge to hands-on experimental techniques.

BC Wang

Index of Advertisers

Candidates for ACA Offices in 2020

The Nominating Committee (Patrick Loll, Amy Sargent & Tom Terwilliger) proposes the following candidates for 2020.

Officers:

Vice-President: Stephen Burley & David Rose

Canadian Representative: Gerald Audette & Dmitriy Soldatov

Committees:

Communications: Rajni Bhardwaj & Indranil Chakraborty

Continuing Education: John Rose & Christine Zardecki

Data, Standards, and Computing: John Bollinger & Paul Boyle

Meetings: Brandon Mercado & Nick Vukotic

To nominate write-in candidates for any office, write to the ACA Secretary: Diana Tomchick, Dept. of Biophysics, University of Texas, Southwestern Medical Center, Irving, TX 75061 (diana.tomchick@utsouthwestern.edu). Letters must be received by September 15, 2019 and must be signed by five ACA members, and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election website. The voting window will open in October 2020.

Stephen K. Burley – Vice President

Director, RCSB Protein Data Bank, University Professor and Henry Rutgers Chair, Institute for Quantitative Biomedicine, Department of Chemistry and Chemical Biology, Cancer Institute of New Jersey, Rutgers, The State University of New Jersey, Piscataway, New Jersey, USA

Education:

Honors B.Sc. (Physics), University of Western Ontario, London, Canada (1980);

D.Phil. (Molecular Biophysics), Oxford University, Oxford, UK (1983); and

M.D., Harvard Medical School, Boston, Massachusetts, USA (1987).

Postdoctoral Training:

Structural biology research with Gregory A. Petsko (Massachusetts Institute of Technology 1983-1987) and William N. Lipscomb (Harvard University 1987-1990).

Clinical Training:

Intern and Resident in Internal Medicine, Brigham and Women's Hospital (1987-1990).

Statement:

It is an honor to stand for election to the post of ACA Vice President. As a member for more than three decades, I have derived enormous professional benefit and much personal satisfaction from the activities of our organization and the manifold contributions of fellow members. "Structure and the ACA have Mattered" at every stage of my career!

I seek a leadership role in the ACA to work closely with the other Officers, the Committees, and the Special Interest Groups to play my part in ensuring that our organization (i) sustains the scientific discipline of crystallography, (ii) embraces the diversity of experimental methods, sample origins, and scientific questions addressed by our members, and (iii) nurtures the careers of the structuralists of tomorrow.

Longevity is testament to the resolving power of crystallography and the enduring impact of atomic level structural information across the physical and natural sciences. This year, the ACA celebrates the 70th anniversary of its launch, following merger of the American Society for X-Ray and Electron Diffraction and the Crystallographic Society of America. The Cambridge Structural Database recently celebrated 50 years of operations, and the Protein Data Bank will turn 50 in 2021. The ACA and these critical data resources persist and thrive in no small part because data integrity and accuracy have mattered to our community since the Bragg father and son team determined structures of diamond and simple salts in 1913. As a future Vice President, President, and Past President of the ACA, you can rely on my enduring commitment to strengthening data standards and preserving crystallographic data and structures of molecules small and large.

Breadth in terms of experimental methods, sample origins, and scientific questions addressed by our members represents an important historical strength of the ACA. I will bring experience in both small-molecule and macromolecular crystallography to the table. I have already proven my openness to embracing new experimental techniques by advocating strongly for inclusion of cryo-electron microscopy, tomography, and diffraction in our annual meetings and supporting the new Cryo-Electron Microscopy Special Interest Group. Going beyond the "resolution revolution" in electron imaging, the next frontier in structural biology will involve integrative structure determination. This new approach combines data from multiple techniques of quantitative measurement and analysis (*e.g.*, cryo-electron microscopy, crystallography, comparative protein structure modeling, evolutionary covariance, small-angle solution scattering, chemical cross linking, fluorescence resonance transfer, electron paramagnetic resonance, and H-D exchange mass spectrometry). As a future ACA leader, my strategic choices will be guided by the evolving wants and needs of our members and the demands of their research programs.

The future of crystallography and of our organization depends critically on recruiting the next generation of structuralists and retaining their interest for decades to come. As a membership, we must work together to pass our collective knowledge and experience on to students, postdoctoral fellows, and early career researchers and educators. To this end, I will commit myself to strengthening the training and outreach activities of the ACA. Building on existing frameworks, it is imperative that we redouble efforts aimed at promoting involvement and inclusion of under-represented minorities in our community of scholars. It is also essential that we improve the way we explain and document the scientific and societal impact of what we do and why it is important to our funders, policy makers, elected representatives, and the tax payers. If elected, I will work tirelessly to make the ACA and its membership valuable to the next generation of crystallographers and those supporting their research and teaching activities.

In closing, I would be honored to serve as the next Vice President of the American Crystallographic Association and I humbly ask for your vote.

Professional Activities:

American Crystallographic Association: Member 1989-Present, Chair, Synchrotron Radiation Special Interest Group, Chair Industrial Special Interest Group, Member and Chair, Data, Standards & Computing Committee, and Co-organizer 2017 ACA Transactions Symposium; **RCSB Protein Data Bank**: Associate Director 2013-2014, Director 2014-Present; **Worldwide Protein Data Bank**: Co-Leader 2014-Present; Worldwide Protein Data Bank Foundation: Vice President 2014-Present; **Biophysical Society**: Member 1984-Present; **American Chemical Society**: Member 2006-Present; **Rutgers, The State University of New Jersey**: University Professor 2017-Present, Henry Rutgers Chair 2017-Present, Distinguished Professor of Chemistry and Chemical Biology 2013-2017, Founding Director, Institute for Quantitative Biomedicine 2015-Present, Director, BioMAPS Institute 2013-2015, and Director, Center for Integrative Proteomics Research 2013-2017; **Rutgers Cancer Institute of New Jersey**: Co-Leader, Cancer Pharmacology Program 2016-Present and Member, Cancer Pharmacology Program 2013-Present; **University of California San Diego**: Adjunct Professor 2005-Present; **Eli Lilly and Company**: Distinguished Lilly Research Scholar 2008-2012; **SGX Pharmaceuticals, Inc.**: Vice-President and Chief Scientific Officer 2002-2008; **Prospect Genomics, Inc.**: Co-Founder 2000-2001; **The Rockefeller University**: Richard M. and Isabel P. Furlaud Chair 1997-2002, Professor 1994-2002, Associate Professor 1993-1994, and Assistant Professor 1990-1993; **Howard Hughes Medical Institute**: Investigator 1994-2002, Associate Investigator 1993-1994, and Assistant Investigator 1990-1993.

Crystallography-related Service:

I currently serve as Director of the RCSB Protein Data Bank (RCSB.org) and Co-Leader of the Worldwide Protein Data Bank (wwpdb.org), the international partnership responsible for joint management of the PDB archive.

In my capacity as Director of the RCSB Protein Data Bank, I oversee:

- Expert validation and biocuration of all PDB structure depositions coming from researchers based in the Americas and Oceania (~5,100 in 2018, ~90% coming from X-ray crystallography).
- Efficient management and secure storage of the global PDB archive numbering >152,000 entries (>10Tb of data in total, as of December 31st 2018, ~90% crystallographic data) as the wwPDB designated PDB Archive Keeper.
- Open access to PDB structure data by millions of RCSB PDB website users worldwide (RCSB.org) at no charge and with no limitations on data usage.
- Download of PDB structure data files (~750 million in 2018) at no charge and with no limitations on data usage.

I also participate frequently in discussions among national and international stakeholders regarding sustainability of digital data resources for the biological and chemical sciences.

Prior to joining the staff of the RCSB Protein Data Bank in 2013, I served as Chair of the organization's Scientific Advisory Committee (1999-2012), Chair of the Worldwide Protein Data Bank Advisory Committee (2002-2012), and Chair of the Board of Directors of the Worldwide Protein Data Bank Foundation (2010-2012).

I am currently serving my second term as Member of the US National Committee on Crystallography (2014-2016, 2018-Present). I represented the United States as a voting delegate for the International Union of Crystallography 2014 General Assembly in Montreal, Canada.

I have been active in co-organizing national and international scientific conferences, and served as a member of the International Program Committee for the 2017 IUCr Triennial Meeting. I have also been an invited speaker at multiple Synchrotron Radiation in Biology Triennial Meetings, and served on the International Program Committee for the 2016 meeting.

Contributions to Structural Biology:

During my career, I have authored/co-authored more than 280 peer-reviewed publications (Google Scholar h-index: 87, i10-index: 213). As a graduate student, I contributed 8 small-molecule structures to the Cambridge Structural Database. In addition, I have contributed 1,238 X-ray crystal structures of proteins and nucleic acids to the Protein Data Bank as an academic researcher, leader of an NIH Protein Structure Initiative structural genomics center, chief scientific officer of a biotechnology company, senior scientist at a large pharmaceutical company, and Director of the RCSB Protein Data Bank.

Since joining the RCSB Protein Data Bank, I have been working to reinvent myself as a computational biologist/data scientist. My current research activities are largely focused on understanding and enhancing the impact of the Protein Data Bank archive, improving the quality of structures contributed to the archive by thousands of Data Depositors worldwide, improving knowledge delivery to millions of Data Consumers worldwide, and mining the archive using machine learning and other statistical tools. Since joining the RCSB Protein Data Bank in 2013, I have published >50 peer-reviewed papers in structural bioinformatics, structural biology, and data science.

David Rose - Vice President

Professor,
Department of Biology,
University of Waterloo,
Ontario, Canada

Education, Career:

BA Biophysics, University of Pennsylvania, 1977; DPhil, Oxford University, 1981, Sir David Phillips; Postdoc, MIT 1981-84, Greg Petsko; Research Associate / Research Officer, National Research Council Canada, 1984-1991; Senior Scientist, Ontario Cancer Institute / Professor, University of

Toronto, 1991-2008; Interim Chair, Department of Medical Biophysics, University of Toronto, 2005-2007; Chair, Department of Biology, University of Waterloo, 2009-2017; Visiting Professor, Département de Chimie, Université Grenoble-Alpes, 2017.

Professional Activities (selected):

ACA: Member since 1986; Canadian Representative on Council, 2 terms; Chair, Canadian Division, 2 terms; Local Chair, Toronto Annual Meeting, 2009; Chair, Fankuchen Award Committee (2015); Member and Chair (2017), Nominating Committee; co-Poster Chair (2018, 2019); ACA Fellow. Other: Canadian National Committee for Crystallography; Co-Founder BHT Regional Crystallography Meeting. Peer Review activities: Canadian Institutes of Health Research, Terry Fox Research Institute.

Research Interests:

Structural Glycobiology: Glycoside hydrolases involved in human health and disease.

Statement:

I love crystallography. What's not to love about collecting data one reflection at a time, spending hours in a darkroom developing films, or solving Patterson's by hand? (Yes, I'm old(-ish) but more on that later.) It's magical to see crystals in your tray, to view the beautiful symmetry of the diffraction pattern, to be the first one ever to see that new structure on the screen. It's pretty much impossible to make a living these days simply as a crystallographer, at least in the biological field. Most students (or even PIs) who publish structures, though they recognize crystallography is 'sweet', don't have the opportunity to fall in love in the same way that we did in "the early days". So where can they get the exposure to that kind of excitement? The ACA is a pretty good place to start.

When I was honoured to be approached to run for VP, the first thing I did was contact a couple of former Presidents to ask what I needed to know. Their positivity and enthusiasm, even after their terms, was convincing. One piece of advice was: don't try to do everything; pick a couple of key issues and focus on those. So, I thought, why do I continue my long association with the ACA every year? (Remember, I'm old-ish.) My number one answer has to be the Annual Meeting. That is where I come to marvel at the new advances in methodology, software and instrumentation at both the academic sessions and the vendor exhibition. (And, of course, to hear Elspeth speak.) Where else can you rub elbows over the course of a few minutes with both a Nobel Laureate and a starting graduate (or even undergraduate) student? I spend so much of the rest of the year thinking about other things, this is my chance to spend a week immersed in crystallography. So, I'll choose the Annual Meeting as my focus for this statement.

I have been impressed with the evolution of the meeting format and a new energy level that I have felt over the past few years. I am not one to fix something that is not broken. However, I am a bit disappointed that more of our colleagues are not attending regularly. An obvious practical consideration is the expense; having just registered for the 2019 meeting, I realized that the M&R cost (Membership&Registration) is now north of $1000 in Canadian funds. I don't know if that is out of line with other sister organizations (anecdotally, it is at the upper end). But the real question is whether it is value for money. In my terms on Council, we had many debates about what might be cut or changed that would make any dent in the meeting costs without having a major effect on the experience, and the answer always ended up being: not much. However, I think it might be worth a renewed conversation among the community and, perhaps, some communication with other sister organizations (most of which are also experiencing decreasing attendance) to see how they operate. After all, an appealing and worthwhile annual meeting is key to retaining and increasing our membership.

On the structure of the meeting itself, I am excited that we have expanded our community to new areas of Molecular Science. The ACA has always been broad in scientific vision: we have incorporated peripheral methods such as powder diffraction, SAXS, computational methods, and even NMR on occasion. Now we are welcoming Cryo-EM, Micro-ED, XFEL and other emerging acronyms, and offering those practitioners a home. This cross-pollination benefits all of us, young and old-ish, as well as keeping the organization current. I would work with the SIGs to think outside the box when proposing sessions to make sure they identify emerging areas and to make those areas feel welcome at the ACA.

There are two unusual strengths of the ACA meetings, in my experience. The first is the equal co-participation of early-career scientists (especially trainees) and senior investigators.

The leadership of YSSIG percolates through the organization and their interest in extra-scientific sessions, such as career development and education, has strengthened interactions across generations and across academic fields. That points to the second, related strength: the breadth of technologies, sectors and research areas. I have learned as much from small-molecule or service talks, and from conversations with vendors, as I have from macromolecular sessions. It is rare to have industrial, vendor and government attendees embedded on equal terms with academics in the organization. Events like three-minute thesis are great, and I would encourage even more such cross-interactions, perhaps through new social or 'fun' activities. (Don't worry – I am not suggesting inter-SIG softball; but maybe curling?). Finally, we made some efforts to revive the accompanying persons programs at recent meetings; a family-friendly meeting not only promotes inclusion, but gives the meeting a more personal feel and has led to many close friendships in the past.

To conclude, for most of us, I think the heart of the ACA experience is the Annual Meeting, and a major priority of mine would be to make sure it is accessible to a diverse range of colleagues, whatever their available funding, and to having attendees leave the meeting feeling inspired and energized. An event to not just hear amazing science, but to socialize and learn from colleagues of all ages and backgrounds, to make career-long connections, to follow new instrumentation and methods and, yes, to fall in love with crystallography all over again.

Gerald F. Audette - Canadian Representative

Associate Professor,
Department of Chemistry,
York University,
Toronto, ON, Canada

Education:

BSc, Biochemistry, University of Alberta (1995); PhD, Biochemistry, University of Saskatchewan (2002)

Professional Activities:

Graduate Program Director, Dept. of Chemistry, York University (2019 -); ACA Meeting Program Co-Chair (2018); Director, Centre for Research on Biomolecular Interactions (2014-15); Faculty of Science Graduate Mentorship Award, York University (2014); Undergraduate Program Director, Dept. of Chemistry, York University (2014); Subject Editor, Crystallography and Structural Chemistry, FACETS Journal (2015 –); Canadian Division of the ACA (Chair, 2012-14); Canadian Light Source User Advisory Committee (2002-2004); Co-Editor in Chief, Journal of Bionanoscience (2006-2010).

Research Interests:

Broadly speaking, my research focuses on understanding at a structural level how microorganisms utilize multi-protein complexes for transferring genetic material and effector molecules across membranes, and facilitate adherence to a variety of surfaces. Using X-ray crystallography and other methods such as SAXS and Hydrogen Deuterium Exchange Mass Spectrometry (HDX-MS), I'm interested in how these dynamic systems are assembled from their component proteins, as well as their effects on infection, adaptation to varying environmental conditions and the development of multi-drug resistance. Understanding of how these systems are assembled from their component proteins, as well as their effects on infection and the development of resistance strategies, is critical to the development of more streamlined approaches to dealing with infection and drug resistance in pathogenic organisms. In addition, understanding how these systems function and assemble at a structural level is central to the development of biological systems for applications such as biosensors.

Statement:

I am honoured to have this opportunity to represent the Canadian crystallographic community as the Canadian Representative on Council. The ACA was the first association I joined as a student, and has been my professional home for well over 20 years. I started in crystallography looking at small nucleoside analogs as anti-viral

compounds (with a CAD-4 diffractometer and NRCVAX and XTAL software packages with the CIF having only recently been introduced), before moving onto macromolecules (first on an Enraf-Nonius FAST system and using O, FRODO and SETOR on an SGI), where my research focus remains. I've recently delved back into the "small molecules" with a colleague who is, oddly enough, exploring anti-viral nucleoside analogs. The experience has re-grounded me in the exquisite detail in which we analyze and report our structures in *Acta Crystallographica* via the CIF, and how our streamlined software can often be a black box for students…getting them to "lift up the hood" sometimes is a good thing that can lead them to ask more in-depth questions about their "molecule(s) of interest." Many of my friends and colleagues of diverse scientific backgrounds, both in Canada and North America, I met through the ACA. I think it's incredibly beneficial for Canadians to be members of the ACA, where chemists, physicists, biochemists, mineralogists etc. come together through the common language of crystallography. This commonality of language allows for the removal of "silos"; crystallography bridges disciplines and the ACA is our venue. I like to think that I have been an active member of the crystallographic community, and within the ACA, and am excited about the opportunity to give back to my community.

A note of thanks to Tomislav Friscic, who has been an excellent voice of the Canadian community on Council for the past 3 years, and before him, Mike James, David Rose and others. I look forward to continuing their work to increase the "Canadian content" in the ACA through engagement of the community and to "reintroduce" my colleagues to what the ACA can offer. As the Canadian attendance at the 2018 Toronto ACA and 2014 Montreal IUCr meetings show, we have a strong and dynamic structural community; I want to thank everyone for making these fantastic meetings. I want to build on these successes and continue to grow our community, particularly with our young scientists. When we look at where our community can grow, the young scientists are the ones who will be our future leaders. They have a diverse spectrum of interests, and often get focused on our particular sub-discipline, be it inorganic catalysts, minerology or structural biology. While this is perfectly normal, most of these interests have structural characterizations as a central component, which is where the ACA comes in – Structure Matters. And when you peruse the programs of the ACA annual meetings, most of these areas are covered, as well as sessions on cryo-EM, hybrid methods, NMR, crystallographic education, inclusivity, and career development are all there. The ACA fosters our building broader connections and relationships within the North American community and beyond, and our meetings are great venues to make those connections. Our ACA community and annual meetings are not so large that one gets lost, and are small enough that there are numerous opportunities for attendees to interact and make professional connections. I look forward to the challenge of (re)engaging my Canadian colleagues, and see how we can be more relevant to their scientific interests. If given the opportunity to represent the Canadian community on the ACA Council, I will encourage more Canadian involvement in the ACA and be an active and enthusiastic voice for Canadian crystallography in the Americas.

Dmitriy Soldatov - Canadian Representative

Associate Professor
and Director of X-Ray Facility
Department of Chemistry
University of Guelph
Ontario, Canada

Education:

MSc in Chemistry, Novosibirsk State University, USSR (1991). PhD in Chemistry, Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences, Novosibirsk and Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw (1995). Visiting and Post-doctoral Fellow with the National Research Council, Ottawa, Canada (1997-2001).

Professional activities:

Member of the ACA since 2001; co-chair of a session in 2018 and 2019. Director of the National Affiliated Centre, Canada for the Cambridge Crystallographic Data Centre (NAC CCDC, 2008-present). Executive Committee Member of the Materials Chemistry Division of the Canadian

Society for Chemistry (CSC): Secretary (2016-2019); Social Media Manager (2019-2022). Member of the Steering Committee for the Crystal Engineering of Emerging Materials Workshop of Ontario and Quebec (CEMWOQ; 2013 – present) and co-chair of CEMWOQ-2 (2015). Member of CSC (2000-2011, 2015-present) and co-organizer of three symposia at the CSC conference (2017, 2018 and 2019). Member of the Canadian Thermal Analysis Society (CTAS, 2009-2014) and organizer of an annual meeting (2011). Member of the North American Thermal Analysis Society (NATAS, 2015-present), IUPAC (2002-2011, 2015-present), All-Russian Mendeleev's Chemical Society (2000-present). Executive English Editor of the Journal of Structural Chemistry (2006-2016) and Guest Editor of two special issues of the journal (1999, 2005). Guest Editor of a Special Issue of Crystals (2017-2018).

Research Interests:

Small molecule X-ray crystallography; solid state organic and metal-organic chemistry; supramolecular chemistry and crystal engineering; molecular self-assembly and design of soft materials; thermal analysis, thermodynamics and sorption; heterogeneous equilibria and phase diagrams. Research objects: molecular crystals and co-crystals, inclusion compounds and porous solids, crystalline and semi-crystalline materials, natural and synthetic polymers, peptides, metal complexes. Teaching: X-Ray Crystallography, Solid State Chemistry, Structure and Spectroscopy, Structure and Bonding, Topics in Nanomaterials, Supramolecular and Nanostructured Materials.

Statement:

It would be a great honor for me to speak and stand for Canadian crystallographic community as the Canadian Representative to Council. Due to my duty as the Director of the CCDC National Affiliated Centre of Canada and various activities within the Canadian Society for Chemistry and beyond, I am very familiar with crystallography and crystallographers across the country, their needs and wants. On the other hand, I have been with the ACA for almost 20 years and could help to strengthen the Association through greater involvement of Canadians in the ACA's community life and activities. The 2018 conference in Toronto was one of the most successful ACA annual meetings over the last several years, with a dramatic spike in the overall number of participants and, needless to say, Canadians. There is a large number of researchers, staff crystallographers and students in Canada interested in learning crystallography and sharing their ideas related to the crystal structure analysis and use. Statistical data show that Canada is over 10% of the USA if one takes into account the overall number of universities, or something more specific to the crystal theme, such as the number of CCDC user sites. One could be tempted to say that greater distances and the border inevitably translate into increased travel costs and other barriers and, as a consequence, lower involvement of Canadians than the bare statistics would suggest. In fact, this may be only half, or even less than half, true. My observations based on the success of CEMWOQ (Crystal Engineering of Emerging Materials Workshop of Ontario and Quebec, 2013-2019) or the series of crystalline materials theme symposia at the Canadian Chemistry Conference (2016-2019) show that once properly "nucleated" and organized, the "crystal" community in Canada grows and evolves. I believe my experience in organizing the above conferences, as well as overall awareness of the crystallography community in Canada will help to attract more Canadians to the ACA. I also believe that my credentials will help me to speak for all Canadians with various research, ethnic and cultural backgrounds.

About myself: From the very first research experience as an MSc student (1989-1991), to present, my research was critically dependent on the crystal structure analysis and understanding the crystallography. I was educated as an inorganic and physical chemist but realized I have to learn X-ray crystallography myself in order to be able to do my studies. The MSc project, and then my PhD research, were devoted to inclusion compounds of metal complexes. The studies required extensive characterization of crystals quickly decomposing in air, often showing disorder of guest molecules in the structure, and presenting other challenges. I started to learn practical crystal structure analysis in Poland, at the Institute of Physical Chemistry with Janusz Lipkowski, who became a co-supervisor of my PhD project. My other mentor in crystallography was Gary Enright at the National Research Council of Canada where I did my post-doctoral studies. I joined the ACA in 2001, when I received the Margaret Etter Award and generous travel support from the ACA to present my post-doctoral research in its Annual Meeting in Los Angeles. The conference felt like an once-in-a-lifetime experience to me, not only due to meeting in person a number of outstanding people,

whose names I knew before I even realized these are real people, alive and active, but also due to a special, friendly atmosphere that prevailed at the conference and that is inherent to the whole ACA community. In 2007 I joined the Faculty of the Department of Chemistry, University of Guelph where I am currently Associate Professor and the Director of the X-Ray Facility. My research is quite diverse, from the design and study of peptide-based inclusion compounds and co-crystals to industrial collaborations on waxes, flours and breads.

Rajni Bhardwaj - Communications Committee

Research Scientist
Solid-State Research Group, Small Molecule Design & Development
Eli Lilly & Co
Indianapolis, IN 46285
USA

Education:

B. Pharm., MDU University (2003), India; M.S. (Pharm) National Institute of Pharmaceutical Education & Research (NIPER) (2005), India; Ph.D. (Pharmaceutical Sciences, University of Strathclyde, United Kingdom (2013); P.G. Diploma in Clinical Research, India (2008); P.G. Diploma in Patents Law, India (2007).

Professional Activities:

Member of British Crystallographic Association (BCA) (2011-2013), Member of Association of American Pharmaceutical Scientists (AAPS) (2012-2014), Member of American Crystallographic Association (ACA), Reviewers to Journal of Molecular Structure, Molecular Pharmaceutics, Journal of Pharmaceutical Sciences, Pharmaceutical Development and Technology & Drug Development & Industrial Pharmacy.

Research Interests:

Structure based solid-state form design, Structure determination from single crystal and powder X-ray diffraction, Structure based property prediction, Chemo and structural informatics, Digital drug product design.

Statement:

It is my honor and privilege to be nominated for a membership in the ACA communications committee. I attended my first ACA meeting in 2013 and was very impressed with the quality of the scientific sessions and the outreach programs. From my personal experience, ACA meetings provide a platform to build professional relationships that last beyond the meetings. One of my favorite and latest addition " Three Minute Thesis" session in ACA meetings provides an excellent forum for students to learn communicating science to general audience without using too many technical jargons.

Working in pharmaceutical industry has made me realized the immense powers of the high-fidelity structures in developing high quality medicine. Being a member of ACA communication committee, I would be in a unique position to provide industrial perspective on finding ways to increase awareness about importance of crystallography and need for continuing student education in this unique area. if elected, I commit to find new ways to increase public awareness of the important work being done by the ACA members and stand by ACA's mission to promote and preserve crystallography.

Indranil Chakraborty - Communications Committee

Research Assistant Professor,
Florida International University,
Miami, Florida

Education:

BSc in Chemistry, with honors and first class distinction, Midnapore College, INDIA, 1996. MSc in Inorganic Chemistry and first position amongst all successful MA/MSc candidates, Vidyasagar University, INDIA, 1998. Ph.D. in Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, INDIA, 2003.

Professional Activities:

Postdoctoral Associate, Department of Chemistry,

University of Puerto Rico, San Juan, PR (2004-2010). Postdoctoral Scholar, Department of Chemistry and Chemical Biology, Harvard University (2010). Postdoctoral Associate, Department of Chemistry, University of Texas at El Paso (2012-2013). Senior Research Specialist, Department of Chemistry and Biochemistry, University of California Santa Cruz (2013-2017). Research Assistant Professor, Department of Chemistry and Biochemistry, Florida International University (2017-till date). X-ray Diffraction Facility Manager at single crystal X-ray facility at UC Santa Cruz (2013-2017). Editorial Advisory Board Member of Crystals (a Journal of Crystallography by MDPI) & Editorial Advisory Board Member of Sci (an international Open access journal by MDPI).

Research Interests:

Research interests primarily involve synthesis of new organic and organometallic compounds, bioinorganic chemistry, medicinal inorganic chemistry and X-ray crystallography. Synthesis of multinuclear iron-oxo clusters and determination of X-ray structures. Redox and electron transfer properties associated with such clusters relevant to iron containing metalloproteins and minerals. Design and synthesis of visible light sensitive carbon monoxide releasing molecules for selective eradication of malignant cells. Synthesis and X-ray structural studies of new organic chelators for efficient and selective extraction of mercury(II) from mixed alkaline nuclear wastes.

Statement:

I have always had the privilege of having great teachers around–starting from the elementary school in Midnapore, India up to the graduate (Ph.D.) studies at Indian Association for the Cultivation of Science, Calcutta (now Kolkata), and during all postdoctoral stints at various Universities throughout the United States. I had teachers/professors/advisors who inspired and led by example. I would have definitely not imagined myself where I am today without them. All these teachers had one thing in common –a passion for teaching and a keen interest in the all-round growth of the students. I as a teacher/mentor would also wish to follow a similar attitude.

From my experience as a postdoctoral mentor to a diverse group of graduate/undergraduate students in chemistry (and Biochemistry), I have learned that engaging the students—to encourage in scientific discussion with each other and with the mentor and also discussion on relevant current developments—works best. It might sound cliché, but getting the student to interact with the teacher in the classroom is quintessential to get the message across and I believe is one of the most efficient methods of learning. Over the years, I have used the pedagogy to teach various concepts to my junior graduate students and also to undergrads. It has been proven very effective.

I have taught inorganic/solid chemistry/general chemistry and various topics in X-ray crystallography. I have conducted lectures and small workshops (as a postdoctoral researcher) on basics of X-ray diffraction techniques and covered also the experimental aspects.

I am an active ACA member and would like to serve this esteemed society in a more profound way in the coming days and years.

In summary, my philosophy is to be proactive, honest, thorough and organized in and outside the classrooms so as to inspire students to learn topics related to X-ray crystallography with interest. My intention will also be to inspire as many students as possible to take on science as their careers. As Carl Sagan once said, “Science is a way of thinking”, and I would like to instill this idea into students and make them informed citizens of the World.

John Bollinger - Data, Standards & Computing Committee

Computing and X-ray Scientist
St. Jude Children’s Research Hospital
Memphis, TN 38105, USA

Education:

B.A. Chemistry, Washington University (1990); B.A. Mathematics, Washington University (1990); Ph.D. Inorganic Chemistry, Northwestern University (1994); Postdoctoral Fellow, Indiana University (1994-1996).

Professional Activities:

Member of the American Crystallographic Association (1997-2005, 2012-present); voting member of the IUCr’s Committee for the Maintenance

of the CIF Standard (COMCIFS; 2012-present).

Research Interests:

Chemical crystallography; crystallographic software development; crystallographic informatics.

Statement:

Software development and data management and analysis have been among my interests since before my first introduction to crystallography, some thirty or so years ago. Those interests played a significant role in my choice to focus my career on crystallography, and efforts in those areas have been a continuing thread running through my work ever since. I have long supposed that if I were to serve the ACA at the committee level then the Data, Standards, and Computing committee would be the one to which I could make the greatest contribution. It is my honor and privilege to now be nominated for such a position.

Among the things I can offer the committee is breadth of experience. Having been trained as an inorganic chemist and chemical crystallographer, and having spent the first part of my career primarily in those areas, I shifted for several years to working outside academia in software design and development before returning to devote the last ten years to supporting a Structural Biology department. I am familiar with the tools, data, and computing practices of all these regimes. Moreover, I bring expertise in software design and development that is no longer common in our profession. A computer scientist colleague once described me as having "the equivalent experience of a computer scientist" – though in fairness, one should take into account that that was on a grant application.

One of my proudest achievements was successfully leading technical development for the Reciprocal Net project (overall project lead: John Huffman). The Reciprocal Net provides a geographically distributed database of crystallographic results provided by multiple laboratories, coupled with a laboratory information management system tuned for service crystallography. Our development team had to address issues of data formats, ownership, versioning, and lifecycle; crystallographic workflow; integration of diverse tools; distributed and high-performance computing; and user interface, among many others. The Reciprocal Net remains in use today.

Perhaps the most consistent theme throughout my career has been the crystallographic information file. It having been unleashed upon the world at about the time I began my graduate work, I am among the first children of the age of CIF. From testing an early version of IUCr software for typesetting articles submitted in CIF format, through developing CIF-handling features for the in-house software of the Indiana University Molecular Structure Center and for the Reciprocal Net, to participating on the committee standardizing CIF 2.0, my efforts seem always to come back to CIF. Indeed, since 2012, I have been one of the five voting members of the IUCr's COMCIFS committee, whose mandate is to maintain the CIF file format and associated technologies, including overseeing CIF dictionaries, which synergizes well with the work of the ACA Data, Standards and Computing committee.

If elected to the committee, I look forward to continuing its work in monitoring and advising Council on issues relevant to crystallographic software, data, and databases. The frontiers in structural science keep advancing, with increasing focus on large data and large numbers of data sets. Ever newer, brighter sources and larger, faster detectors mean new challenges for data and computing, and as techniques such as serial crystallography and Cryo-EM move toward the mainstream, issues of standards for publication and deposition, and of cataloguing and documenting software arise anew. There's plenty of work to be done, and I stand ready to do my part.

Paul Boyle - Data, Standards & Computing Committee

Manager, X-ray Facility, Department of Chemistry, University of Western Ontario, London, Ontario, Canada

Education:

B.S. magna cum laude, Chemistry, (1983), Syracuse University; Ph.D. Inorganic Chemistry (1988), University of Minnesota; Post-doctoral: with Hans-Beat Bürgi, (1988-89), Universität Bern.

Professional Activities:

Member, American Crystallographic Association, past chair of the Canadian Division (2016-17), member of Small Molecule and Service

Crystallography SIGs, instructor for the Canadian Chemical Crystallography Workshop.

Research Interests:

Small molecule structure determination, weak hydrogen bonding interactions, thermal motion analysis, computer programming.

Statement:

I am honoured to be nominated as a candidate for the Data, Standards, and Computing Committee, and would be pleased to serve the ACA in this capacity. I have a long standing interest in crystallographic and scientific programming. As an early adopter of the Linux operating system as a platform for crystallographic computing, I also have a continuing interest in the issues of open source software and accessibility of source code for crystallographic programs.

X-ray crystallography is a field which generates an abundance of data and numerical results. For the data to have maximum usefulness, they must be accessible to researchers beyond the original scientists who generated data. This accessibility manifests in two ways: First, direct access to the data files. Second, the data file formats must be readable by different software packages. The development and implementation archival policies as well as the development and implementation of open standards for data formats is therefore key for maximum usefulness of crystallographic data. The ACA and other crystallographic professional organizations should play a key and leading role in the development of these standards.

Dissemination of data and interoperability of software challenges our community in a number of ways. These challenges include: developing and implementing standards for archiving data and the facile retrieval of archived data, encouraging instrument vendors to provide seamless support of one another's data formats or developing common open standards for image data, continuing to develop and refine automated methods of detecting erroneous or fraudulent structures, and developing and maintaining standards for publication and deposition of crystallographic information.

I look forward to the opportunity to work with other members of the Data, Standards, and Computing Committee on these challenges, and to working with the broader ACA community on other areas they identify for growth.

John P. Rose - Education Committee

Associate Professor of Biochemistry and Molecular Biology, University of Georgia, Athens, GA, Associate Director for Program, Southeast Regional Collaborative Access Team, Advanced Photon Source, Argonne National Laboratory.

Education:

Ph.D. (1980) in Physical Chemistry (small molecule crystallography), Rutgers University, Newark NJ with Prof. Roger A. Lalancette, B.A. in Chemistry (1974) Benedictine College, Atchison KS.

Professional Activities (related to education):

Member American Crystallographic Association, Local organization ACA Annual Meeting, Pittsburgh (1992), Tutor ACA Summer Course for Crystallographers (1992-1997), Lecturer ACA Summer Course for Crystallographers (1997-2001), Co-Chair, Symposium on Crystallographic Education, Congress of the International Union of Crystallography, Geneva, Switzerland (2002), Co-organizer with Dr. Bi-Cheng Wang and others, One-day Workshop on Sulfur SAD Data Collection and Phasing, Annual Meeting of the American Crystallographic Association, Chicago, IL (2010), Co-Organizer with Dr. Wendy Dustman the one-week UGA Biotech Boot Camp for GA high school science teachers (2010 – 2018), Co-organizer with Dr. Bi-Cheng Wang, 5th Winter School on Soft X-rays in Macromolecular Crystallography, University of Georgia, Athens, GA (2019) and President Pittsburgh Diffraction Society (2012, 2014).

Research interests:

Diffraction-based structural biology, methods development for macromolecular crystallography in the areas of soft X-ray data collection and phasing, Native-SAD structure determination, high throughput methods for structural studies, remote/automated systems for synchrotron data collection.

Statement:

Crystal structure determination is becoming a more general tool for the scientific community.

The current generation of sources, improved optics and instrumentation coupled with powerful phasing methods, data processing and structure determination software now gives the novice user the ability to collect and process data, solve and refine the structure producing a publication quality structure in a matter of hours. The success of these pipelines may give novice users the false impression that understanding the theory and principles used to generate the structure is unimportant. But what happens when the pipeline fails. This was the topic of a recent presentation "The next generation of X-ray structural biologists: button pushers or crystallographers?" I presented at the 2016 ACA meeting in Denver.

Training the next generation is of paramount importance to the field. However, fewer universities offer formal courses in the theory and practice of crystal structure determination. I applaud and support the ACA's focus on education and will strive to provide more educational opportunities in terms of summer schools, workshops and meeting sessions, including resurrecting the much-needed ACA summer course in Macromolecular Crystallography.

I have over 40 years' experience in crystal structure determination (both small and macro molecules), have crystal structures in both the CCDC (9) and PDB (138) and a strong interest in crystallographic education. I believe that my experience and interest in crystallographic education should be of benefit to the ACA.

Christine Zardecki - Education Committee

Deputy Director, RCSB Protein Data Bank
Institute for Quantitative Biomedicine;
Department of Chemistry and Chemical Biology;
Rutgers, The State University of New Jersey,
Piscataway, NJ, USA

Education:

B.A., Rutgers, The State University of New Jersey (1994)

Professional Activities:

Member, American Crystallographic Association,

American Association for the Advancement of Science, American Society for Biochemistry and Molecular Biology; Executive Director/Secretary/Treasurer, wwPDB Foundation.

Statement:

I am delighted by this nomination to serve on the Education Committee. While I originally planned a more traditional career in Education, it has been exciting to instead develop education and outreach efforts focused on structural biology. In my current role as Deputy Director of the RCSB Protein Data Bank (PDB), I support all aspects of the organization with particular focus on our Outreach/Education efforts. This includes the PDB-101 website (http://pdb101.rcsb.org), which supports 600,000 students and teachers annually, and in-person activities including science fairs, Science Olympiads, and undergraduate research experiences.

I first volunteered with the ACA in 1996 to help with the IUCr meeting in Seattle, WA and was inspired by dedicated leadership and attendees. Since then, I have exhibited and presented at ACA meetings; mentored undergraduate students that presented at the meeting; led hands-on activities for students visiting the meeting; helped develop the Discovering Biology Through Crystallography coloring book for the ACA (http://pdb101.rcsb.org/learn/coloring-books/discovering-biology-through-crystallography), and co-chaired an education session at IUCr in 2017 (https://cdn.rcsb.org/rcsb-pdb/general_information/news_publications/newsletters/2017q4/corner.html).

One of my goals with the RCSB PDB is to promote structural biology to a broader audience. The structure of DNA is easily recognizable to non-scientists; we would like to expand this familiarity to larger macromolecules. It would be an honor to combine this work with the ACA.

Brandon Mercado - Meetings Committee

Research Support,
Chemical and Biophysical Instrumentation Center
Yale University,
New Haven, CT

Education:

B.A. with distinction in Chemistry, Vassar College, 2006; Ph.D. in Chemistry (outstanding dissertation award), University of California, Davis, 2011; Energy Efficiency & Renewable Energy Postdoctoral Research Fellow, University of California, Irvine, 2012-2013.

Professional Activities:

Manager of the X-ray diffraction laboratory in the Chemical and Biophysical Instrumentation Center housed in the Chemistry Department at Yale University since 2013. Member of the ACA since 2009. ACA Service SIG (Secretary 2016-2017). ACA General Interest SIG (Chair 2020). ACA Small Molecule SIG (Chair 2020).

Research Interest:

Small molecule diffraction with X-rays, neutrons, and electrons; small angle X-ray scattering of oriented nanoparticles, quantum dots, and inorganic thin films; endohedral and exohedral fullerene chemistry.

Statement:

I am honored that the ACA nominating committee has asked me to stand as a candidate for the ACA Meeting Committee. I believe our annual meeting is one of the most important events planned by the ACA. I attended my first ACA meeting in Toronto in 2009 as a graduate student. The inclusive and educational environment fueled my interest and desire to pursue a career in crystallography. I was excited to return to Toronto in 2018, where I saw many of the people I met for the first time nearly a decade prior.

Having grown closer with the members of this community, I have come to appreciate the herculean effort and time it takes to plan and coordinate a successful meeting. Continuing the tradition of fantastic meetings will not be a small task. I believe that expanding the diversity of sessions, encouraging young scientists, and emphasizing education are major components in the plan for a successful and productive annual meeting.

I have experience with conference planning on a targeted, regional scale. I have been planning the Rigaku Symposium Series at Yale University since 2014. I am directly responsible for inviting speakers and poster presenters, planning the workshops, and organizing the social events. I would look forward to the opportunity to apply

my skills in programming to our national meeting.

One of the committee's missions is to highlight opportunities to enhance the attendee experience at the annual meetings. There are many exciting elements that are already established. For example, the Young Scientist SIG mixer and poster prize awards cater to young investigators at our meetings. With the recent inclusion of the three-minute thesis session, I would be excited to identify additional ways to expand the scope of programming for young scientists.

I am also interested in working with session chairs to continue the trend of including more structural characterization sessions that go beyond traditional crystallographic methods. Our upcoming meeting has representation for solid state nuclear magnetic resonance, cryo electron microscopy, and micro electron diffraction.

Finally, the educational sessions and workshops provide a crucial forum where participants can learn and discuss pedagogy and advancements in our field. If selected as a committee member, ensuring that the annual meeting maintains a strong educational mission would be a core focus I would maintain during my tenure.

Nick Vukotic - Meetings Committee

Assistant Professor
NSERC/PROTO Industrial Research Chair
Department of Chemistry and Biochemistry
University of Windsor
ON, Canada

Education:

B.Sc. Biochemistry (Honours) University of Windsor (2009), Ph.D. Chemistry, University of Windsor (2014), Industrial Post-doctoral fellow with PROTO Mfg. Ltd. (2014-2016)

Professional Activities:

Member of the (CNCC) Canadian National Committee for Crystallography (2019-), Member of the (CIC) Chemical Institute of Canada (2007-), Member of the Royal Society of Chemistry (2017-)

Research Interests:

Powder X-ray diffraction, in-situ XRD, small molecule crystallography, materials chemistry, stimuli-responsive crystals, high-throughput screening, nanoporous adsorbents, metal-organic frameworks, chemical sensors, biomaterials, crystal engineering.

Statement:

I would like to thank the nominating committee for considering me as a candidate for the ACA meeting committee. I would be happy to support the ACA and its activities in this capacity. My passion for X-ray diffraction and crystallography started very early in my research career after I solved my first structure of a hydrogen-bonded network. The ability to visually observe the interactions between molecules and deduce the fundamental driving forces for molecular self-assembly were simply fascinating to me. As an undergraduate student, I was fortunate enough to attend some wonderful conferences and workshops focused on crystallography which further spurred my interest in the field. My graduate work on incorporating dynamic interlocked molecules into metal-organic frameworks then exposed me to powder X-ray diffraction as an extremely valuable method for studying the structure property relationships of materials.

After graduate school, I decided to pursue a career in industry working for PROTO Mfg. on specific applications of XRD in industry and developing X-ray diffraction instrumentation. This was extremely gratifying, as the environment allowed me to learn much more with respect to how XRD is used in various industries around the world and also gave me a much deeper understanding and appreciation for the X-ray sources, goniometers, optics, and detectors required for XRD instrumentation. Currently, I run a research program at the University of Windsor dedicated to developing new stimuli-responsive crystalline materials, in addition to developing XRD instrumentation and in-situ devices with the help of PROTO Mfg. I am also a current member of the Canadian National Committee for Crystallography which promotes the advancement of crystallography in Canada and throughout the world. I believe that my previous industrial experience and being an early career academic researcher allows me to bring a unique perspective to the ACA meeting committee.

The 2019 joint meeting of the Pan-African Crystallography Conference and the African Light Source

Group photo of the PCCr2/AfLS2 participants. Photo by George Dwapanyin.

Teeming with excellent science and rich cultural experiences, the joint meeting of the Pan African Conference on Crystallography (PCCr2) and the African Light Source (AfLS2) held in early 2019 in Accra, Ghana was truly a conference like no other. Build around the theme "Crystallography, a tool for sustainable development in Africa", many of the scientific presentations included work that highlighted the unique opportunities found across the African continent. One example with potential economic impact is the work by Mark Bediako in which he illustrates how calcined clays from Ghana may be used as supplementary cementitious materials. While exciting keynote presentations are always a pleasure, I was particularly moved by several of the student presentations. Witnessing young students deliver, in English (for many their non-native language), a presentation that was for many their first was as inspirational as it was humbling.

A small sample of the many performers integrated into the conference. Photo by George Dwapanyin.

However, the theme of sustainable development echoed well-beyond individual scientific advances and exhibited notable resonance when presenters discussed a synchrotron in Africa – or more to the point – the lack thereof. With the exception of Antarctica, Africa is the only continent on the planet without a synchrotron. In order to conduct the cutting-edge research that these facilities enable, African researchers must leave not only their home country but their continent. As the audience heard from several participants, many times these researchers do not return – an emigration termed the African Diaspora. A large portion of the meeting was thus devoted to highlighting and promoting efforts to establish a light source on the African continent. Part of this effort involves creating and/or sustaining important scientific organizations like the ACA, that will help organize the existing community of scientists and also train and grow the next generation. Given the unity and shared sense of purpose on display by meeting participants, an African synchrotron seems inevitable and when completed will dramatically enhance the growth and opportunity that is being realized through the exciting crystallography of this truly inspirational continent.

Jason Benedict with PCCr2/AfLS Local Organizing Chair Robert Kingsford-Adaboh from the University at Ghana.

Jason Benedict

Some of the awesome student helpers serving up great traditional eats which included banku and fufu! Photo by George Dwapanyin.

2018 U. S. Crystal Growing Competition

"We restructured our curriculum to accommodate crystal growing and it made for a fun year. Can't wait to do this again!" – Thank You note excerpt from educator Laura McMillen of Powdersville High School in Greenville, South Carolina.

I've said it before, and I'll say it again: Kids and teachers love growing crystals! Nearly 260 teams from schools and households in 42 states (up from 160 teams in 36 states in 2017) signed up for the fifth running of U.S. Crystal Growing Competition (USCGC, http://www.uscrystalgrowingcompetition.org/). Hundreds of kilograms of alum went out, and over 150 crystals were sent back to the University at Buffalo (UB)! In fact the contest is growing so much, we welcomed a new assistant, Tasha Benedict (UB)! And we're sending out so much alum that some of it is now being shipped by the three regional coordinators: Michael Nippe (Texas A&M University, TAMU), Fernando Uribe-Romo (University of Central Florida, UCF) and Karah Knope (Georgetown University, GU). Sponsored in part by ACA, the USCGC continues to bring the science of crystals into America's classrooms. As we've observed previously, the crystal growing abilities of the participants continues to improve!

Chemistry professor Jason Benedict (center) at the start of the judging of the 2018 U.S. Crystal Growing Competition. Photo by Douglas Levere/UB.

The 2018 USCGC, which once again began during National Chemistry Week in mid-October and concluded in early December, was judged by a number of veteran judges that included UB Professors from Chemistry: Timothy Cook, Ekin Atilla-Gokcumen, David Lacy, and Luis Velarde. The contest welcomed back veteran USCGC judge Andrea Markelz, UB Professor of Physics. The contest was aided by some new judges: Graduate students Nicole Vanagas (GU), James Vanjak (TAMU), and Demetrius Vazquez-Molina (UCF).

Winner of the 1st place Overall for grades K-8, 6th grader Dimitri Agdanowski from Kalamazoo, MI with Krystle Dorris of The Weather Channel's "Prospectors," Steve Arnold from The Science Channel's "Meteorite Men," and Eric Rintamaki who discovered "Yooperlite" showing off his 2018 USCGC certificate at the Kalamazoo Geological and Mineral Society's Rock Show on May 4, 2019. Photo by Keith Agdanowski.

No longer does the northeast dominate the USCGC - winners dotted the entire nation! For grades K-8, 6th grader Dimitri Agdanowski from Kazoo School (Kalamazoo, MI) won 1st place Overall. Mr. Walstrom's 3rd grade class from Monte Vista Elementary School in Albuquerque, NM won 2nd place Overall. And we had a tie for 3rd place Overall: 3rd grader Benjamin Muchnik from Manhattan School Plus (New York, NY) and 5th grader Tim Yap from Windermere Elementary (Williamsville, NY). A team of Chris Ann Slye's 7th graders from Maumee Valley County Day School took home 1st place quality!

10th graders and winners of 1st place Overall for grades 9-12, (Left to Right), Juliette Atkinson, Ava Berry, Sadie Frankel, Emma Boardman from Lucy Walter's class at Old Lyme High School in Old Lyme, CT. Is that a USCGC slideshow in the background?!? Awesome!!! Photo by Olivia Stack.

All entries are on display on the 7th floor of the Department of Chemistry Natural Sciences Complex at the University at Buffalo. Photo by Jason Benedict.

In the 9-12 grade section, 1st prize Overall ($200) went to Lucy Walter's 10th grade students from Lyme-Old Lyme High School (Old Lyme, CT). A pair of 12th graders from Donna Malkmus's class at Francis Howell North High School (St. Charles, MO) won 2nd place Overall grades 9-12. Gwendolyn, Gregory, and Peter from the Trinity Academy Homeschool (Moore, OK) won 3rd place Overall. Taking home 1st place quality were a team of 11th grade students from Bradley Miller's class at J.C. Harmon High School (Kansas City, KS).

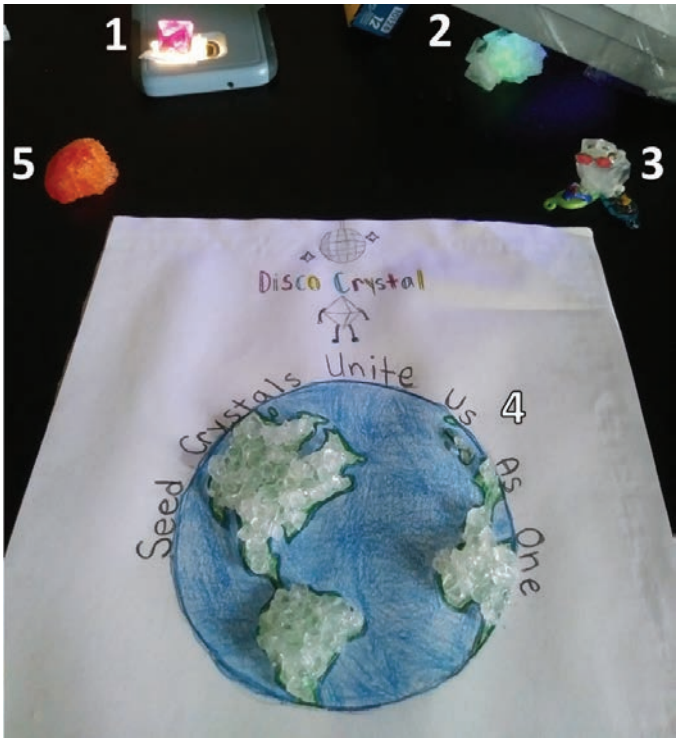


Image of the top five 'Coolest Crystals' for2018. Photo by Gage Bateman.

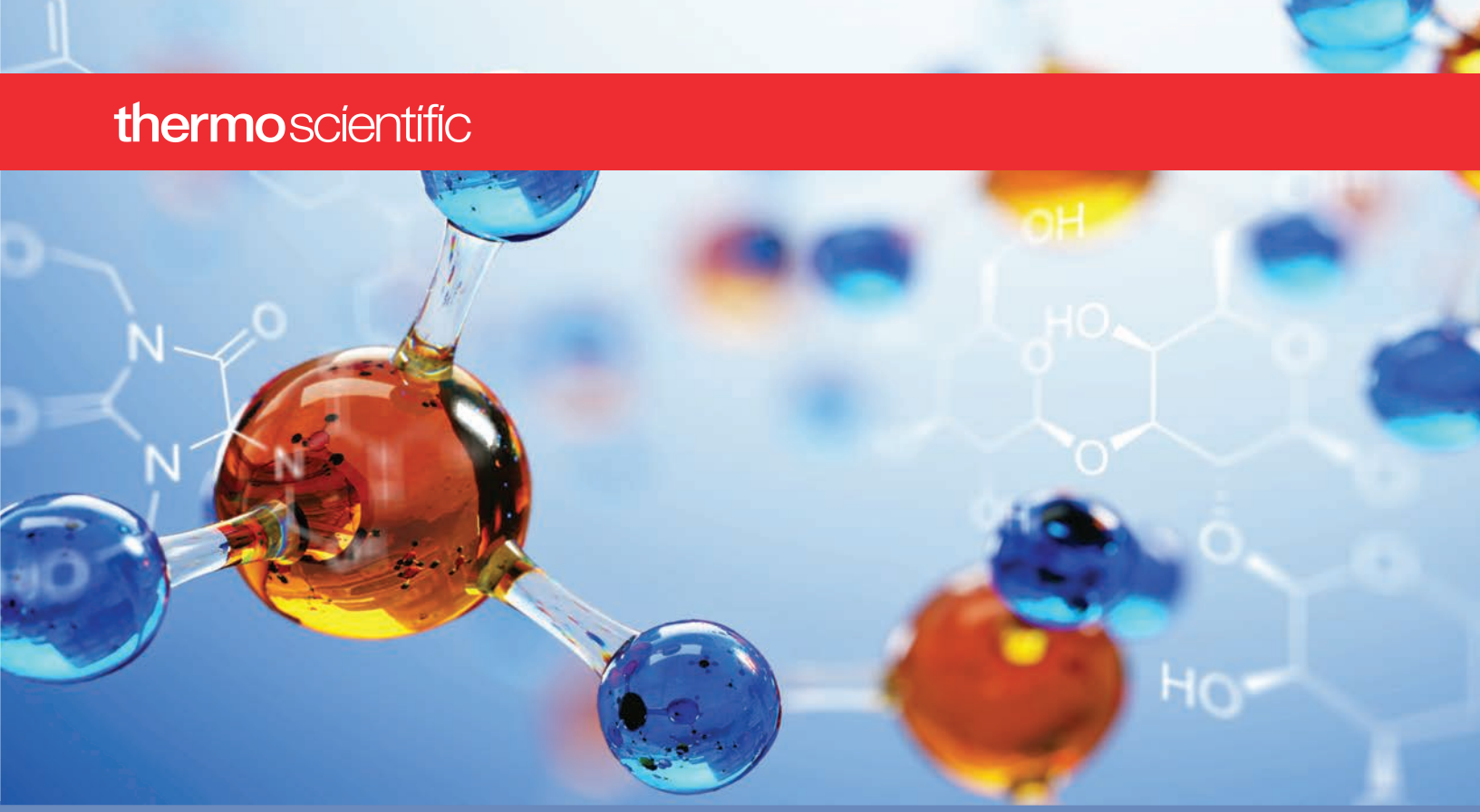
The 'Best Teacher Crystal' was won by John Thurmond of the Illinois Mathematics and Science Academy (Aurora, IL). And finally, with their submission of a beautiful purple/crimson crystal of alum, the winners of the 2018 Coolest Crystal was a team of 10th and 11th graders from Laura McMillen's class at Powdersville Highschool in Greenville, SC!

Social media remains one of our best tools for advertising and providing contest updates! The winners were announced via the contest Twitter account, @USCrystalComp. Check out all the winners and some great participant posts (e.g. Jim Burdick's dissolving crystal data!) at ***#2018USCGC*** on Twitter!

The USCGC helps raise public awareness of the importance of crystal-based research and the organizations, including the ACA, that promote and support these important activities. The USCGC gratefully acknowledges the Benedict Research Group graduate students, and the support of our sponsors: ACA, National Science Foundation, Ward's Scientific/VWR, Bruker AXS, Krackeler Scientific, Cambridge Structural Data Centre, the Western New York section of the American Chemical Society, the Departments of Chemistry of UB, GW, UCF, and TAMU. Please consider making a tax-free donation to the 2019 contest! For more information, please visit the USCGC website or e-mail Jason Benedict at jbb6@buffalo.edu.

Jason Benedict

thermo scientific



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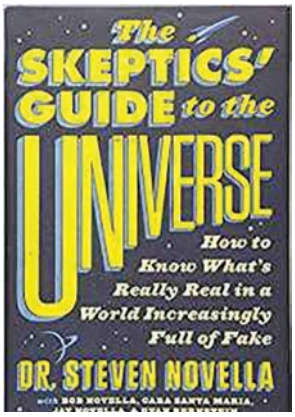
Book Reviews

The Skeptics Guide to the Universe: How to Know What's Really Real in a World Increasingly Full of Fake

Dr. Steven Novella with Bob Novella, Cara Santa Maria, Jay Novella, and Evan Bernstein
(ISBN: 978-1-5387-6053-6)



The Skeptics Guide to the Universe is a wonderfully comprehensive work for anyone who already identifies as a skeptic or who wants to become a well-informed one. Podcast fans might recognize the title—it is shared with a weekly show hosted by Dr. Steven Novella and his team of co-authors.

The book will probably take longer to read than listening to an episode of the podcast--or even several. Coming in at almost 450 pages, The Skeptics Guide delivers just what its name implies: a guide to the universe for those of a more skeptical nature. The book is broken down into 5 sections: Core Concepts Every Skeptic Should Know, Adventures in Skepticism, Skepticism and the Media, Death by Pseudoscience, and Changing Yourself and the World.

The first of these sections, Core Concepts Every Skeptic should know, is the longest and most densely packed with information. In the first 316 pages of the book, Novella lays the fundamental groundwork for skepticism. This section is subdivided into the following categories: Neuropsychological Humility and Mechanisms of Deception, Metacognition, Science and Pseudoscience, and Iconic Cautionary Tales from History.

Novella uses a lot of technical jargon, especially in these earlier chapters, while laying the foundational groundwork for a healthy understanding of skepticism. Novella does an excellent job explaining this jargon, and illustrating each term through vivid examples, but if you don't pay attention in the first section, you will be lost in the latter part of the book. The first section almost feels like a very reader-friendly, well-written textbook on skepticism, and the latter sections are more like a work of popular science that could be titled Skepticism and the Real World..

It's these later sections, especially "Adventures in Skepticism," where the book really captures the reader's attention. Once Novella is done teaching the fundamentals of skepticism, he applies them to entertaining and exciting real-world scenarios. "Adventures in Skepticism" brings each co-author to the fore, with an anecdotal adventure into skepticism. One of these, told by Evan Bernstein, involves ghost hunters Ed and Lorraine Warren. You might recognize their names from The Conjuring film franchise. Several of the films in the franchise, which includes spin-offs like Annabelle, focus on real cases the Warrens worked on--although the "realness" of the supernatural events depicted should be approached with a healthy dose of skepticism.

Given the author's role as host of a podcast of the same name, the structure of The Skeptics Guide makes sense. Treat each subdivision of the first section as its own section, and each subsequent shorter section (2-5) as their own, as individual episodes of a podcast if you will. Stop reading to pause and contemplate what you have read before diving into the next section, and you will probably have a more fruitful reading experience that someone who tries to read the whole book in one sitting.

Jeanette S. Ferrara, MA

Broken Ballots: Will Your Vote Count?

Douglas W. Jones and Barbara Simons
(ISBN 978-1-57586-637-6)

Broken Ballots: Will Your Vote Count? is the product of a collaboration between Douglas W. Jones, a computer science professor at the University of Iowa, and Barbara Simons, a former IBM Research employee. Broken Ballots takes a deep, methodical dive into the popular vote tradition in American electoral history and the automation of the voting process, making certain repeating patterns of election controversy quite clear.

Jones and Simons begin with a brilliant opening line: "This book should never have been written." It's a bold opening statement that's immediately followed up with a detailed explanation: "In 1934, the Brookings Institution published a great book by Joseph Harris, entitled Election Administration in the United States. Had people followed Harris' advice, there would be no need for our book." However, to state the obvious, people—namely the government officials making election-related decisions for the past eighty years—did not follow Harris' advice. It's startling to consider that election tampering and voter fraud was enough of a concern 80 years ago for someone to write a book about it. And these election-related cracks in American democracy were not new then—they'd been slowly spreading since the birth of the nation. How far we simply haven't come becomes quite apparent the further the reader gets into Broken Ballots.

Given the extensive government inquiry following the 2016 presidential election and the level of turmoil regarding the validity of each American's vote, one might suspect that Broken Ballots was published in the aftermath of that election. They would be incorrect.

Broken Ballots was published in 2012—and the tumultuous election to which the authors make the most reference is that of 2000. For those readers who need a refresher on what made the outcome of that election so contentious, Al Gore lost the electoral college vote to George W. Bush thanks to Florida even though he won the popular vote. After a recount and a Supreme Court decision, Bush was declared the winner. But many suspected that certain discrepancies in the voting process could be attributed to flaws in the Votomatic machines that many Floridians used to cast their vote.

Swap out Bush for Trump, Gore for Clinton, and the Florida debacle with Russian election tampering, and the overall outcome of the 2016 election parallels that of the 2000 election quite eerily. Even though Simons' and Jones' book is almost 7 years old at this point, the content is hardly dated. If anything, it should be required reading for high school students taking AP Government. Jones and Simons address the dangers of online voting and the ease with which voting machines can be tampered with and internet voting can be hacked by a third party. More than 4 years before the 2016 election, they were basically telling their readers how it would end.

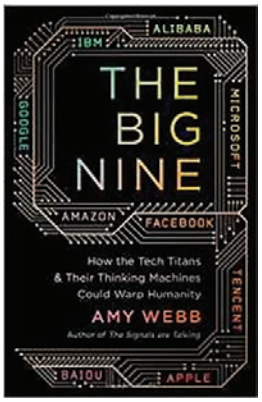
It's not clearly marked which chapters or sections were authored by Jones or Simons. The writing is clear and seamless—no one section seems more or less well written than any other. Anytime either author appears as a character in the narrative, so to speak, they are referred to in the third person. The rather interesting narrative decision has the effect of conveying to the reader both that Jones and Simons themselves have nothing to hide and emphasizes their importance in the perhaps rather small sphere of academically-inclined experts in electronic voting.

Simons and Jones have the unique talent of taking a rather pedantic subject and making it more than palatably interesting. I recommend reading Broken Ballots before the next time you cast a vote.

Jeanette S. Ferrara, MA

The Big Nine: How the Tech Titans and Their Thinking Machines Could Warp Humanity

Amy Webb (ISBN: 978-1541773752)



Forget Stephen King. If you want to read something nightmare-inducing, pick up Amy Webb's newest book, The Big Nine. Webb, a quantitative futurist and professor of strategic foresight at NYU's Stern School of Business, presents a vision of humanity's future that doesn't have much humanity in it. It is scary—real world scary, not vampires and haunted hotels scary.

The rise of artificial intelligence in recent years (newsflash: it's already here) gives many in the academic community like Webb reason to pause. For a lot of laypeople, their understanding of artificial intelligence—and perhaps fear or skepticism of it—stems from representations in popular culture, like HAL in 2001: A Space Odyssey. The concern that AI is ultimately created by humans, who are inherently flawed, and therefore, AI might be inherently flawed, is a real one. However, as Webb herself notes in the introduction, "This is not a book about the usual AI debates." Instead, "it is both a warning and a blueprint for a better future."

The Big Nine refers to the nine big tech companies

around the world that are at the forefront of artificial intelligence research and development. They are: Google, Microsoft, Amazon, Facebook, IBM, Apple, Baidu, Alibaba and Tencent. The first six of these form America's "G-MAFIA," as Webb calls it. The latter three form China's "BAT"--and Webb suggests they are the ones we should really be concerned about. In America, the AI business is driven by capitalism and the desire to be better and faster than the competition. Here, it's all about the bottom dollar. In China, it's about something else entirely.

But before Webb really digs into these companies, their corporate missions, and the future impact of their actions on humanity, she steps a few centuries back, providing her readers with a brief history of AI. The first part of her book, "Ghosts in the Machine," begins with a deep dive into the philosophical debate regarding mind, man, and machine. In other words, if man has a mind, and man makes machine, can the machine have a mind? René Descartes, in his Treatise of Man, expressed his belief that even if humans could make a believable automaton (or robot), it would never pass as a human because it would lack a human mind and therefore a human soul.

Technology has advanced significantly since Descartes' time. The first computational machines were invented, automation made industrial work more efficient and oftentimes safer. However, computer scientists and researchers have always strived to bridge the gap Descartes described between machine and mind. And that's where the Big Nine come in.

The Big Nine are all about pushing boundaries and surpassing the limit of previously developed technologies. Webb introduces each of the companies in the G-MAFIA and BAT, and describes their role in AI research and development, as well as her concerns regarding each of them. One of the most interesting concerns Webb expressed regarded the limited pool of people culled to work on AI projects, especially in the United States. The G-MAFIA's AI divisions consist largely of people with degrees from elite East Coast and occasionally West Coast universities. They typically have a liberal political perspective. But humans are diverse—and as a corollary, human thought is diverse. So, shouldn't the pool of people developing artificial intelligence—artificial thought one might say—be more diverse?

In the second part, "Our Futures", Webb describes three possible (and seemingly probable) future states of humanity. Webb's writing is so descriptive and detailed it's easy to forget that these events haven't happened yet. It feels like reading a history textbook where our future is already the past. Or like something Aldous Huxley and George Orwell co-wrote with Isaac Asimov about a future where artificial intelligence overrides human intelligence. If Part One didn't spook you out of your skin, Part Two will.

In Part Three, Webb hits rewind, bringing her readers back to the present, and reminding them that the future isn't set in stone. It is an admirable attempt at optimistic pragmatism, but I had a hard time feeling like anything could substantially change. Unless some kind of technological plague wipes out all our electronics, parts of what Webb describes seems inevitable. AI is already here—and the responsibility for making sure that it doesn't wipe out humanity (not humans, just humanity) lies not only on the shoulders of these tech giants, but on the shoulders of individual consumers. Holding these companies—and the AI they develop—accountable to an ethical and moral code of conduct is our responsibility.

Jeanette S. Ferrara, MA

Puzzle Corner

For summer, we have a *Crystal Connections*, a DISORDERED puzzle and a *Crystoquote*, along with the solution to the previous *Crystoquote*.

Crystal Connections #16

Find the answers to these clues and how they are connected.

1) Year in which space shuttle Columbia crashed
2) Recipient of the Buerger Award in that year
3) Originally the Red Stockings (not to be confused with the Red Sox), later the Big Red Machine
4) 1965 movie starring Steve McQueen as a poker player
5) Her wedding ceremony was held at an ACA meeting
6) The only person to be both president of the USA and the Chief Justice of the Supreme Court
7) Opened in 1866, crossing the Ohio River
8) "Happy Trails" singing cowboy
9) A good method for eating ice-cream cones

Crystoquote #4

Letter substitution reveals a quote by a well-known crystallographer

W RICA BPDEWTCF B PICKWORTH OCR RIBR GBO ORJTCF EAFCT

KH LCF BAF GBO BLMC RJ KWS PICKWPBMO BAF KBQC

GJAFCTUEMMH PJMJTCF OJMERWJAO BAF CZWM-OKCMMWAV

XTJFEPRO. - *YCAAH VMEOQCT*

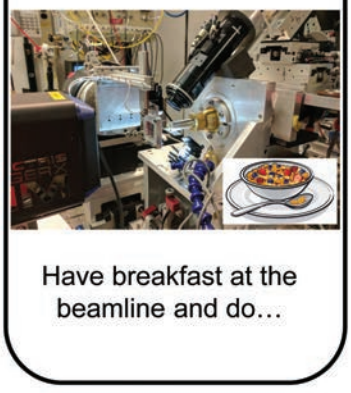
DISORDERED

Shoot at these random words sequentially to make the full pattern

GASLINC	
RTCLASSY	
GILYOOB	
SHAPING	
CROTLENE	
AGREES	

Answer:

" "



Joel Harp (Vanderbilt University Center for Structural Biology) provided the solution to *Crystoquote* #3.

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

Solution to *Crystoquote* #3:

In fact, it is the exceptions or outliers that ignite our curiosity and lead us to new experiments, new theories, and new developments. - *Joel Bernstein*.

JULY 2019

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

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

AUGUST 2019

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

OCTOBER 2019

7-10 **4th Meeting of the Latin American Crystallographic Association,** Bucaramanga, Colombia
https://www.lacacristalografia.org/

DECEMBER 2019

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

17-20 **Asian Crystallographic Association,** Singapore
http://www.asca2019.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

JULY 2021

30-3 Aug **ACA 2021 Annual Meeting**. Baltimore, MD
http://www.AmerCrystalAssn.org

JULY 2022

29-2 Aug **ACA 2022 Annual Meeting**. Portland, OR
http://www.AmerCrystalAssn.org

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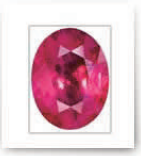

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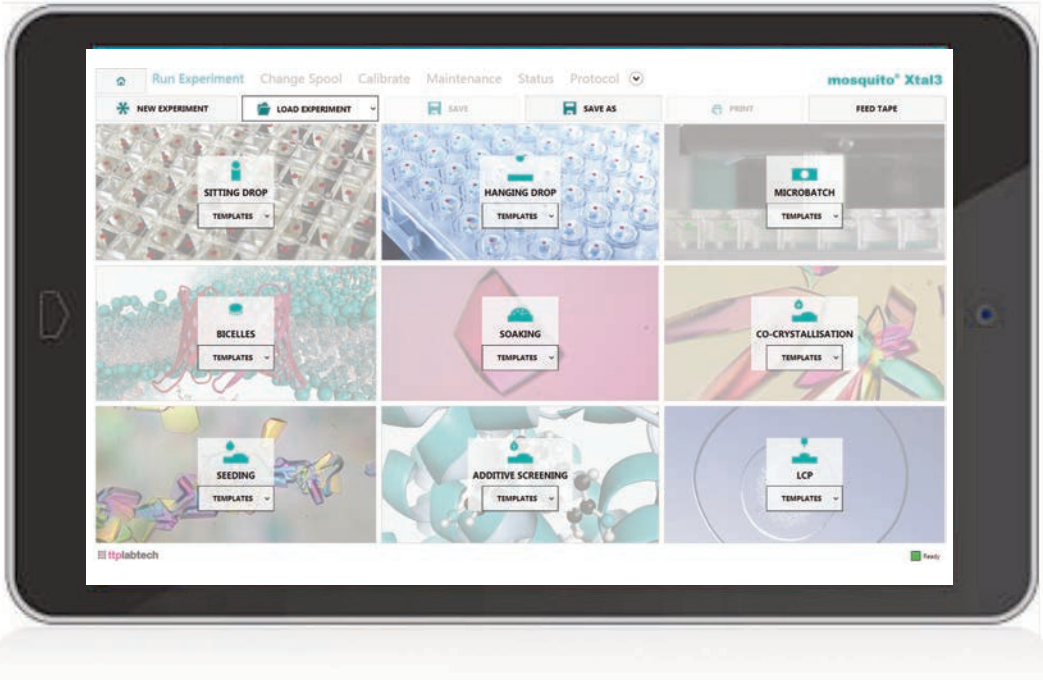

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