ACA RefleXions

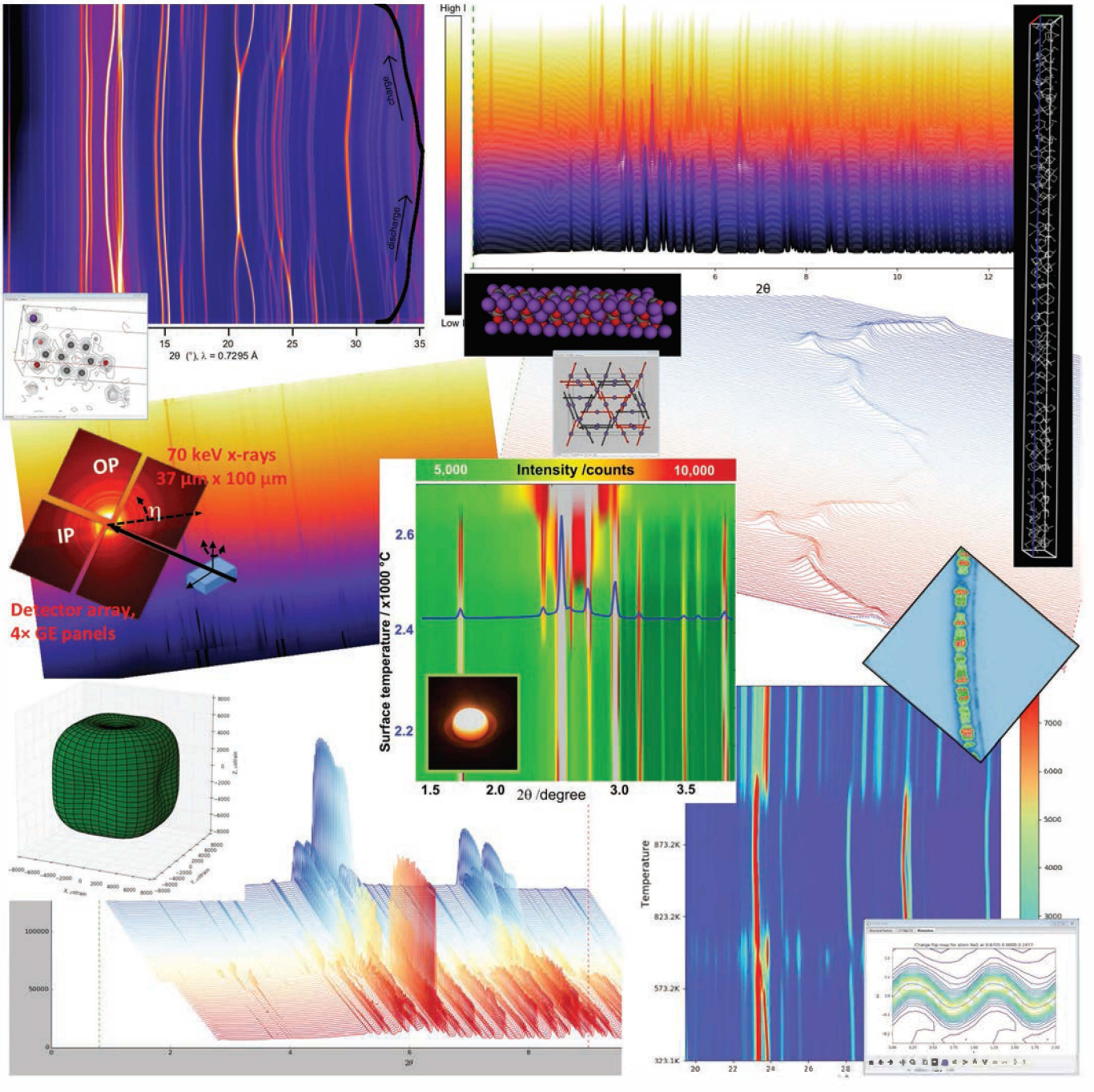
American Crystallographic Association

Structure Matters

Number 3

Fall 2019

Graphics from GSAS-II Users



Robert Von Dreele and Brian Toby Receive Trueblood Award

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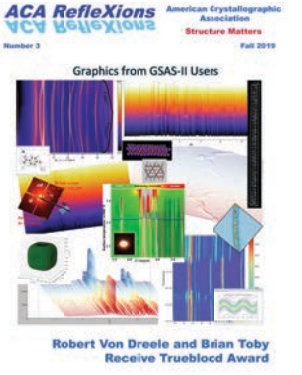
Joseph Ferrara
2019 ACA President



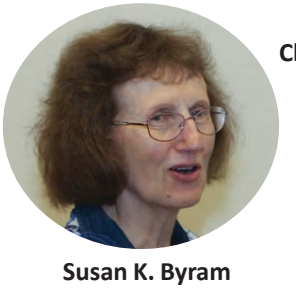
Robert Von Dreele and Brian Toby received the Trueblood Award for 2019. The cover images are described in the 'What's on the cover' page 5.

2019 ACA Fellows

Craig M. Brown

Elspeth F. Garman

Charles W. Carter, Jr.



Susan K. Byram

Xiaoping Wang

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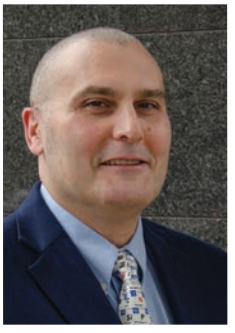
President's Column



Joseph Ferrara

It is hard to believe that this is my last column as President of the ACA. As I write this I still have 5 months to go in my term, so I may take the liberty of a short Past President's column in November.

This column comes just after the 2019 Annual Meeting in Covington. All indicators suggest it was a success, both from scientific and financial points of view. The scientific program drew over 550 people. As a result, we expect some net income, which will help offset ACA operating expenses.

On July 19, we held Bystander Training for a group of about 30 people, including Council, SIG chairs and vendors. It was a success and I look forward to more activities like this that enhance the meeting experience. In addition to the bystander training we received on the 19th, we have more tools coming from the Societies Consortium on Sexual Harassment in STEMM in 2020.

The opening session, celebrating the life of **Michael Rossmann**, was well received. I have to admit the humor in **Jack Johnson**'s eulogy made it a very tough act to follow, but the last speaker left us in awe with the placement of Michael on a "special position".

The Class of 2019 Fellows was announced at the opening ceremony. They are **Craig Brown**, National Institute of Standards and Technology; **Susan Byram**, Bruker Corp.; **Charles Carter, Jr**., University of North Carolina; **Elspeth Garman**, University of Oxford; and **Xiaoping Wang**, Oak Ridge National Laboratory. This year, at the Fellows Reception, every Fellow, past and new, received a certificate and pin.

At the meeting, Council learned about the Education Committee's proposal for a Certified Crystallographer. This is exciting because earning and maintaining certification can really benefit members, particularly those early in their careers. Furthermore, the IUCr is interested in creating a similar program based on ours. The Education Committee will provide more details in a future issue.

The Business Meeting was held on the 23rd. While we had a reasonable turnout, I would like to see more members participate. Thus, next year we will hold the meeting orthogonal to all other activity to maximize participation. At the business meeting this year we announced the 2020 award winners: A. L. Patterson Award to **Václav Petříček** of the Institute of Physics of the Czech Academy of Sciences; David G. Rognlie Award to **James Holton**, Lawrence Berkeley National Laboratory and the 2020 Margaret C. Etter Early Career Award to **Nozomi Ando**, Cornell University.

One of the topics we broached at the business meeting was the question of whether a name change would better reflect the broad nature of the science being done by the members of the ACA and presented at our meetings. This includes, but is not limited to, X-ray, neutron and electron diffraction, small angle scattering -- both neutron and X-ray, NMR structure determination and cryo-electron microscopy, where all the methods are being employed to determine the structure of molecules and materials. This is not going to be an easy task and we welcome meaningful suggestions.

I had hoped we would end the year with a surplus in the budget. Current projections indicate we will end with a small deficit. While disappointing, it is a marked improvement over last year's large deficit. The good news is that the bookkeeping is now transparent with QuickBooks Online and next year's budget will be more accurate.

Council has been looking at ways to increase membership, to bring in more revenue, and find cost saving measures to reduce expenses. One example of the latter is that through the year Council has been meeting electronically for an hour every month to conduct business. The result is that our face-to-face meetings are more productive and timely and we can decrease travel expenses. We will delay the next face-to-face Council meeting to early January, rather than October, to both reduce expenses and do a better job of onboarding the new members.

Council realizes the recent changes to the tax code make it less appealing to make tax deductible donations. Nevertheless, donations to the general fund allow us to conduct outreach and education, and provide travel grants to students and postdocs. We very much need your donations, but ask they be made to the general fund so they can be used towards the three aforementioned activities. The award funds are producing sufficient income for the awards and the principal for each award is secure.

This is the penultimate issue of RefleXions that will be printed en masse. We will switch to an e-version of the newsletter at the beginning of 2020. We realize that this may be an unpopular change, but will save the association between $14,000 and $16,000 per year. For those that still insist on a print copy, we will assess a fee of $100/year for printing and postage.

Council met with the IUCr Executive Committee as well. We learned that the Mexican Crystallographic Association and the Latin American Crystallographic Association are planning a bid to hold the 2026 Con-

gress in Mexico. The ACA and USNC/Cr are in discussion with the MCA to determine the best way to support the bid. **Peter Strickland** provided information on a number of cost savings available to ACA members as well as Associate Members of the IUCr. Members of the ACA receive a 30% discount on the International Tables and at least a 50% discount on publication fees for hybrid IUCr journals. The IUCr would like to encourage all ACA members to maintain an entry in the World Directory of Crystallographers (https://www.iucr.org/people/wdc). Further, if you become an IUCr Associate (US$200/3 years regular and US$60/3 years student) your benefits will include a 20% discount on open-access fees for articles in IUCr journals, 6 free article downloads from Crystallography Journals Online, a 50% discount on individual price of print copies of the International Tables (for personal use) and discounts from other publishers including Wiley, CRC Press and Elsevier.

I would like to remind you to renew your membership and come to meetings, convince your colleagues to join or renew and come to meetings. Most importantly, the ACA cannot function without volunteers. I invite you to organize a session or workshop, nominate a colleague for ACA Fellow or ACA award, and bring ACA promotional materials to other meetings.

Since this is my last column as President I need to say thank you to everyone who made my year as President so productive. **Lisa Keefe** and **Diana Tomchick** who have been on Council in the past and provided great advice and institutional knowledge, **Brian Toby** who provided fresh insights, and **Tomislav Friščić** who provided the Canadian perspective. I want to thank **Ilia Guzei** for taking such a keen interest in the books and ensuring the transition to QuickBooksOnline would be successful. I also need to thank **Steve Ginell** and **Vivien Yee** for putting together a great Annual Meeting and **Kristin Stevens** and **Kristina Vitale** for doing such a good job running the office. I can't forget to thank ALL the volunteers without whom the ACA would cease to function.

It has been a fun and productive year. Brian Toby will do a great job as President and I look forward to working with him as Past President.

Past-President's Column

Lisa J. Keefe

As the sun sets on my term as Past President, I share with you the vision for ACA that we on Council have been cultivating these past several years. Along with a steady migration from a burdensome managing role to a more effective governing role for Council, there has been a transition in focus strategically aimed at increasing the value of membership and shoring up ACA for an enduring future.

The harsh reality is that membership is declining and meeting attendance is too low to compensate for the revenue needed for ACA to thrive. Council, which includes management from ACA headquarters, has worked long and hard over recent years to implement significant cost-saving measures; at this point in time, ACA operations are exceedingly efficient and there is minimal space in which to execute further reductions. This predicament prompts us to scrutinize the value offered to our structural community both through membership and by attending our annual meeting, and to develop fresh and innovative initiatives to revitalize interest in ACA and reinvigorate engagement.

We are listening to you: lower the cost of meetings, offer more educational programs, provide more opportunities to promote our science, recognize our achievements, facilitate effective networking, expand the reach of structural science, advocate for resources that support our structural science, and the list goes on. Council has been diligently improving communications, striving for transparency and inclusivity while working to maintain the momentum of this dialogue and respond to the needs of our community.

Council's efforts have been significant. Recognizing that strong leadership is essential, Council has embraced a cohesive and collaborative governing model that has strengthened each year, from when I first joined under the leadership of Amy Sarjeant, growing throughout my tenure, reinforced during the present term of Joe Ferrara, and with confidence it will endure under the next president Brian Toby. This approach has enabled Council to make noteworthy strides in evolving the ACA and bolstering relevance.

Reflecting on recent years' efforts of Council, committees, SIGs, and a cohort of active members, the following accomplishments are noteworthy: broadened reach of structural science to embrace the cryoEM and microED communities; attractive

locations for future annual meetings (including San Diego, Baltimore, and Portland, OR) that meet ACA's space requirements while reining in costs; strategic fiscal management; modern website and tools for effective and timely communications; comprehensive and easy-to-navigate history portal for sharing legacies of structural scientists; mechanisms for integrating interactive workshops into the annual meeting; enhanced promotion of scientific accomplishments highlighted by ACA awards and recognition of ACA fellows; partnership with the new Structural Dynamics journal to regularly publish the Transactions Symposium in a dedicated issue and to highlight hot trends at the annual meetings; more avenues for member engagement including the establishment of the new Meeting Reorganization / Enhancement Committee; and the development of a variety of initiatives to increase speaking opportunities at annual meetings, facilitate meaningful mentoring activities, and augment networking to foster collaborations.

Under development are initiatives to further enrich the annual meeting experience. The banquet format has been evolving to enhance networking, first sparked by former president Chris Cahill when he replaced the Past President's speech with a dance band, and further advanced this year by changing the event to a buffet dinner on a riverboat. To augment educational activities this year, the cryoEM workshop was offered for no additional fee and, rather than be scheduled on the traditional workshop day prior to the annual meeting, it was embedded in the meeting, occurring in sessions on two separate days.

New and exciting ideas have emerged to integrate more interactive learning sessions into the annual meeting, such as workshops and short courses, in a predominantly workshop-style conference to be offered perhaps every several years. Recognizing that speaking opportunities are essential to increasing meeting attendance, coupled with the success of the 3-minute thesis competition and the keen interest of senior researchers to participate in this challenge, future session organizers are encouraged to convert some longer talks into several shorter presentations for participants at every level of their professional development. There is an upswelling of interest in developing a certification program to recognize attained knowledge in the fundamentals of structure determination and other key areas.

As I leave ACA Council, I now pass the baton to you, as a member of the ACA, to continue building on these efforts. Offer to lead a workshop or short course at an upcoming ACA meeting. Nominate a mentor or colleague for an award or for recognition as a Fellow. Renew your membership annually, which grants you access to the online resources available only to members. Contribute to the ongoing growth of ACA's online resources. Express your interest in serving your ACA and volunteer in a variety of capacities. Ensure annual representation of your lab at the annual meeting and reap the benefits of your science being highlighted. Support your students and postdocs in participating in the breadth of upcoming workshops and short courses. Attend the annual meeting yourself and engage in the multitude of networking events—benefit from the significant opportunities for cultivating new collaborations and for advancing your professional career. Join the effort to evolve the ACA.

Together, let's keep the dialogue active, explore new initiatives, develop innovative strategies to maintain relevance, and strive for a fiscally healthy and enduring ACA.

Lisa J. Keefe

What's on the Cover

The art on the cover was created using the GSAS-II package, the latest program from two careers worth of software generated by the 2019 co-winners of the Kenneth Trueblood Award, Robert B. Von Dreele and Brian H. Toby, both of Argonne National Lab's Advanced Photon Source.

One goal in the design of GSAS-II was that any intricate collection of numbers used in the program should be accompanied by a graphical display that helps make sense of those data or results. Brian commented that "most of these graphics were received in a matter of hours after a broadcast to our mailing list asking for contributions for this cover. Receiving them was also educational for me as it shows how many people are using GSAS-II for processing large collections of powder diffraction data, which I had not fully appreciated."

The credits for the figures are:

1) Kent Griffith: Operando synchrotron diffraction data during electrochemical discharge and charge of high-rate lithium-ion battery electrodes comprising complex niobium tungsten oxides. Data from APS beamline 17-BM. (Griffith et al. Nature, 2018, 559, 556-563.)

2) Georgiy Akopov (Kirill Kovnir Group): "Sunrise in a Forest of Peaks." Heating and cooling of a metal tetrel pnictide, synthesized during a reaction of a pre-arc-melted cerium monosilicide and phosphorus, APS 17-BM.

3) Gabriela B. González: area detector measurements for indium oxide thin films. (González et al., J. Appl. Phys. 121, 205306, APS 1-ID)

4) Shannon Lee (Kovnir Group): heating and cooling of a metal tetrel pnictide in a Sn flux, APS 17-BM

5) Vanessa Peterson, Christophe Didier, Zaiping Guo, & Wei Kong Pang: Sequential neutron diffraction data from a commercial battery during cycling. WOMBAT (ACNS, Australia)

6) Riley Hanus: Anisotropic strain in PbTe. This figure explained the origin of the internal-strain that softens the material's elastic moduli. (Hanus et al. Adv. Mater. 2019, 1900108)

7) Sergey Ushakov: Cubic to hexagonal phase transformation in Er2O3 above 2000 °C from diffraction on a laser heated levitated sample, collected at APS 6-ID-D.

8) Matt Kramer: Detail from Spinodal decomposition of Fe-Co-Al-Ni alloy, as cooled from 1250 to 800 C, APS 1-ID

9) Bryan Owens-Baird (Kovnir group): variable temperature reaction of Cs_xSb_y, Zn_8Sb_7, and Sb to form a single phase $Cs_8Zn_{18}Sb_{28}$ clathrate structure at circa 450 C, APS 17-BM

10) Ivan Trussov: Interesting phase transitions in sodium super-ionic conductor (NASICON).

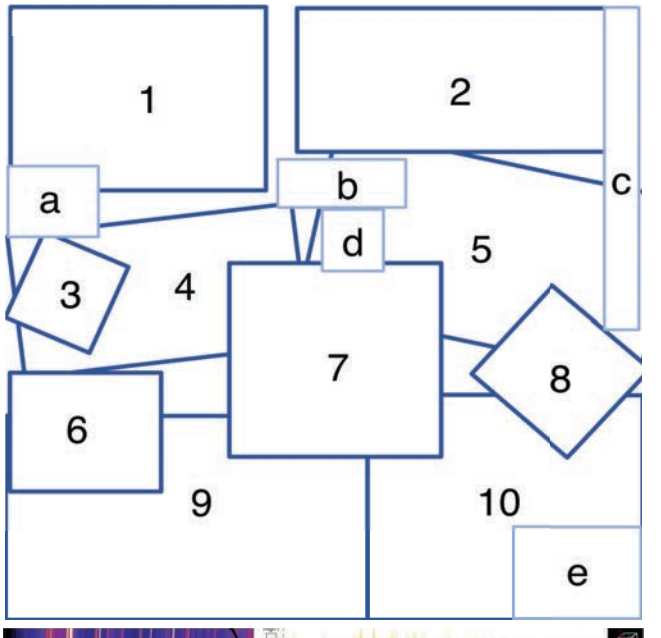
Bob wanted to showcase some of the other types of graphics available in GSAS-II and provided these images:

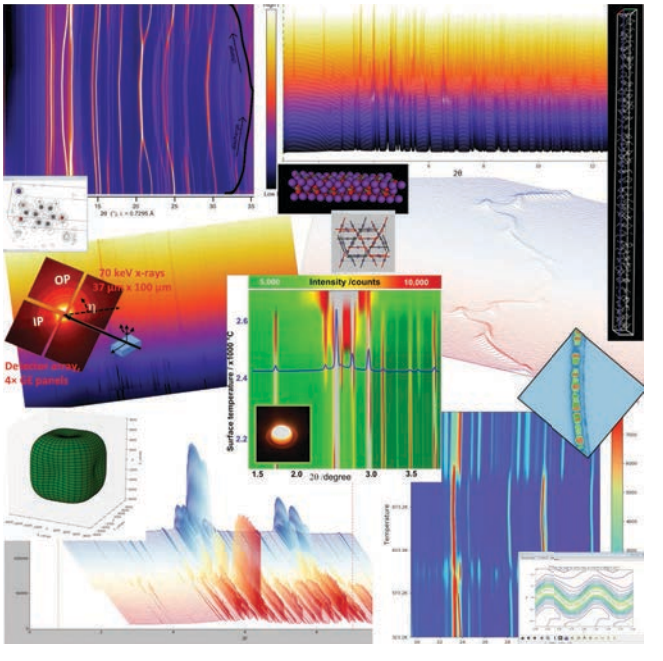
a) An electron density contour map of Na benzoate made from structure factors extracted from powder data superimposed on its three-dimensional structure (data from Peter Stephens).

b) The four-dimensional modulated structure of Na_2CO_3. This figure is actually a movie, but we do not have the appropriate technology from Harry Potter to show that. GSAS-II charge flipping result for solving structure of mcgovernite with an 8 x 8 x 200 Å rhombohedral unit cell using high resolution powder data from APS 11-BM (with Charles Lake).

d) A three-dimensional structure of Mn_3O_4 (hausmannite) with superimposed magnetic spins, solved via web interface between GSAS-II and k-SUBGROUPSMAG (Bilbao Crystallographic Server).

e) A τ-y slice in the xyzτ space from a four-dimensional charge-flipping structure solution map for Na_2CO_3 showing modulation of one Na atom position.





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Crystallography

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2019 ACA Fellows

ACA Fellows who were present at the Covington Meeting (Photograph by Richard Bromund)

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

For 2019 five new fellows have been elected: Craig M. Brown, Susan K. Byram, Charles W. Carter, Elspeth F. Garman, and Xiaoping Wang.

Craig M. Brown is Team Leader for Structure and Dynamics of Materials in the Center for Neutron Research (NCNR) at the National Institute of Standards and Technology (NIST). He manages a vibrant team that supports a suite of 7 cutting-edge, neutron instruments, 2 diffraction related and 5 spectroscopy oriented. As well as maintenance, this team continues to design, develop and improve this unique neutron instrumentation. Craig is also responsible for the well-known diffraction mail-in program at the NCNR, user support that makes the NCNR one of the most popular neutron facilities in the world.

Craig is a skilled scientist who has focused on the structure and dynamics of novel materials using mainly neutron radiation. He is at the forefront of understanding how structure correlates to properties in functional materials. Besides being a noteworthy scientist in his own right, Craig also maintains an extensive collaborative network through which some of his most important work has been carried out. For instance, Craig and his close collaborator from UC Berkeley, Jeff Long, were recognized by the DOE Hydrogen and Fuel Cells Program with its Hydrogen Storage Award "for their decades of dedication and achievements in adsorbent-based hydrogen storage materials development and characterization." He has used the infrastructure he has developed for *in-situ* neutron diffraction measurements to study the atomic nature of industrially important gases for adsorption and separation technologies. As a collaborator, Craig brings not just expertise but broad knowledge in inorganic chemistry that allows him to contribute to material design.

Training, mentoring and motivating future scientists is very important to Craig. He holds an appointment as Affiliated Assistant Professor in the Chemical and Biomolecular Engineering Department at the University of Delaware and also mentors graduate students and post-docs who go to the NCNR to collect data. He is an excellent and patient teacher who has taught hands-on approaches to analysis of powder diffraction data at a number of workshops. He has been the president of the Powder Diffraction SIG and was a session organizer for the Philadelphia ACA meeting as well as co-organizing several international symposia. He is currently a Guest Editor of the journal *Powder Diffraction* for a series of publications entitled "Crystallography and properties of metal organic framework (MOF) compounds."

Craig's publication record, his excellent technical ability, and his deep interest in educating the scientific community, current and future, in the power of neutron diffraction and crystallographic methods have made a significant contribution to the crystallographic community.

Susan K. Byram has been integral to many of the developments that have shaped modern x-ray

diffractometers. She has always been an overachiever earning undergraduate degrees in Mathematics, Physics and Chemistry from the University of Toronto and, upon graduating, being recognized by the Chemical Institute of Canada as top chemistry graduate in Canada. While an undergraduate, Sue was drawn to crystallography because of its capability to give definitive information about materials. This fascination led to her earning a Master of Science degree, also at the University of Toronto, which emphasized x-ray crystallography. Her natural affinity was for the software side of crystallographic research.

Sue's career really began when she took a position at Syntex doing software development. (Ask her about getting this job.) She was reporting to Bob Sparks and together they automated single crystal diffractometers and wrote the first commercial, minicomputer-based structure solution and refinement suite called XTL. After several years at Syntex, she became a co-founder (with Bob Sparks and others) and Operations Manager of a company that provided advanced software and automation for powder diffraction systems. This company was acquired by Nicolet and Sue became Product Manager for Powder Diffraction and then Product and Applications Manager for X-Ray Diffraction at Nicolet. Subsequently she was Product and Applications Manager of Single Crystal Diffraction at Siemens Analytical X-ray Systems, Inc. and then at Bruker AXS. In 2001 she became Business Manager of Crystallographic Systems. This position put her in control of Bruker's crystallography sales force in the USA and Canada. She also coordinated global sales activities and managed the crystallographic application laboratories and Application Scientists for activities such as demonstrations, new product testing and application courses. Throughout her career she has continued to aid all the crystallographers she encounters.

Besides all the worthwhile scientific work she has done, Sue is known for her deep interest in helping members of the crystallographic community. She is a great resource since she knows so many in the community and what they are doing. She is always – and to everyone – a welcoming presence at ACA meetings. She is known for even greeting new participants at ACA meetings who work for competitor companies. She has been a stalwart at ACA meetings since 1970 and has been an invaluable support for the ACA throughout this time. She has both presented her work and volunteered her time, most recently as Treasurer of the ACA. She taught for ten years at ACA Summer Schools.

Sue truly embodies the spirit of an ACA Fellow: great science and insight, exceptional service to the ACA and passionate outreach to the scientific community.

Charles W. Carter, Jr., Professor of Biochemistry and Biophysics at the University of North Carolina – Chapel Hill (UNC), has made contributions to science in a number of diverse fields including structural biology, experimental design, mechanistic enzymology, and the origin of genetic coding. He earned his PhD at the University of California at San Diego (UCSD) under the mentorship of Joe Kraut. During this time, he was part of the team that determined the structure of high-potential iron protein (HiPIP), one of the first protein structures to be deposited in the PDB. After post-doctoral stints at UCSD and at the MRC Laboratory of Molecular Biology at Cambridge under the mentorship of Aaron Klug, Charlie established his own laboratory in which he uses protein engineering as well as mathematical and myriad biophysical techniques to pursue his goals.

Charlie's development and study of "urzymes" – *ur* meaning earliest or primitive - and their role in evolution of the genetic code has challenged the "RNA World" hypothesis that posits that RNA alone triggered the rise of life from a sea of molecules. His work pointed out what small primordial proteins can do in the evolution of the genetic code. He was elected a Fellow of the American Association for the Advancement of Science on this basis of this work.

In addition to his significant research program, Charlie has been an exemplary contributor to the American Crystallographic Association (ACA) and also to its parent organization, the American Institute of Physics (AIP). In 2002 Charlie served as President of the ACA and from 2003-2012 he was an associate editor for *Acta Crystallographica A*. He served two terms on the US National Committee for Crystallography. Since 2004 he has held various roles in the AIP including as a member of its Board of Directors and, most recently, on the Publishing Partners Advisory Committee. His work on AIP committees has been particularly important since the AIP is the publisher of the ACA's journal *Structural Dynamics*.

In 2003 Charlie proved himself to be one of the most artistic of the members of the ACA; his past-president's talk took the form of a modern dance performance. No one who saw it will ever question

his creativity. Charlie's influential and forward-looking research, his on-going service to the ACA and his creativity in communication show him to be a talented contributor to the greater crystallographic community.

Elspeth F. Garman, Professor of Molecular Biophysics at Oxford University, is an acclaimed figure for both her high-level scientific achievements and her willingness and ability to communicate science. She has made invaluable contributions to the field of macromolecular crystallographic methods by developing tools and methods for improving the quality of diffraction data. Her pioneering efforts in developing methods to cryo-preserve macromolecular crystals have had a profound effect on the field. This is evidenced by the fact that around 90% of the more than 131,000 macromolecular x-ray structure determinations in the Protein Data Bank use these methods. Her methods are now routinely used beyond the field of macromolecular crystallography and with both laboratory and synchrotron sources. Another of her significant accomplishments that has affected the entire protein crystallography community is her development of methods for both monitoring and mitigating radiation damage of crystals. As an acknowledgement of the importance of this work, the radiation dose limit of a cryo-cooled protein crystal is called the "Garman limit." She has received several awards for her work on improving the quality of diffraction data, including the I. Fankuchen Award of the ACA and the Max Perutz Prize of the European Crystallographic Association.

Elspeth's science has included the elucidation of many important biological structures, among others, the structures of neuraminidases linked to pandemic influenza viruses and bacteria.

In addition to her influential scientific contributions, Elspeth is internationally known for her role in communicating science both to the next generation of structural scientists and to the public. Besides the teaching she does at Oxford, she is a much sought-after speaker for workshops, conferences, and distinguished lectures. She has also played a major role in the public communication of science. She is a knowledgeable, ever-willing and engaging media presence who has been interviewed on topics both specific, e.g. like avian flu, and general, e.g. *The Life Scientific*. To ensure the spread of knowledge, she has organized numerous conferences and meetings and is willing to lecture anywhere - in schools, in pubs, in museums. Her editorial roles have been another way she has given her time in service to the communication of science. Among them are the co-editorship of *Acta Crystallographica D* since 2008 and the co-editorship of the *Journal of Applied Crystallography* from 2008 – 2013.

Elspeth's extensive engagement in communicating crystallography, and science more generally; her excellent mentorship of the next generation of scientists; and her work that has dramatically changed the way macromolecular crystallographic data is collected show her to be a significant contributor to the crystallographic community.

Xiaoping Wang is Senior Scientist in the Neutron Scattering Division at Oak Ridge National Laboratory ORNL. He was originally an inorganic chemist, earning his PhD and holding a postdoctoral appointment with F.A. Cotton. In his book, *My Life in the Golden Age of Chemistry*, Cotton applauds him as making critical contributions to the most difficult structures. As a complement to his inorganic work, he took a postdoctoral position at the Intense Pulsed Neutron Source at Argonne National Laboratory with Arthur Schultz. He started his career as Director of Crystallographic Computing at Texas A&M University and, subsequently, as Director of the X-ray Diffraction Laboratory at the University of North Texas becoming an experienced chemical crystallographer who used both x-ray and neutron diffraction.

While working as Director of the X-ray Diffraction Laboratory, he became a member of the Instrument Development Team for the SNS-single-crystal neutron diffractometer TOPAZ. In 2008 Xiaoping took a position as Senior Scientist at the Spallation Neutron Source (SNS) at ORNL, becoming the SNS

TOPAZ Point of Contact. The commissioning of TOPAZ was difficult but Xiaoping played an essential role in making the SNS TOPAZ single-crystal instrument the leading facility of its kind in the US and one of the premier facilities in the world. As Point of Contact for TOPAZ, he has done a superb job of working with the community to leverage TOPAZ's unique capabilities, e.g. of neutron time-of-flight single-crystal diffraction.

Xiaoping is an active volunteer. He was Chair of the Small Molecule SIG and is currently a member of the Editorial Board of *Acta Crystallographica C, Structural Chemistry*. He is an enthusiastic and informative speaker and is frequently invited to lecture. He has given numerous workshop presentations on the use of TOPAZ and has organized sessions at the ACA.

Xiaoping has demonstrated a high level of excellence in neutron chemical crystallography research and has taken a leading role in making it accessible and understandable to other scientists. His professional service has expanded the neutron user community both among senior and junior researchers.

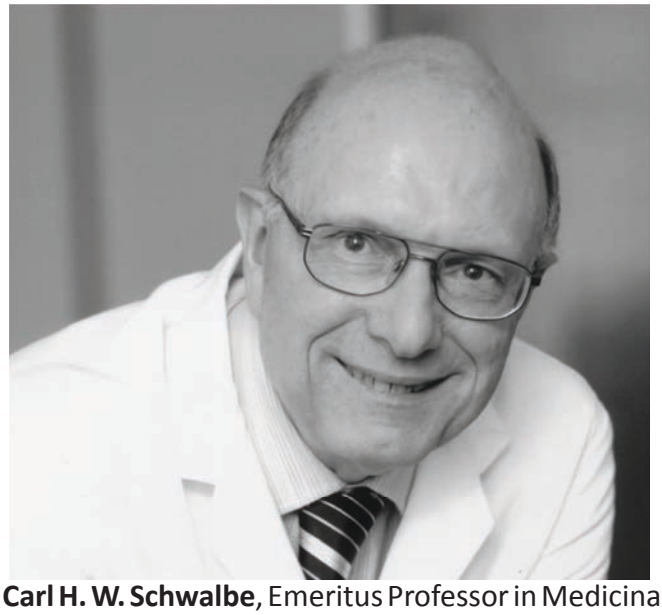
Kay Onan

Obituary – Mark Beno

Mark Beno, Senior Chemist at the Advanced Photon Source at Argonne National Laboratory, passed away suddenly on August 24, 2019 at the age of 68. Mark earned his PhD at The Ohio State University with a focus on chemical crystallography. A postdoctoral appointment at Argonne National Laboratory led to a career there. He carried out neutron and x-ray crystallography, moved to becoming Group Leader of the Basic Energy Sciences Synchrotron Radiation Center and then moved, with his group, to the X-ray Science Division. His leadership roles have included Deputy Division Director, Associate Division Director for beamline operations and, most recently, Interim Associate Division Director.

Mark was well-known for the time he spent on the APS experimental floor, walking around talking with all the staff and users about the beamlines, projects and current experiments. He was always ready to share ideas and give advice. It was important to him that everyone felt comfortable and respected. The APS community will miss him.

Obituary – Carl Schwalbe



Carl H. W. Schwalbe, Emeritus Professor in Medicinal Chemistry, Aston University, and Emeritus Research Fellow, Cambridge Crystallographic Data Centre, passed away on August 1, 2019, following a short illness. Carl was well known to many in the international crystallographic community, and especially to those in the British Crystallographic Association. For the past 10 years he was the much-loved editor of their news magazine, Crystallography News.

Born in 1942 in Ohio, USA, Carl studied at Oberlin College (AB in chemistry) and Harvard University (PhD with William Lipscomb) and then took a post-doctoral position at the Max Planck Institute for Experimental Medicine. It was there that his interest in applying crystallography to drug discovery and dosage form design was stimulated. He followed this interest to an appointment in Aston Pharmacy School at Aston University in Birmingham, UK, where he spent his entire career, as Lecturer, Senior Lecturer, and then Professor of Medicinal Chemistry.

Carl regularly attended IUCr Congresses and American Crystallographic Association (ACA), European Crystallographic Association (ECA), German Society for Crystallography (DGK) and British Crystallographic Association (BCA) meetings. After he retired in 2010, he continued to enjoy these meetings as a way to extend his academic life and scientific community. He also continued scientific work; his last research project looked at the challenges of correct tautomer determination which led to questions of how best to remediate those, and other, problematic cases contained in the Cambridge Structural Database.

Kay Onan

Anton Paar

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Trueblood Award Acceptance Talk

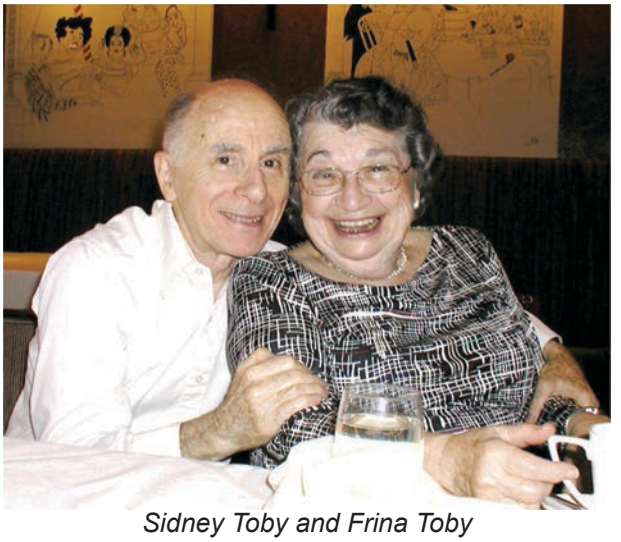
Brian Toby, co-recipient (with Robert Von Dreele) of the 2019 Ken Trueblood Award, made the following presentation at the award ceremony in Covington.

Brian Toby

APS Chief Computational Scientist,
Senior Physicist, Group Leader
Argonne National Laboratory

ACA Vice President

As I was preparing to give this talk, being so honored by my professional peers with the Trueblood award, I thought about some of the lows and highs I have seen in this journey. I regularly speak with young scientists who are struggling with launching their careers – and I do believe it has gotten harder – but I want to hold out hope that the wonderful level of recognition that I am experiencing with this award is not reserved only for those who have charmed career trajectories, consisting of successive breakthroughs and recognitions. I have worked hard, but recognize that my career was driven as much by things I could not control. I have benefitted from chance opportunities and the kindness of mentors. This award talk provided an occasion where I could thank some of those people who influenced my career the most, though not everyone deserving, alas. Finally, I can't give a talk without some science content and I used the lecture to talk about subgroups and supergroups and how that relates to getting structures right.



Sidney Toby and Frina Toby

So, launching into the people I wanted to thank, let me start with my parents. I did not grow up with much self-confidence, in part because I was a terrible student from early grades through high school (I even repeated 3rd grade). Nonetheless, each of my parents were very important in launching my interests in science. My father, 89 in May, is a retired physical chemistry professor from Rutgers who always enjoyed his work, had a constant interest in learning more and was willing to teach me how things work and how to fix things, both around home and occasionally in his lab. Having now raised children of my own, I admire his patience with "let me help daddy." My favorite thing to do when in his charge as a child was sit in his lab doing glass blowing or wander around collecting the little beads of mercury that were scattered all about his lab into an empty squeeze bottle. (All contemporary safety officers are now shuddering.)

My father was born in London and as a school child there experienced the very severe bombings of WWII. After a short post-war stint in the Royal Air Force, and an undergrad degree from Queen Mary College, he then came to McGill for his Ph.D., where he met my mother who was getting her B.A., also at McGill. My mother, who just turned 90, wanted to be a physician, but that was prevented by "kind" relatives who did not believe in educating women for a profession. She did enroll later to get a Ph.D. in biochemistry, when my sister and I were quite young. Our demands were no doubt partly responsible for her "flunking out with a masters." Having trouble finding a job, but wanting to do something in science, she started volunteering in my father's lab, where she initiated his group's use of the Rutgers' computer (yes, there was only one back then) for data analysis. From her I got my first exposure to computing. By the time I was in high school, I was writing programs and my mother was getting paid to teach Freshman Chemistry.

In the talk I did note that my mother's family fled from Romania just before WWII started. At the time, U.S. immigration policy strongly disfavored European Jews attempting to flee. Few imagined how bad it would actually become. Fortunately, Canada had much more open borders. Thanks to Canada, my mother's family settled in Quebec, later moving to Montreal. What would have happened without Canada? I probably would not be around to say.

My undergrad years were the first high-point in my life. As freshman (taking advantage of the Rutgers faculty brat discount), I was able to pick courses with subjects that I wanted to learn, and my grades surprised everyone – most of all me. Not mentioned in the talk was that my first publication to be written started from a dinner conversation where I suggested optimizing one of my mother's APL programs (Toby, Toby and Toby, 1978, Int. J. Chem. Kinetics, 10, 417). Interestingly, my optimization there used the same multi-dimensional linear algebra strategy we now use

with NumPy in GSAS-II.


Joseph Potenza

The summer after my freshman year, I went looking for a research job. Not so much because I expected to like it, but because I knew the salary would be low, but enough to get my parents off my back and besides if I was not paid that much I would not need to work that hard. Of the faculty I spoke to, crystallographer Joseph Potenza (himself a student of William Lipscomb) gave me the same tour of his labs that he would have given a prospective grad student, and I still remember his words, "if you choose to work here…" With just that I was sold. He was able to offer me that job because he paid me from a grant written by Harvey Schugar. Joe and Harvey ran a lab together and co-supervised students. Their lab changed my life. It was a fun group of people and we all enjoyed the research. Collaboration was the rule in Joe and Harvey's group, both internally and with the rest of the department. I ended up as a coauthor on seven more papers, which included a total of seven Rutgers faculty members (not counting the Tobys).


Harvey Schugar

Joining the group that summer were two other 1st year undergrads, Bill Schwindlinger and Steve Rudich (now both M.D.-Ph.D.s). Sometime during that summer, the professor in charge of freshman chemistry, Lester Morss, totaled up the scores for the year and told us that out of ~800 students, Bill, I and Steve had scored 1, 2 and 3, respectively. Harvey jumped on that and Number-One, Number-Two,… became our nicknames -- until I did something dumb (no memory of what) and Harvey started calling me Two-Bar, which he still does. Remembering Lester, who I very much miss, brings to mind Dan Nocera, a fairly recent ACA Wood prize winner. Dan was a year ahead of me at Rutgers, and then worked for Lester and later joined Joe's group to do magnetic spectroscopy. Dan was very impressive even back then.

Crystallography just made sense to me and the work was a good match for my strengths and weaknesses (such as I'd rather spend a day coding to avoid an hour or two of tedious work). During that time, I got to know grad students Tim Fawcett, John Rose and Bill Furey; I'd like to think that my ORTEP previewer shaved months off their grad careers. I also taught myself digital electronics and PDP-8 assembly language from schematics and source code labeled in Dutch while troubleshooting a CAD-3 diffractometer, given up for dead, that Nonius would no longer service. There were cheers around the lab when I found and replaced the bad chip and the CAD-3 again worked, (but I was still Two-Bar).


Dave Cox

When pondering grad school, I accepted the advice I got, which was that it was hard to find a job in crystallography. That advice was partly correct. It was much harder back then than it had been a few decades earlier. The less said about my grad studies perhaps the better. Grad school was an amazing time of growth for me, but that cannot be said for my thesis work in surface science. I can now see the fraction of the blame that I own, but reminders of those days still bring on PTSD symptoms. Graduating, I did not see much value in myself as a scientist and I was happy to accept a job at Union Carbide, Inc. (Rest in Pieces) that suited my self-appraisal. Fortunately and unplanned by me, Carbide wanted me to learn more about powder diffraction, and sent me to work with David Cox at Brookhaven (who invented high-resolution synchrotron powder diffraction), just as the NSLS was coming on-line. I learned so much from Dave, but more importantly, I discovered that research was as fun there as it had been in my undergrad work. I finally knew what I wanted to do and that it was not going to happen at Carbide.


Takeshi Egami

Takeshi Egami, who I met as a user on Dave's beamline, rescued me from Carbide with generous research associate and later lecturer positions at the University of Pennsylvania. I went planning to work on quasicrystals but instead got diverted to working on inventing PDF analysis techniques for studying local order in (the then brand-new) high-Tc superconductors. With Takeshi, I had the opportunity to return to NSLS, but also make many visits to IPNS at Argonne and even the ILL in Grenoble.

I can categorically say that without the mentoring of Dave and Takeshi, I would not have become the scientist that I am now; I want to thank them so much. While working at Penn I went to my 1st ACA meeting and found my professional community. Also, while in Philadelphia, I met my wife and life-partner Diane Pies Toby. More on that later.

Still, at that point in my career, I still did not see myself as being able to do academic-level science on my own and took a job at Air Products & Chemicals, Inc., which hired me to attack some cutting-edge powder crystallography problems. Despite my fears, I succeeded with them. It was a great place to work. I continued to do work at Dave Cox's beamline, but APCI also sent me often to collect neutron data at the NIST Reactor, where I gained much from the very wise and experienced crystallography team of Judith Stalick, Tony Santoro and Ted Prince.

Judy Stalick *Tony Santoro* *Ted Prince*

To my amazement, the NIST Reactor's Science Director, the late Jack Rush, invited me to interview for the position created by Ted Prince's retirement. Diane was willing to close her psychology private practice if I got that job, which is what happened. In retrospect, I would likely have stayed at APCI out of loyalty, if not for a rather needless layoff that occurred shortly before I interviewed. Such loyalty would have been quite misplaced. By now, I think every one of my coworkers from those days is no longer an APCI employee and many did not leave by choice.

Mike Rowe *Jack Rush*

Jack and NIST Reactor director, Mike Rowe, were benign despots; as a team leader I could not sign for a postage stamp, but both were also excellent managers and selfless in promoting all the good science and scientists at the superb facility. At NIST I finally started to see myself as a full-fledged scientist and I gained very much from the opportunity to work closely with Judy, from whom I also learned much.

Diane Toby

I cannot talk about my career and life journey without thanking my family. My wife Diane has been my partner in my career for about half my life now; I'd like to believe I have reciprocated. Diane is a Ph.D. psychologist who has made many sacrifices in aid of my career, including four moves that included three states (which required closing practices and retaking licensing exams.) Somehow on this journey we found ourselves joined by Jason (now 25), Josh (now 21) and our dog Rocky and each has added much to my life. My family provides me with a sense of internal security, drive and inner peace that helps me feel rooted in a way I have trouble articulating.

Josh and Jason Toby

Finally, I need to thank my co-winner in this award, Bob Von Dreele. Around the time when we each started using e-mail in the late 1980s, I began asking him questions about crystallography, Rietveld and GSAS. I have never stopped asking him questions, but now he asks me a few too. In 2005 we started working together at Argonne and it is no coincidence that soon after we envisioned the GSAS-II project.

Bob Von Dreele

I very much associate the Trueblood award with its first winner, Dick Marsh. While in grad school I had the chance to be his teaching assistant and created an undergrad p-chem lab experiment that was done (with film!) in the magnificent x-ray lab that he and Sten Samson ran. He was also on my thesis committee. Dick had a personal commitment to scouring the literature, correcting where structures could be improved by finding missing symmetry. I feel very lucky to have had the chance to meet and learn from one of the great crystallographers of my lifetime.

Dick Marsh *Linus Pauling*

Moving from Dick Marsh to incorrect symmetry, I think that the difficulty of this problem is heightened because as crystallographers we tend to look at space groups as the "rules" that structures follow and not as mathematical groups formed by collections of generators. I suspect that few people pay any attention to the International Tables Volume A section that shows what happens as generators are added or removed. As I will cover, that information is important but hard to use.

Definition: *To Marsh (verb)*

- *1) to find missing symmetry in someone's paper*
- *2) to find and publish the correct space group*

Related: to be Marshed (see embarrassment)

Crystallographers know that there are 230 distinct space groups, but thinking about them as fixed entities ignores how space groups form interconnected families. This can be seen with the graph in figure 1, which shows how about a dozen space groups are related by addition of symmetry (supergroups) or removal of symmetry (subgroups). Note how one of Dick's favorite "wrong" cases, Cc, is closely related to his common correction, C2/c.

Dick was justifiably concerned with neglected symmetry. Nothing good comes from this, as due to correlation, our programs fit the data badly and often produce implausible results. Much more accurate structural models are found after "Marshing" when the model is simplified and correlation is removed. This process is the exploring of supergroups, which Dick could likely do in his head, but myself, I need tools.

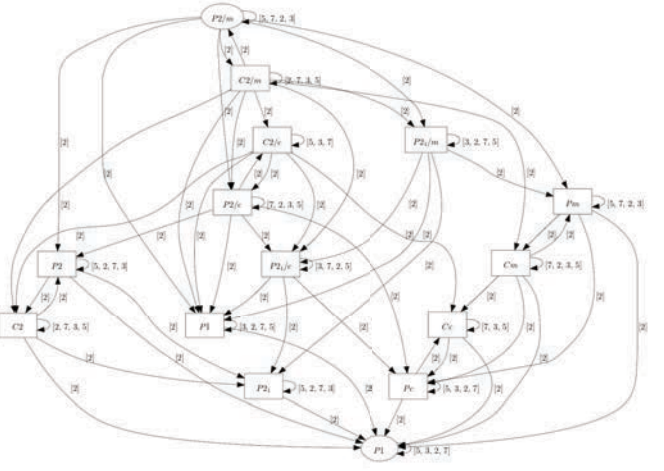


Figure 1. (generated by the Bilbao web site, www.cryst.ehu.es)

However, assuming too much symmetry can also be just as bad, but with different results. Superposition of unrelated entities can masquerade as disorder. Likewise, important useful physical properties may be missed, for example when a center of symmetry is not actually present. I like Frank Fronczek's term "Inverse-Marshing" to describe the process of determining that a lower-symmetry structure fits the data much better. Good practice in crystallography is to consider both subgroups and supergroups as possible improved models.

The problem with the subgroup/supergroup information in Volume A is that the axes redefinitions and origin shifts needed to apply them are left as "an exercise to the reader." For this reason, I.T. Volume A1 was later produced, which tabulates this much-needed information. Nonetheless, applying these transformations is still far from simple.

Fortunately, the world's heroes of crystallographic symmetry, the group of Bilbao, Spain have produced a wonderful web site, the Bilbao Crystallographic Server, www.cryst.ehu.es, which can find and transform subgroups and supergroups and much, much, more. Cutting and pasting information into this site can still be well beyond my tedium limit, but they make this treasure trove accessible to all.

Facilitating these transformations has long been a goal for me and we have made a start on implementing this in GSAS-II (figure 2). With some initial help from me in creating a mechanism for communicating with the Bilbao web site, Bob recently created a very nice interface in GSAS-II for utilizing their results for treatment of color space groups in magnetism. My

suggestion to Bob was to reuse much of that code for finding subgroups. Bob did all the work, but I will use my supervisor's prerogative of claiming partial credit for his work (but don't tell him I said that.) I also implemented one of their web methods for searching for higher symmetry cells in GSAS-II – I think Dick would be pleased.

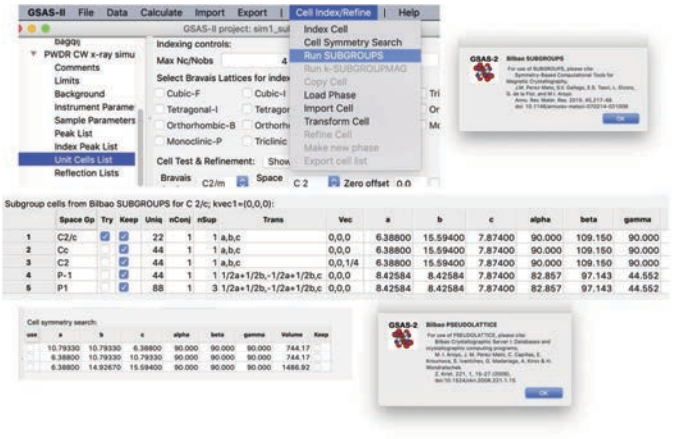


Figure 2. GSAS II support of Bilbao

For the future, there is yet another Bilbao program (PSEUDO) I want to implement for finding supergroups. When that is done, Bob and I have talked about the need for a tool for comparing different GSAS-II refinements. This will get done, but when is not clear, as ACA Council seems to be soaking up a lot of my programming "play" time.

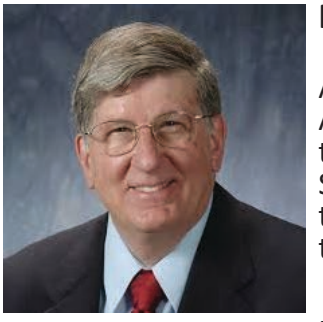
As a few concluding comments: I hope I left my audience and readers here with an understanding of how subgroups and supergroups are an important part of the crystallographic bag of tricks; I'd like to see them be better understood and easier to use. Also, with the wisdom of hindsight, I'd modify the advice I had gotten to say, while it does pay for students to think about the prospective job market, it is even more important to pick something that one likes and wants to work hard doing. I hope that the experiences I have shared will make it easier for early career scientists to understand that they too may end up, like me, behind the ACA awards podium, even if the early stages of their career are not going as desired. Finally, I want to thank the ACA and the awards committee. This award means more to me than I feel able to put into words.

Brian Toby

Trueblood Award Acceptance Talk

Robert Von Dreele, co-recipient (with Brian Toby) of the 2019 Ken Trueblood Award, made the following presentation at the award ceremony in Covington.

From 1972 to GSAS-II



Robert Von Dreele

Advanced Photon Source, Argonne National Laboratory
Senior Physicist, Computational Scientist and Computational X-ray Science

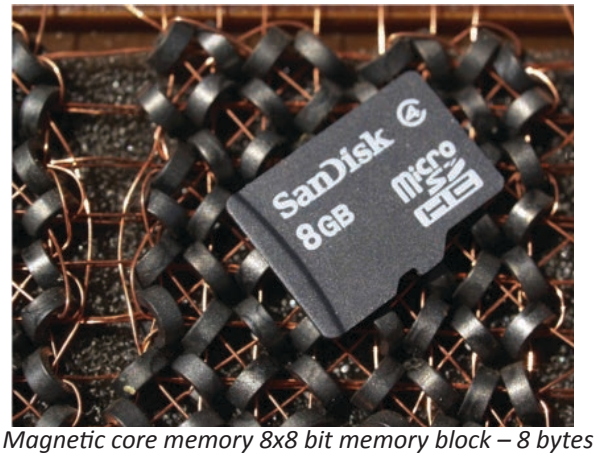
I am honored to be this year's co-recipient of the Trueblood Award and particularly want to thank those who in a timely way helped me on my way to here. Tony Cheetham for his suggestion about doing a neutron powder diffraction experiment, Allen Larson for his mentorship in crystallographic computing while creating GSAS, Brian for his collaboration on GSAS-II, Peter Stephens for his willingness to entertain a crazy experiment involving protein powders on his beam line, Hans Bunge for his guidance in doing texture analysis, Bob Blessing and Jim Jorgensen for their encouragement. Finally I must thank the US DOE for its support without which the work would not have been possible.

PLUTO Reactor AERE Harwell

In late 1972 while I was a postdoc in J.S. Anderson's lab at Oxford, Tony Cheetham stopped by to ask if I was interested in doing a neutron powder diffraction experiment. He had a copy of a new computer program from Alan Hewat written by some Dutchman (Hugo Rietveld). The PLUTO reactor was close by at Harwell and had a powder diffractometer that might suit. So we made two samples of titanium-niobium oxides and did the diffraction experiments – each run was 3 days. The object was to determine the metal site distributions in these "block" structures

that were all the rage at the time. One could see the blocks in electron microscope images.

Hugo's program was a typical crystallographic one with decks of cards as the code and input. The program punched a new set of cards to be used for the next iteration (it was a least squares refinement process) along with a line printer output for us to peruse – including a line printer rendition of the 600-700 point powder pattern – to decide what to try next.



Magnetic core memory 8x8 bit memory block – 8 bytes

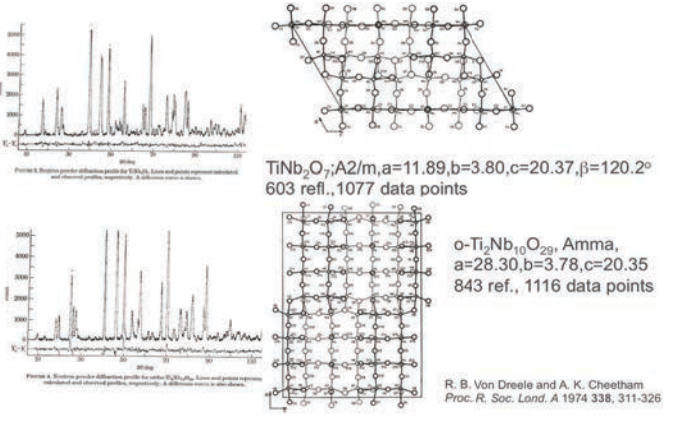
(Cf: modern 8Gb chip)

The manual was typical of that era; details of each line of input controls and data with a listing of the code at the back.

The biggest change during my career has been in computing. The machine at Oxford was a huge main frame machine with magnetic core memory; the scale in memory size shown here covers 9 orders of magnitude in almost 5 decades – that's Moore's Law.

Oxford ICL1906a – Banbury Rd, Oxford

The titanium-niobium oxides Tony & I worked on were too large for Hugo's program as written. It couldn't handle more than 300 reflections within the Oxford computer and these problems were much larger. So I had to modify the code to use a window of reflections that moved across the pattern as it was processed. This allowed much larger problems to be addressed; these two were some of the largest structures refined from powder data for many years after until folks began working on e.g. zeolites.



Some of the largest structures done by powder diffraction for many years

When I got back to Arizona State University, I gave a copy of this code to Ray Young (Georgia Tech). It included my attempt at fitting laboratory X-ray powder data (I had used data from an old GE goniometer set up in the Oxford Geology Department) which didn't work because the peaks weren't Gaussian. Ray & his students found a number of functions that fit the peaks – most especially the pseudo-Voigt; a linear combination of Gaussian & Lorentzian profiles still in use today. This effort resulted in the DBW & DBWS programs they adopted for the IBM PC computers. With that in hand Ray, Tony & myself went to several places around the world to educate students in this new method of structure analysis from powder data. We called it the Rietveld Refinement Road Show and went to Poland, Russia, Brazil & Argentina to spread the word. The DBWS code (NB: open source) became the core of several other packages including fullprof and LPHM (there may be others). Later I used my version (before DBWS) to create a working code for Rietveld refinement using neutron time-of-flight data. This became the basis of the tofpref/tofls package used for many years at IPNS (Argonne Natl. Lab.)

```
EXPEDT data setup option (<?>,D,F,K,L,P,R,S,X) >
EXPEDT data setup options:
 <?> - Type this help listing
 D   - Distance/angle calculation set up
 F   - Fourier calculation set up
 K n - Delete all but the last n history records
 L   - Least squares refinement set up
 P   - Powder data preparation
 R   - Review data in the experiment file
 S   - Single crystal data preparation
 X   - Exit from EXPEDT
```

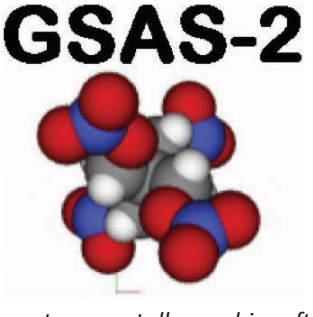
Menu-driven editor – EXPEDT - state of the art in 1980's

In the early 80's I was spending summers in Los Alamos (Phoenix is too hot in the summer!) as a part time contractor. The group leader, Richard Silver, asked

Allen Larson and I to support the data analysis for the single crystal and powder diffractometer instruments at the WNR spallation neutron source. We decided to combine our efforts and do one code that did both tasks – after all the math was the same. Thus the Generalized Structure Analysis System – GSAS – was born. It had to deal with multiple data sets because that's what neutron TOF data was. Powders were also frequently multiphase mixtures so that added to the complexity. We immediately recognized that an editor with error checking would be needed to give the user any hope of successfully setting up the control file; so we created EXPEDT – a state of the art user interface for the 1980's computing. Its type ahead feature was especially useful. Later (early 1990's) Brian Toby created EXPGUI, a more modern user interface that gave the novice a less imposing way into GSAS.

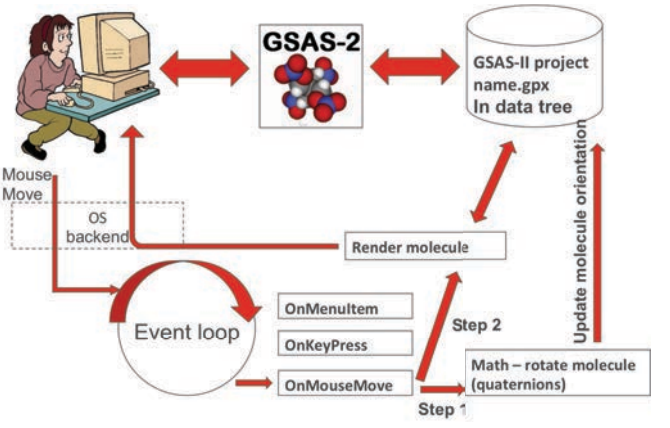
GSAS Manual (seven editions; 1985-2004)

I then moved GSAS from its original computer platform (DEC VAX machines) to Silicon Graphics IRIX and then to Microsoft MS-DOS & Windows. Many additions & changes to the code were made as the scope expanded and improvements were made to the powder profile functions. This is reflected in the change in number of pages for the manual (150 in the 1986 edition to 250+ in the 2004 one). However, it clearly had limits especially in the number of data sets that could be processed and the lack of structure solution tools.



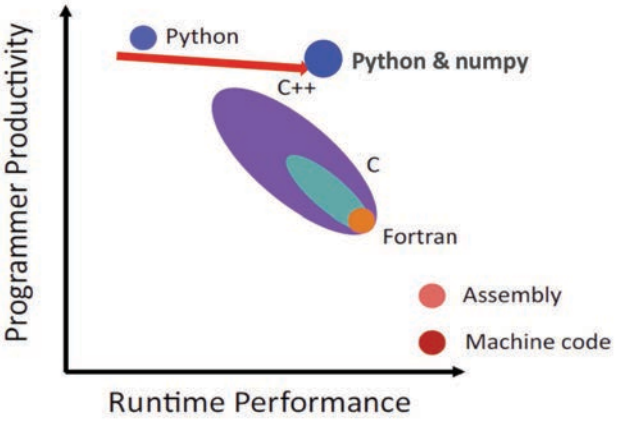
21st century crystallographic software

Clearly something new was needed. Today's computer users are not tuned into the old paradigm of manuals, card oriented control files & batch programs. Computer speed had made the need for that almost obsolete. Thus the new code is based on an "event loop system".



event loop systems – what you see

The way this works is that the user, say, moves the mouse (with a button down) wanting to rotate a drawing of a molecule shown on the screen. This creates an event (mouse move/button down) that is seen by a routine specifically written to handle it. The routine then calls the various utility routines (some with math) to convert the mouse move (from a previous saved point) to a vector which is used to rotate the object (via a quaternion), update the data and finally send new drawing instructions to the graphics hardware so the user sees it to move as desired.



Why python?

Based on: RW Grosse-Kunstleve, TC Terwilliger, NK Sauter & PD Adams, Source Code for Biology and Medicine 2012, 7:5

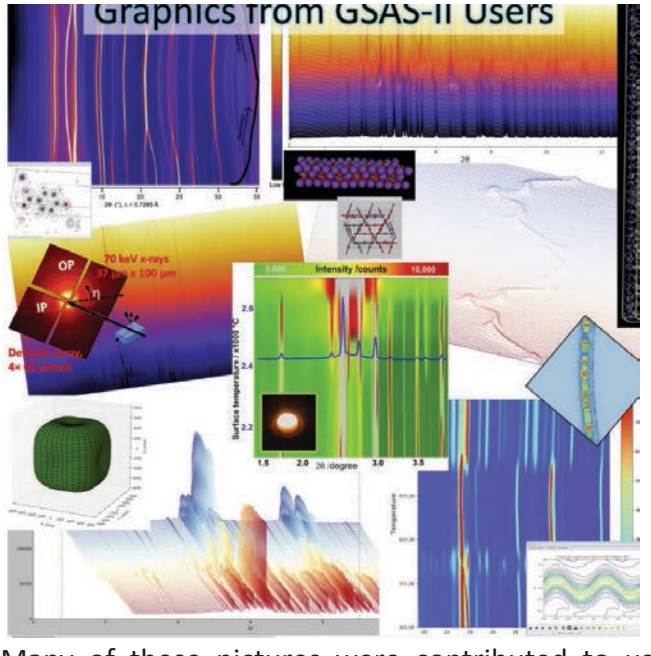
A good language for doing this is python because it and the available packages for it cover all that is needed to quickly and easily create a modern GUI event based package. The inclusion of numpy for numerical array calculations gives properly written python speed that is comparable with code in other languages along with easily integrated graphics for data plots and crystal structure drawings.

```
CErho = np.real(fft.fftn(fft.fftshift(CEhkl)))*(1.+0j)          #fft Fhkl → ρ(xyz)
CEsig = np.std(CErho)                                           #get σ(ρ)
CFrho = np.where(np.real(CErho) >= flipData['k-factor']*CEsig,CErho,-CErho)   #CF ρ → ρ'
CFrho = np.where(np.real(CErho) <= flipData['k-Max']*CEsig,CFrho,-CFrho)      #U atom CF!
CFhkl = fft.ifftshift(fft.ifftn(CFrho))                         #fft ρ(xyz) → F'(hkl)
CFhkl = np.where(CFhkl,CFhkl,1.0)                               #avoid divide by zero
phase = CFhkl/np.absolute(CFhkl)                                # get ϕ(hkl) from F'
CEhkl = np.absolute(CEhkl)*phase                                #apply ϕ to F
Ncyc += 1                                                       #count tries
sumCF = np.sum(np.array(np.absolute(CFhkl),mask=Emask))         #Σ F
DEhkl = np.absolute(np.absolute(Ehkl)/sumE-np.absolute(CFhkl)/sumCF)   #ΣDF
Rcf = min(100.,np.sum(ma.array(DEhkl,mask=Emask)*100.))         #R-value for CF
```

Code snippet – charge flipping all inside a "while" loop

For example, this is a bit of code for charge flipping in python. The entire algorithm is in 8 easily understood lines; there are 4 extra ones for house keeping (on the fly calculation of residuals).

I don't show the code here but an OMIT map is easily done in python and it's inclusion in GSAS-II means it could be used for any structure beyond its original intent for protein rebuilding.



Many of these pictures were contributed to us by users. We were amazed at how many of them featured hundreds of powder patterns showing things like phase transitions or chemical reactions all being analyzed by GSAS-II.

Robert Von Dreele

International Union of
CRYSTALLOGRAPHY

Can you be found in the World Directory?

As a member of the ACA, you are eligible to be included in the International Union of Crystallography's World Directory of Crystallographers [and of Other Scientists Employing Crystallographic Methods] (WDC, https://www.iucr.org/people/wdc). Are you there? If not, how will crystallographers and other scientists who are looking for somebody with your expertise find you? Creating a new entry is a quick process. Much professional information can be supplied, but little more than your name, job title and mailing address are required. The directory is used for dissemination of IUCr news and promotions, but only to people that opt in. Likewise, you have to give permission if you wish the IUCr to allow commercial providers of services to the crystallographic community to access this information. However, armed with this entry, crystallographers around the world will be able to contact you.

Do you have an old entry which badly needs an update? In writing this, one of us (BHT) discovered several items to change. To edit the entry you need your IUCr id number (which you can find from the directory) and password. If you do not remember your password, you can have a password reset link sent to the e-mail address on record. If your e-mail has changed and you don't have your password, you will need to send an e-mail to support@iucr.org where you can also get help with other problems.

If nothing else, the WDC can allow you to discover that there are only four crystallographic professionals with a first name of Hanna, and only one with a last name of Toby, but the WDC is one of many tools that helps the IUCr create a world-spanning community in our profession.

Brian Toby and Hanna Dabkowska

Help someone find a job in structural analysis. If you know of a crystallography related job - at any level - please ask the person posting the job to contact the ACA office at aca@hwi.buffalo.edu and get it on our web site. This also increases the value of ACA membership.

SIGs and other stuff that goes on at the ACA annual meeting.

Another ACA annual meeting has gone by; talks, posters, drinks with old friends and new, with ideas generated as a result. Have you ever wondered how you can shape the program of the next meeting? The answer is you can do this with very little effort. During lunch breaks and before poster sessions there are multiple Scientific Interest Group (SIG) meetings. Each of these SIGs (14 at last count) represents a community within the ACA that defines the scientific sessions for the next ACA meeting.

The SIGs are open to all, you can belong to multiple ones, and they don't cost anything to join; just indicate your interests through ticks on your annual renewal. Irrespective of whether you have formally identified yourself with a SIG, you are welcome to attend their meetings. The SIGs have a chair, vice–chair (sometimes) and secretary elected from their members. During each annual SIG meeting session topics for the following year are discussed and chairs for the sessions suggested. Topics should be of interest to the members with potential speakers to spare and posters also; even better if they are likely to also be of interest to other SIGs. If you've always wanted to see a topic but haven't seen it yet, the SIG meeting is the place to get this started. They are very democratic and in our combined experience (too many years to think about) everyone's voices are heard. If you make a strong enough suggestion you may end up being nominated as the chair.

The SIGs also discuss potential workshops. They sponsor workshops and help put together proposals which are passed to the ACA Education Committee for selection. If there is a burning topic you want to learn, help suggest an idea. Workshops are a good place to meet the experts and make connections to others with similar needs.

Unfortunately, SIG meetings generally have a low attendance; we note there was a period a few years back when the BioMolecules SIG had pizza as part of their meeting that increased participation (a hint for the future). Although many SIGs also solicit ideas for sessions before the meeting, ultimately it is the small number of attendees that make the key decisions about which sessions will become part of the following years ACA program. If you want that future to reflect your interests, go to a SIG meeting. If it's boring, do something about it, if it's interesting, engage, get noticed, and use it to build a career.

Finally the SIGs meetings nominate new members for election. If you have an interest in knowing members of the field better, getting involved with chairing a session or standing for election is a great way to make new contacts.

What happens after the conference is finished, after decisions on sessions have been made? Next year's program is settled the day following the ACA meeting through what is sometimes called the Thursday food fight. The morning after the talks have all finished there is a planning meeting. Sessions have to be suggested to cover all the days of the next meeting and so as not to produce too many clashes between the same audiences being interested in two or more simultaneous sessions. Some SIGs will have suggested too many sessions for the slots available, perhaps some will have suggested too few. SIGs who have done their homework may combine so that multiple SIGs sponsor a session. A table for the next meeting is slowly populated through several rounds of negotiation and discussion. Sessions with chairs and good sponsorship are strong, others fall by the wayside, and by the time the meeting finishes, well before lunch, the skeleton of the next ACA is ready for session chairs to start populating the following meeting. The SIGs have done their job until next year.

Another thing happens at ACA meetings, this being the general meeting. This is open to all members and provides a statement of the health of the association and news on any initiatives that may be coming down the line. There is opportunity for anyone to make their voice heard. In the Cincinnati meeting there was discussion about how to increase association membership, the change of the newsletter to an electronic format, and the effective use of social media among other things. The latter point was interesting as very few in that audience were new to the ACA, or one might add, completely up to date with the true potential of social media.

So this article is written to describe some of our experiences with SIGs and with a nod to how that process leads to bigger and better things within the ACA and outside. We absolutely encourage you to join a SIG or several, communicate with the SIG executives, and come to one or more of the SIG meetings. As a bonus, and this is intended for newer ACA members, try the general meeting – stand up and say something. Shape your association and help it grow and represent you for the future.

Edward Snell and Carrie Wilmot

ttplabtech

leaders in integrated structural biology

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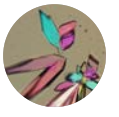
automated plunge freezing for cryo-EM

- blot-free high speed plunging
- automated grid handling
- grid screening based on vice thickness



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2019 ACA Transactions Symposium
Best Practices: Current State and Future Needs

The ACA Best Practices for Data Archival and Analysis Scientific Interest Group (SIG) was established in 2018 to join the major effort by the international community to standardize best practices in data analysis and archival and to improve our community's involvement in these best practices.

The 2019 Transactions Symposium "Data Best Practices: Current State and Future Needs" represented the first session hosted by the SIG at an ACA meeting. The full day session focused on how the wide variety of data collected by ACA members, from different fields, was (1) being archived and analyzed, (2) what data analysis problems the community is currently facing and (3) what the community sees as their future needs. The session was also timely in that the funding agencies would soon require the deposition and archival of the raw (e.g. images) and meta (e.g. program data processing input) data that the resulting publications were based on.

The session (see below) was developed by **Nicholas Sauter** (LBNL), **John Rose** (UGA) and **Talapady N. Bhat** (NIST). Papers based on the authors' Session presentations will be published in a special edition of the Journal of Structural Dynamics. The cost of a free-access publication is $1,000 (with ACA discount) and the SIG is trying to raise $14,000 to support publication costs. Any tax-free donation from the community for the publication costs is highly appreciated.

Best Practices: Current State and Future Needs

The morning session began with a Welcome and Introductory remarks by ACA President Joseph Ferrara followed by six presentations. **John Helliwell** (Chairman of the IUCr Committee on Data, and IUCr Representative to CODATA) introduced concepts of FACT [Fair, Accurate, Confidential, Transparent] and FAIR [Findable, Accessible, Interoperable, Reusable], and how these concepts apply to crystallography. **Nadia Zatsepin** (La Trobe University, Australia) reported on the challenges of optimizing data quality and data archival in injector based SMX. **Thomas Proffen** (ORNL) described how FAIR data will accelerate scientific discovery at national neutron scattering facilities. **Brent Nannenga** (Arizona State University) introduced MicroED methodology and current developments for both small and large molecules. **Michael Wall** (LANL) made a strong case for saving the raw diffraction data with respect to diffuse scattering where what lies between the spots can give important clues to structural dynamics. **Catherine Lawson** (Rutgers University) spoke on the evolving data standards for cryo electron microscopy important for standardizing and validating this new and exciting approach. The morning session concluded with a general discussion and SIG business meeting. The general discussion and business meeting focused mainly on the cost of raw data archival, who will oversee the archives and where the money will come from to do this. The discussion was tabled to allow discussion about session topics for the 2020 meeting in San Diego and the election of new officers.

The afternoon session had eight speakers and began with the Etter Student Lecture by **Jorge A. Diaz** (Rochester Institute of Technology) who presented his work on "Migrating the fast_dp software package for Python 2 and 3 compatibility. **Andreas Förster** (Dectris, Ltd.) provided a vision for macromolecular crystallography over the next five years based on new detector technology and other developments. **Filip Leonarski** (Swiss Light Source) presented details about the New Dectris Jungfrau detector and how it will impact both MX and the storage, processing and transfer of the data. **Herbert J.Bernstein** (Ronen Institute) provided updates on HDRMX and the best practices for high data-rate macromolecular crystallography. **Wladek Minor** (University of Virginia, School of Medicine) reported that the Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC) accepts raw image data for long term storage. **Doeke Hekstra** (Harvard University) introduced Electric-Field Stimulated Time-resolved X-ray Crystallography and its data analysis challenges. **Stephen Burley** (RCSB Protein Data Bank) provided an update on PDB ligand validation and new tools available to the user. The afternoon session concluded with a presentation by **Amy Sarjeant** (formerly of the Cambridge Crystallographic Data Centre) who described the challenges and opportunities in curating one million crystal structures.

The Transactions Session was well attended given the competition from other sessions. The Chair would like to thank the speakers for their excellent presentations, and **James Holton** (University of California San Francisco) and **Nadia Zatsepin** (La Trobe University, Australia) for their excellent job

of moderating the morning and afternoon sessions, such that we finished on time. The Chair would like to thank **Nicholas Sauter** and **Suzanna Ward**. Nick for playing a major role in developing this outstanding session and who unfortunately was unable to attend the Session at the last minute to see the fruits of his hard work and Suzanna for her notes from the business meeting which were essential in preparing our ACA SIG report.

We will have a session at the 2020 ACA meeting:

The 2020 ACA SIG Symposium

Meeting the Challenges of Raw Data Deposition

Chair - Wladek Minor

All science is based on data, which needs to be properly curated and archived. The half-day symposium will explore how to best accommodate the deposition of raw data, soon to be required by funding agencies. To do this we will bring together (1) Experts in long-term data storage/management, (2) High throughput data producers (light sources, cryoEM centers) and (3) Large data storage providers. The session will also invite funding agency representatives to learn community concerns as to how the long-term raw data archive will be managed and supported.

John P. Rose

Kenneth N. Trueblood Award: To recognize exceptional achievement in computational or chemical crystallography. The award is established in memory of Professor Kenneth N. Trueblood, UCLA 1949-1998, who was a major force in the early use of computers and the development of crystallographic computer programs. He applied these programs to the examination of chemical and molecular details of many structures at the frontiers of research.

Robert von Dreele & Brian Toby - Trueblood Award Winners (Photograph by Richard Bromund)

Fankuchen Memorial Award: To recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Established in 1971 in memory of Dr. I. Fankuchen, Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964.

ACA President, Joseph Ferrara, presenting the Fankuchen Award to Eaton Lattman (Photograph by Richard Bromund)

Bau Neutron Diffraction Award: The award is in memory of Professor Robert Bau, University of Southern California (1969-2008) and President of ACA in 2006. A much beloved teacher and mentor, Professor Bau made major contributions to the development of the technique of single-crystal neutron diffraction and to its applications in chemical and biomacromolecular crystallography.

ACA President, Joseph Ferrara, presenting the Bau Award to Bryan Chakoumakos (Photograph by Richard Bromund)

Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award is established to honor the memory of Professor Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. She had a love for people, for science, and especially for people who do science, that we honor.

ACA President, Joseph Ferrara, presenting the Etter Award to Efraim Rodriguez (Photograph by Richard Bromund)

Michael Rossmann Legacy Session

L to R: Eddie Arnold, Hao Wu, S. Saif Hasan, Rui Zhao, Tonia Key, Karen Bogan, Jack Johnson and Janet Smith (Photograph by Richard Bromund)

Michael Rossmann eagerly accepted an invitation to open the 2019 ACA Annual Meeting with a plenary lecture, but passed away two months before the meeting at the age of 88. To memorialize his legacy to crystallography, five alumni of Michael's research group at Purdue University spoke in a Rossmann Legacy Session, describing his scientific achievements related to their research and sharing personal reminiscences of him as a scientific leader, mentor and friend. The large audience, which included Michael's wife **Karen Bogan** (West Lafayette, IN) and his daughter and son-in-law **Heather and Dennis Bossé** (Brewer, ME), appreciated the scientific and personal stories from alumni spanning five decades of the Rossmann lab at Purdue. The speakers are among Michael's legacy of leading scientists: **Jack Johnson** (The Scripps Research Institute, postdoc in the 1970s), **Eddy Arnold** (Rutgers University, postdoc in the 1980s), **Hao Wu** (Harvard Medical School, grad student in the 1990s), **Rui Zhao** (University of Colorado, grad student in the 1990s), and **S. Saif Hasan** (University of Maryland, postdoc in the 2010s). The talks covered key aspects of Michael's seminal contributions to crystallography, and each speaker captured his enthusiastic, energetic and innovative spirit with entertaining personal recollections. The audience, family members and speakers continued sharing stories of Michael at the conference opening reception, which immediately followed the session. The session was recorded by Virginia Pett and Richard Bromund, who quickly posted a video to the ACA history website (https://history.amercrystalassn.org/michael-g-rossmann).

Janet Smith

1.1.1: Macromolecular Structure Under Physiological Conditions

L to R: Matthew McLeod, Takashi Kumasaka, Aaron Finke, Rob Thorne, Richard Gillilan, Silvia Russi, Michael Thompson and Timothy Stachowski

Most high-resolution structures have been obtained at cryogenic temperatures, far from the conditions where the molecules function at all, let alone optimally. It is increasingly appreciated that these extreme conditions may bias our understanding of biological function.

Richard Gillilan (CHESS) opened the session with brief welcome entitled "A Word About Physiology." The label physiological is too often applied loosely to refer to samples measured at room temperature in the liquid state. More specifically, physiological can imply a particular range of temperatures, pH's, ionic strengths, and concentrations.

Often physiology means human physiology. But it is now widely appreciated that a great deal of the biomass on Earth lives under many extraordinary conditions: corrosive springs, permafrost at -17 C, superheated water (122 C!) in hydrothermal vents, rock pores in deep coal beds, and under 11 km deep (105 MPa) of ocean pressure. Pressure and temperature "extremes" are really the norm for most microbial life on earth and may well have been the conditions under which life and much of our molecular biology first evolved. This session focused both structural techniques and model systems in a wide range of conditions where water is in the liquid state.

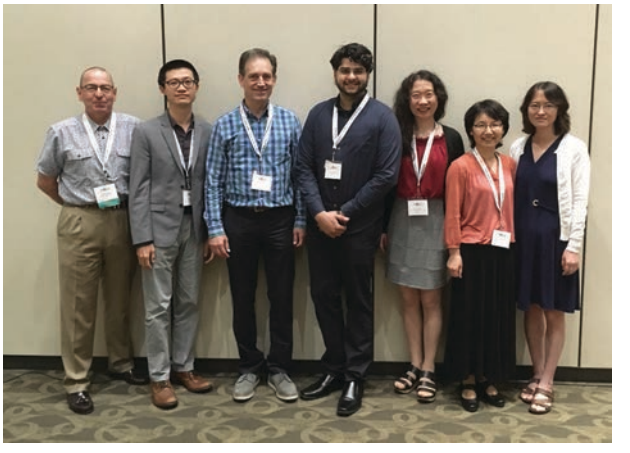
Michael Thompson (UCSF) described experiments at RIKEN and SLAC/LCLS in which an IR laser pulse creates a rapid (ns) temperature jump in a crystal that can then be probed by ultrafast X-ray pulses. Conformational changes in two model enzymes, cyclophilin A and lysozyme corresponded to functionally significant collective motions, validating this method for time-resolved studies. **Robert Thorne** (Cornell) has studied water structure in protein crystal solvent cavities. He discussed collecting diffraction data on the short timescale of supercooling with reduced X-ray damage

and better B-factors than conventional flash-cooling methods. This nanoconfined water apparently freezes into a stacking-disordered mixture of cubic and hexagonal planes, with a 6 Å layer near the protein remaining uncrystallized. Evidence of solvent flow at cold temperatures was observed.

Silvia Russi (SSRL) described new automation and equipment available at SSRL-SMB and LCLS-MFX for automated room temperature data collection under humidity-controlled conditions. Controlled dehydration of crystals can induce changes in crystal packing, unit cell dimensions, and mosaicity that may result in improved diffraction resolution. Upgraded equipment will enable remote SSRL users to rapidly switch between ambient temperature and 100 K and data collection. A new plate designed for crystallization, transport and mounting of samples under humidified ambient conditions was passed around for the audience to view. **Aaron Finke** (MacCHESS) unveiled the new room temperature serial crystallography capability that will be made available to CHESS users. Microcrystals are loaded onto special silicon microchips that separate and hold the crystals for rapid oscillation data collection. The oscillation technique combined with proper data processing maximizes data quality while minimizing the total number of crystals needed to complete the structure. **Timothy Stachowski** (HWI) examined an extracellular protein signaling complex, Latent-TGFβ-1, involved in the cellular response to low-dose (therapeutic) radiation exposure. Unlike conventional damage which often causes aggregation, this system undergoes a functionally-significant dissociation that initiates signaling pathways in the cell. SAXS was used to characterize changes induced by radiation exposure, look for regions most affected by radiation, and understand the radiation chemistry. **Matt McLeod** (U. Waterloo) introduced an enzyme, phosphoenolpyruvate carboxykinase (PEPCK), that contains a 30 Å long loop that opens and closes to control pyruvate production. Adaptation of enzyme function to different temperatures is thought to involve modulation of the degree of flexibility of the loop. In addition to the mesophilic form of the enzyme, they have now crystallized a psychrophilic (cold-adapted) form which can be used to investigate the effect of the adaption. **Takashi Kumasaka** (Japan Synchrotron Radiation Research Institute) at Spring 8 closed the session with a description of a unique mounting system for serial crystallography that combines humid air with a glue coating – the HAG method. They have successfully studied the H-Ras protein using this system of scanning and rotation at room temperature.

Richard Gillilan and Aina Cohen

1.1.2 Cutting edge studies using Cryo Electron Microscopes



L to R: Stephen K. Burley (Session Co-Chair), Wei Jia, Todd Yeates, Ali Punjani, Hao Wu, Peijun Zhang, Rui Zhao (Session Co-Chair)

Session 1.1.2 included talks describing cutting edge cryo-EM techniques and biological insights obtained therefrom. Dr. **Ali Punjani** from University of Toronto and Structural Biotechnology, lead author of cryoSPARC (the popular cryo-EM structural determination package), described recent algorithmic advances for single particle cryo-EM. Dr. **Peijun Zhang** from the Electron Bio-Imaging Center at the Diamond Light Source in the United Kingdom presented exciting technology developments in cryo-electron tomography and sub-tomogram averaging, and explained how these techniques were used for in situ structure determination of virus assemblies inside human cells. Dr. **Todd Yeates** from the University of California at Los Angeles addressed some of the challenges involved in using cryo-EM to study smaller macromolecular systems by designing modular scaffolds that enable higher-resolution imaging of cargo proteins. Dr. **Hao Wu** from the Harvard Medical School described how her laboratory uses cryo-EM to study supramolecular complexes contributing to the innate immune response, including the inflammasome. Dr. **Wei Jia** from Dr. Liang Tong's lab at Columbia University demonstrated the exciting possibility of using cryo-EM to reveal the action of small molecule inhibitors of human ATP-citrate lyase. Dr. **Rui Zhao** from the University of Colorado School of Medicine presented recent unpublished work on the cryo-EM structure of the spliceosomal E complex, which enabled her to propose a unified molecular mechanism for intron definition, exon definition, and back-splicing, all supported by complementary biochemical analyses.

Rui Zhao and Stephen K. Burley

1.1.3 Morphological Characterization of porous Materials

First row: from the left, Dr. Lilin He, Prof. Greeshma Gadikota, Dr. Byeongdu Lee, Dr. Charl Jafta, Dr. Petra Bombicz

Second row: from the left, Dr. Andrew Allen, Dr Albrecht Petzold, Dr. Rui Zhang

This session brought together more than 30 researchers from universities and national laboratories performing research in experimental characterization using a broad range of techniques in porous materials. The session consists of three invited talks and five contributed talks. The invited talks lasted 25 mins and the contributed talks lasted 17 minutes each.

The invited talk given by Dr. **Byeongdu Lee** from Argonne National Naboratory discussed Scattering functions of polyhedra. Dr. **Andrew Allen** from National Institute of Standards and Technology reported how his group used scattering methods to investigate the structural basis of CO2 adsorption in a porous metal-organic framework material. After that, Dr. **Charl Jafta** from Oak Ridge National Laboratory (ORNL) presented his research on the SEI formed by bis(fluorosulfonyl) imide based electrolyte on ordered mesoporous carbons using in situ methods. The second invited talk was given by Dr. **Albrecht Petzold** from Martin-Luther University, Halle-Wittenburg, Germany. He discussed a model free analysis of Small Angle Scattering data of mesoporous and microporous carbons. Then Dr. **Petra Bombicz** from Hungarian Academy of Sciences, Hungary, presented the talk on structural features of the formation of iHOF materials, which was quite interesting to the audience. Another contributed talk given by Dr. **Lilin He** from ORNL showed their exciting results on the enzyme encapsulation in MOF materials using scattering methods. These results were expected to guide us to prepare new porous materials with optimum morphologies and mechanical properties for enzyme industries.

The third invited talk was given by Prof. **Greeshma Gadikota** from University of Wisconsin–Madison. In her talk she discussed how she could advance the understanding of reactive fluid induced chemo-morphological changes in multi-phase environments using X-Ray and Neutron Scattering techniques. The last talk given by Dr. **Rui Zhang** from Penn State, was about characterization of pores of shales using small angle neutron scattering. Shale gas will be a main energy source in the near future in US. However, how the gas is stored in the shale pores and how the gas interacts and moves in the sales remains unclear. SANS with contrast matching technique can provide unique phase behaviors of gases and pore structure, pore connectivity, pore accessibility, which is vital for the shale gas industry.

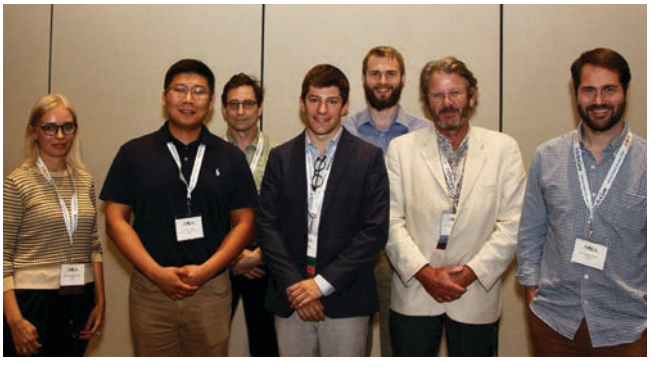
Lilin He

1.1.4 Crystallography in the Geosciences

★No report submitted★

Nichole Valdez and J. Caleb Chappell

1.2.1: Structure Without Structure



L to R: Emma Danelius, Zhijie Li, Tobin Sosnick (back), Garrett Ginell, Justin Porter (back), George Phillips and Jonathan Clinger (Photograph by Richard Bromund)

The Structure Without Structure session held on Sunday July 21st, distinguished as the Structural Dynamics Session, encompassed seven speakers and provided a platform to present new ideas and novel research related to the study of conformational heterogeneity and dynamics in molecules. To start the session **George Phillips**, of Rice University, set the stage providing an excellent background covering disorder, heterogeneity, and intrinsically disordered proteins (IDPs) in his talk entitled “Determining the Structure of a Protein When it Doesn’t Have One”. To follow postdoctoral fellow, **Zhijie Li**, from the Carter

lab at the University of North Carolina-Chapel Hill provided an example of such molecular dynamics during his talk "Aminoacyl-tRNA synthases may have evolved from molten globular precursors". Directly after, the audience learned how to identify cryptic pockets, conformational switches, and allosteric coupling through cooperative changes in solvent exposure in an excellent talk given by **Justin Porter** a postdoctoral fellow from the Bowman lab at Washington University in St. Louis. Looking towards the future, **Emma Danelius** in the Gonen lab at the University of California in Los Angeles, explored the future possibilities for use of MicroED in studying intrinsically disordered regions (IDRs) during her presentation. Following a short intermission for coffee, **Tobin Sosnick**, from the University of Chicago, explored the importance of measuring the solvent quality of unfolded proteins during the Judith Flippen-Anderson memorial lecture. Following this, a PhD candidate, **Nir Salinas** at Technion Israel institute of Technology, spoke on Extreme Amyloid Polymorphism in Staphylococcus Aureus Virulent PSMα Peptides. The session concluded with postdoctoral fellow from the Phillips lab at Rice University, **Jonathan Clinger**. Clinger delivered a fascinating presentation on Cryo-trapping Crystal Studies of Photoreceptor PixJ to yield new insights into its Photoconversion Mechanism, and was awarded the Etter Student Lecturer Award by the ACA. This session dedicated to structural disorder, dynamics, and heterogeneity was sponsored by the journal Structural Dynamics and Rigaku.

Garrett Ginell and Gerald Audette

1.2.2: Crystallography at Extreme Conditions

An "extreme" condition can be anything that varies from standard conditions by an order of magnitude or more. This term is most often found in the geosciences, due to the fact that most of the mass of the planet is subjected to conditions which are much hotter and more pressurized than what we enjoy on the crust. In this session, we invited abstracts from any crystallographic discipline, allowing a broad view of extreme conditions. Unfortunately, we were saddened to have a number of presenters unable to join us; however, the resulting, shortened, session was very enjoyable.

Fahima Islam from Oak Ridge National Lab shared her experiences using high performance computing to optimize a collimator for the neutron beamline SNAP. In many in situ experiments performed with neutrons, the sample container can produce more scattering signal than the sample, unless collimation is used. Fahima detailed her methods for creating this collimator in a 4 step process; she simulated the SNAP instrument using ray tracing, optimized the many variables of the collimator design using the supercomputers available at ORNL, produced a collimator using additive manufacturing, then tested the collimator on the instrument. Her presentation showed the possibilities that high performance computing aligned with engineering design can offer to central facilities, resulting in better crystallographic outcomes for the end users.

Richard Gililan from CHESS was next up, with his intriguing title of "Structural Biology in the Abyss." He runs the high pressure biological SAXS beamline at CHESS, which exists to watch the effects of pressure on biomolecules, e.g. unfolding or denaturing. He shared some enjoyable insights on the shifts in thought that have occurred in the last four decades in biology: before the 1980's the bottom of the ocean was thought to be a barren place, devoid of life; deep-sea life and thermophiles were discovered and then the discovery of archea re-wrote the tree of life. The HP BioSAXS beamline can help researchers understand how life adjusts to these extremes.

Angus Wilkinson from Georgia Tech described his recent brush with an unexpected hybrid perovskite. Angus is an experienced explorer of negative thermal expansion, which is an uncommon phenomenon where the unit cell volume decreases upon heating. Thermal expansion, he explained, is due to thermal energy promoting electrons into higher order excited states, which produces longer bonds due to anharmonicity. Negative thermal expansion(NTE), when heating produces no expansion or a contraction, occurs due to entropically favourable librations, which can also drive high pressure phase changes. While exploring a perovskite NTE material at high pressure using neutron diffraction, Angus and team observed the unit cell volume decreasing as the pressure increased, then with further pressure increases, it began to increase. The sample had been loaded in helium as the pressure transmitting medium, and it soon became obvious that, at high pressure, the helium had invaded the sample, which was considered non-porous! They were able to model helium atoms on the A site, using the neutron diffraction data, and learned that N2 would not penetrate the sample, and that the He-doped material is stronger and more robust to higher pressures.

Branton Campbell from Brigham Young University closed the session with a delightful anecdote about a compound, $CsCoO_2$, which has a painstaking synthesis, where one tries to not explode an azide starting material, as well as topotactic phase change behaviour. The β form, which is stable at room temperature and pressure can be transformed into the γ phase at high temperatures and modest high pressures, which are both achievable in a large volume press. The γ phase is quenchable, and can be recovered back to ambient pressure and temperature. More

on this fascinating system can be found in the recent publication where Branton is a co-author: Acta Cryst. (2019). B75, 704-710

Christine M. Beavers, Camelia V. Stan, Joe Tanski

1.2.3: Understanding Polymer Structure and Dynamics During and After Processing

L to R: Juan David Londono, Allison Domhoff, Byeongdu Lee, Thomas Fitzgibbon and Joseph Kline. Anne Gohn not pictured.

The session on polymer structure and dynamics featured participants from industry, synchrotron and neutron sources, and academics to discuss new advances in understanding the structure of polymeric materials. Industrial participants **Juan David Londono**, DuPont, and **Thomas Fitzgibbons** (Dow Chemical) provided insight into the work the respective companies perform at the DuPont-Northwestern-Dow Collaborative Access Team (DND-CAT) at the Advanced Photon Source. Londono showcased the use of a spinneret system that was installed within the hutch to characterize polymer orientation and crystallization during the fiber spinning process. Fitzgibbons showcased the work that Dow has done on characterizing the crystallinity and morphology of polyolefin systems under strain at DND-CAT. **Byeongdu Lee** from sector 12 of the APS gave a talk showcasing the new advances in direct electron density mapping using small angle scattering. The talk featured recent work on how the tool can be applied to describe the morphology exhibited in block copolymer systems. **Allison Domhoff**, a graduate student from Clemson University, provided insight into the work she has been doing on the role of electrostatic interactions and nanoparticle dispersions on ionomer nanocomposites. The work described the use of SANS to describe the structure of these membranes with a goal of reducing breakthrough of ions form one side of the membrane to the other. **Anne Gohn**, a researcher from Penn State, showcased the use of flash DSC in conjunction with WAXS to describe how specific nucleators effect the phase of polypropylene. The final talk in the session was given by **Joseph Kline** from the National Institute of Standards and Technology (NIST). In his seminar, Joseph described using soft X-rays to characterize the directed self-assembly in block copolymer thin films. This field has a lot of interest in the semiconductor world as a way to increase the density of electronic components through novel photolithographic routes. The CD-SAXS technique developed by his team has been instrumental in understanding the packing and order present through the thickness of the film.

Thomas Fitzgibbons

1.2.4 : Magnetic, quantum, and electronic correlated materials

L to R: Rebecca Smaha, Benjamin Frandsen, Rebecca Dally, Jared Allred, Efrain E. Rodriguez, Matthew Davenport, Branton Campbell, Daniel Phelan and Huibo Cao

This half-day symposium deals with the relationship between crystal structure and the properties of a class of materials broadly termed quantum materials. Symmetry plays a large role in the underlying physics of these new materials, which can exhibit phenomena such as frustrated magnetism, quantum spin liquid behavior, and superconductivity. Many of our speakers represent young leaders in this field who use neutron and X-ray diffraction along with crystallography to advance the boundaries of quantum materials.

Our session began with a focus on a concept known as 'magnetic frustration'. In certain crystal structures, the magnetic ions cannot satisfy their pairwise interactions equally well, hence the frustration, due to their special distribution. Our first speaker **Gabriele Sala** (ORNL) introduced such a model for frustrated magnetic interactions, the Shastry-Sutherland lattice is substantially more complicated the simple hexagonal lattice, but still has known analytic solutions for the

magnetic ground state. Sala described and explained the magnetic structures and properties of two very different frustrated systems whose moments lie on such a lattice: Nd2Ni2In (metallic, Ising-like, and antiferromagnetic) and BaNd2ZnO5 (ferromagnetic dimers). **Huibo Cao** (ORNL) then described the relationship between magnetic frustration and the presence of direction-dependent magnetization plateaus in bilayered perovskite system Tb2SrFe2O7. **Rebecca Smaha** (Stanford) presented compelling evidence for quantum spin-liquid (QSL) behavior, which is related to magnetic frustration but on a quantum rather classical level. Smaha showed that highly frustrated S=1/2 spins on a Kagomé layer, as found in Zn-substituted barlowite (Cu3.44Zn0.56(OH)6FBr), are prime candidates for the QSL state which was characterized by long-range quantum entanglement in the absence of long-range magnetic order. Smaha was also presented with the Etter Student Lecturer Award in Neutron Diffraction during this session.

Continuing with the theme of magnetic frustration, **Benjamin Frandsen** (Brigham Young U.) demonstrated that unconventional ways to look at diffraction data could help understand the physics at the local level. Frandsen presented how pair-distribution function (PDF) methods with neutron powder diffraction data can be used to reliably extract the details of the local magnetic structure of a frustrated systems such as NaMnO2 and a highly-complex pyrochlore oxide. This approach opens the door to a wide range of previously inaccessible local structure-property relationships. After reviewing the toplogical properties of magnetic textures in condensed matter systems, **Rebecca Dally** (NIST NCR) presented small angle neutron scattering (SANS) data to illuminate the dynamics of a topological feature that occurs in complex antiferromagnets known as the skyrmion. In particular, Dally showed how the relaxation of such skyrmions in the lacunar spinel, GaV4S8, which occur near the cycloidal-skyrmion phase boundary. This vanadium sulfide is one of the only non-centrosymmetric materials to host skyrmions.

Non-magnetic local order was also featured prominently in the session. **Jared Allred** (U. of Alabama) and **Matthew Davenport** (ANL) presented a remarkable way to visualize x-ray single crystal data using the three dimensional (3D)-ΔPDF method. In this way of analyzing the single crystal data, the diffuse scattering from local order rather than the Bragg reflections is the star of the show. Allred and Davenport demonstrated that the 3D- ΔPDF data from single crystals of molybdenum-doped VO2 reveal a variety of local Mo-site orderings that potentially influence its metal-insulator transition. These orderings were then classified among the possible symmetry modes dictated by group representation theory. **Daniel Phelan** (ANL) then presented x-ray diffuse scattering evidence of charge stripes arising at the semiconductor-insulator transition of an orbitally polarized trilayer nickelates. These nickelates are materials that attempt to reproduce similar coordination geometry and electron count for the transition metal as the high-Tc superconducting cuprates. Phelan presented their work specifically on the nickelate La4Ni3O8, where such orbitally driven stripes are mutually commensurate with and likely coupled to previously-observed antiferromagnetic spin stripes.

Efrain E. Rodriguez and Branton J. Campbell

2.1.1: Symposium on Structure in Cancer Biology I

Betsy Goldsmith and John Tainer organized a highly successful 2-session symposium on Structure in Cancer Biology. The first session focused protein kinases and G-proteins, with a data-rich presentation on Hippo pathway components from **Xuelian Luo** from UT Southwestern Med, and structural analysis of RAF cancer mutants by **Mike Eck**. **Betsy Goldsmith** described the exciting structure-based discovery of pressure-sensing for activation of an important kinase. **Chris Brosey** combined X-ray scattering and crystallography to examine the NADH-mediated allosteric monomer to dimer switching by apoptosis-inducing factor. **Steve Sprang** presented a tour-de-force crystallography and EM analysis of a soluble GEF, and Xiaoshan Min from AMGEN presented on the new strategy of chemibody screening for drug discovery.

Betsy Goldsmith and John Tainer

2.1.2 Micro-Electron Diffraction

★No report submitted★

Tamir Gonen and Gerd Rosenbaum

2.1.3: Diffuse Scattering for Biological Structure and Dynamics

This session focused on the interpretation and potential applications of diffuse scattering from protein crystals for dynamical studies. The pattern of diffuse scattering between the Bragg peaks, ignored during conventional data processing, contains information about displacement correlations that cannot be obtained from the Bragg data alone. The interdisciplinary session included perspectives from structural biology, materials science, computational chemistry,

and coherent imaging.

L to R: David Wych, Ed Lattman, Richard Welberry, Loes Kroon-Batenburg, Steve Meisburger, Michael Wall, David Case and Mark Wilson (Photograph by Richard Bromund)

Richard Welberry, Australian National University, opened the talks with an account of the development of the experimental recording of diffuse scattering from the early work of Kathleen Lonsdale using 1D detectors, through 2D area detectors that allowed complete 3D data to be measured, and finally the latest methods using continuously rotating crystals and high frame rate area detectors. Examples of Monte Carlo modeling were described including harmonic springs connecting rigid fragments and a global semi-empirical pair potential related to the Buckingham potential.

Mark Wilson, University of Nebraska, Lincoln, spoke about cysteine modification-gated protein dynamics in isocyanide hydratase, an enzyme involved in the detoxification of isocyanide natural products. Ambient temperature X-ray diffraction showed that ICH exhibits a correlated displacement of an alpha-helix that occurs as a consequence of radiation-driven oxidation of the active site cysteine residue. X-ray free electron laser (XFEL) serial mix-and-inject crystallography established that ICH forms a transient thioimidate intermediate at the active site cysteine residue, triggering the alpha helical displacement. Analysis of ICH X-ray diffuse scattering data suggested that the data may be suitable for more detailed studies of how proteins respond to functionally important perturbations.

Eaton Lattman, Hauptman-Woodward Medical Research Institute and University at Buffalo, opened the floor to discussion of time-resolved diffuse scattering with X-ray lasers. He asked participants to imagine illuminating a small crystalline volume with a coherent, femtosecond x-ray pulse, removing the effects of temporal and spatial averaging. He reasoned that the entire scattering pattern observed in such an experiment would have defined phase, anchored by the phase of the diffraction pattern at the Bragg peaks, and that the full scattering pattern, Bragg and non-Bragg alike, could be calculated for all the atoms in the illuminated volume, and not just for those atoms in a single unit cell.

David Wych, University of California, Irvine and Los Alamos National Laboratory, presented a molecular dynamics simulations study of X-ray crystallographic diffuse scattering. He compared the effects of various choices made in the preparation of crystalline MD models, and found that the systems are fairly robust to changes in equilibration time, force-field, and restraint procedure. He also analyzed the full 2x2x2 supercell C-alpha covariance matrix, and compared alternative methods for computing the cumulative diffuse scattering.

Loes Kroon-Batenburg, Utrecht University, presented a recent paper on rigid body motions modeling of diffuse scattering in protein crystals. Diffuse scattering was modeled for cyclophilin A (CypA) and hen egg white lysozyme using ensembles of molecules representing translational, rotational, and internal motions, with amplitudes of the various motions based on B-factors from structural refinement against Bragg reflections. A supercell approach was used to calculate diffuse scattering in between Miller indices of the lattice, and models were compared to experimental data. The paper argues that rigid body motions, and especially translations, dominate the diffuse scattering signal.

Finally **David Case**, Rutgers University, presented results of molecular dynamics simulations of lysozyme in a crystal environment, with a "supercell" of up to 343 unit cells as the repeating unit. The simulations provide a plausible, if imperfect, model for conformational heterogeneity in biomolecular crystals. He showed that thermally-activated phonon-like modes, "trapped" lattice distortions, and more localized protein and solvent conformational disorder all contribute to diffuse scatter. Comparisons were made to recent experimental diffuse maps collected and analyzed by co-authors Steve Meisburger and Nozomi Ando.

Although extracting information of biological relevance from diffuse scattering remains an unsolved problem, it is clear that better computers, X-ray sources, and detectors have allowed the field to make rapid progress. Importantly, the gathering of speakers has created new opportunities for advancing the field.

Mike Wall and Steve Meisburger

2.1.4: Solid State NMR Crystallography

★No report submitted★

Manish Mehta and Tomislav Friscic

2.1.5: Crystal Structure Solution from Powder Data

★No report submitted★

Fernando Uribe-Romo and Shoji Hall

TMT2: Three Minute Thesis 2019

L to R: Victor Young, Chelsy Chesterman, Aparna Annamraju, Riley Metcalfe, Rebecca Smaha, Rebeccah Warmack, Nir Salinas and Qingyun Dan (Photograph by Richard Bromund)

This year we held the second annual three-minute thesis competition at the ACA annual meeting. This event for students and postdocs is organized by the Young Scientists Interest Group and generously sponsored by TTP Labtech. We had many great presenters who rose to the challenge of communicating their research in only 3 minutes. We are proud to congratulate this year's winner **Rebeccah Warmack** from the University of California, Los Angeles and this year's runner-up **Rebecca Smaha** from Stanford University.

Chelsy C. Chesterman, Korey Carter and Victor Young

2.2.1: Powder Diffraction in Industry

L to R: Jim Kaduk, Yuanpeng Zhang, Elena Kabova, Rajni Bhardwaj

Powder diffraction is utilized in a wide variety of industries for a very wide range of materials, including pharmaceuticals, polymers, pigments, ceramics, cements, catalysts, petrochemicals, batteries, and minerals. As such, it is unsurprising that one of the catchphrases used in the field is "everything's a sample".

This session took a pharmaceutical flavor, but included examples of the application of powder diffraction to other practical problems. Its use along with other complementary techniques, such as DFT-D, to tackle challenging structures, was included in multiple presentations.

Rajni Bhardwaj (Eli Lilly) illustrated a variety of applications of powder XRD in the pharmaceutical industry. **Jim Kaduk** (Poly Crystallography, Illinois Institute of Technology, and North Central College) presented several new crystal structures of commercial pharmaceuticals, determined using synchrotron powder diffraction data. **Yuanpeng Zhang** (NIST) discussed the local magnetic cluster size identified by neutron total scattering in site-diluted spin glass SnxFe4-xN for x = 0.88. **Elena Kabova** (U. Reading) presented "Powder diffraction - pragmatic, precise, or both?" in which she showed both new structures and the application of density functional theory to assess the accuracy of such structures.

James A. Kaduk and Elena Kabova

2.2.2: New toys: Sources, Beamlines and Detectors

The purpose of the session was to highlight recent advances in sources, beamlines and instrumentation. **Sol Gruner** opened the session with a talk about new developments in imaging radiation detectors, designed with wider dynamic ranges to take advantage of beams from x-ray free electron lasers, low emittance storage rings, and aberration-corrected electron microscopes. He discussed the relationship of the dynamic range with other detector characteristics. **Karol Nass** followed with an update on the SwissFEL facility for structure determination of microcrystals and time-resolved crystallography (TR-SFX), that has been used successfully for several user and commissioning. He described the supported sample delivery techniques, sample environment, pump and probe possibilities and the capabilities of the new JUNGFRAU X-ray detector. **Joe Ferrara** presented the first Ultra High Speed System (UHSS) hybrid photon counting detector detector developed at Rigaku. The detector, capable of collecting 50 kfps at continuous mode, or 1 Mfps in burst mode, is well suited to use for time resolved experiments in the submicrosecond time scale.

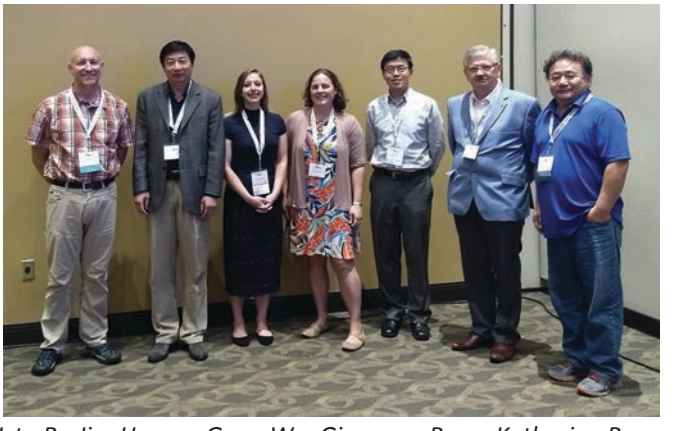
On the subject of synchrotron beamline facilities,

Aina Cohen talked about progress on the new undulator beamline at the Stanford Synchrotron Radiation Lightsource. This beamline is optimized for serial crystallography experiments, with a broad bandpass multilayer monochromator option and a high frame rate EIGER detector; it is also meant to function as a gateway for users of the Macromolecular Femtosecond crystallography (MFX) instrument at LCLS. **Scott Classen** presented ALS-ENABLE, a new NIH-funded program to support the joint operation of MX and SAXS beamlines at the Advanced Light Source, and the plans for a shared computing, data storage and networking infrastructure to cope with increasing data collection rates and carry out real time data processing. He also gave a historic perspective on structural biology at ALS and an update on the ALS-2 upgrade. **Masaki Yamamoto** gave an overview of the automated data collection and data analysis software ZOO in use at the microfocus beamline BL32XU at Spring-8. The software is capable of automated sample selection and consecutive data collection from crystals present in the same mount. It also performs data processing and merging of data from several samples. He also described the conversion of the SAXS beamline BL45XU to a MX beamline. **Marian Szebenyi** described the recently completed Cornell High Energy Synchrotron Source upgrade to a dedicated high-flux, high energy 3rd generation source. Half of the beamlines are brand new, while the others have undergone extensive renovation. She gave a brief description of the beamlines already allocated, dedicated to MX, SAXS, X-ray spectroscopy and material science using scattering and other techniques. **Wuxian Shi** talked about the new macromolecular crystallography beamlines at the National Synchrotron Light Source II, FMX and AMX. These beamlines are characterized by high flux and micron-sized beams. AMX is focused on automated experiments and high throughput. The frontier micro-focus beamline, FMX, is designed to tackle challenging problems. She illustrated the capabilities of the beamlines with a couple of successful experiments, involving multicrystal data collection and serial crystallography approaches.

Ana Gonzalez

2.2.3: Locating and Refining H Atoms using X-ray, Neutrons and Solid-State NMR

The ACA session "Locating and Refining H Atoms using X-ray, Neutrons and Solid-State NMR" was held on July 22, 2019. The session had six speakers including three solid-state NMR spectroscopists, two speakers describing neutron diffraction methods and applications and one discussing x-ray diffraction techniques for locating hydrogens. The session represents a variation on the NMR crystallography session and one of the first to bring together into the same session speakers using both diffraction and NMR methods.



L to R: Jim Harper, Gang Wu, Giovanna Pope, Katharine Page, Xiaoping Wang, Krzysztof Wozniak and Yu-Sheng Chen

The work presented makes clear that x-ray diffraction methods can now provide hydrogen positions approaching the accuracy of those derived from neutron diffraction data. Remarkably, all of the NMR methodologies presented also provide hydrogen positions while representing a very different time scale than diffraction. The NMR work was also shown to provide very accurate anisotropic displacement parameters for hydrogens. Attendance of the session was over 30 people and the format appeared to be an effective way to engender discussion among the practitioners of the different techniques.

Jim Harper and Yu-Sheng Chen

2.2.4: General Interest I

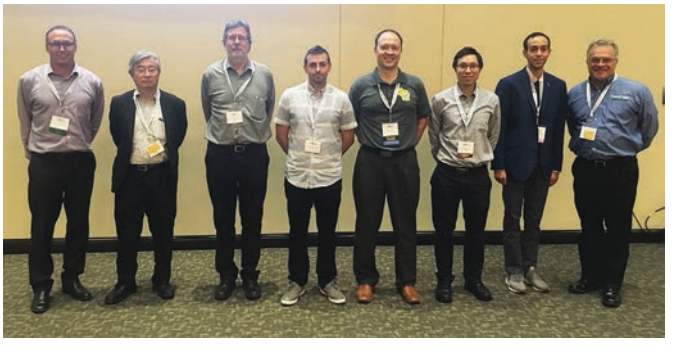
L to R: Gregory Powell, Bruce Noll, Suzanna Ward, Kevin Gagnon, Carolyn Brock, Winnie Wong-Ng and Peter Corfield

Suzanna Ward (Cambridge Crystallographic Data Centre) discussed the impact that having a curated

database of one million small molecule structures has had on crystallographic research. **Carolyn P. Brock** (University of Kentucky) explained how Z>1 structures arise from approximate symmetry in the P1 space group using an impressive data set drawn from the CCDC database. **Kevin Gagnon** (Vertex Pharmaceuticals Inc.) presented an in-depth examination of an example of enantiomeric enrichment via crystallization and the resulting (extremely complex) solid solution continuum. **Peter Corfield** (Fordham University) conducted an examination of a series of copper cyanide coordination polymers and the diverse topologies they can form. **Winnie Wong-Ng** (National Institute of Standards and Technology) presented a detailed examination of Ca-M-Co-O systems and the relationship between their crystal chemistry and a wide range of physical properties. **Gregory Powell** (Abilene Christian University) showed how he uses disomium sawhorses and a series of inexpensive ligands to make metal organic frameworks for solvent capture. **Bruce Noll** (Bruker Nano, Inc.) made most of the room jealous of the capabilities of the PHOTON III CPAD detector and its photon-counting capabilities. **Joerg Wiesmann** (incoatec GmbH) then further impressed the room with his description of the Diamond Hybrid Anode microfocus X-ray tubes incoatec has created.

Matthew L. Brown, Joe Tanski, Brandon Mercado

2.2.5: Crystallization on the International Space Station



L to R: Marc Giulianotti, Hiroaki Tanaka, Timothy Mueser, Jose Manuel Martin Garcia, Ilia Guzei, Albert Chan, Kristofer Gonzalez-DeWhitt, Ken Savin

The use of microgravity to improve the quality and size of crystals for structural determination studies has been explored since the days of Mir and the Space Shuttle Program. Now, with the availability of a long-duration microgravity environment onboard the International Space Station (ISS), space-based crystallization experiments have both continued and expanded. This ACA session provided a forum for topics that ranged from how to access the ISS for research purposes to the use of the space station for growing large crystals for neutron diffraction; utilization of commercial off-the-shelf (COTS) hardware and space station crew members for crystallization on the ISS; and how to engage students in crystallization-related science, technology, engineering, arts, and mathematics (STEAM) education.

The session began with an overview of recent and upcoming crystallization experiments supported by the ISS U.S. National Laboratory. Following that, University of Toledo researcher **Timothy Mueser** gave a presentation on his team's custom-designed crystal growth apparatus, the Toledo Crystallization Box. This apparatus is being used for capillary counter diffusion experiments on the ISS, with the goal of generating crystals of sufficient size and quality for neutron crystallography studies. Mueser's presentation was complimented by a talk from **Tanaka Hiroaki** of Confocal Sciences Inc., in which Hiroaki described a novel device for growing large crystals both in Earth-based laboratories as well as onboard the ISS. The first half of the session closed with a STEAM presentation from **Ilia Guzei**, from the University of Wisconsin–Madison, who described how he has expanded his successful statewide STEAM program focused on crystal growth to now include an ISS experiment component. This marked the second year Guzei's education program has utilized the ISS National Laboratory.

The second half of the session focused on describing the use and application of COTS hardware for crystallization experiments on the ISS. By using COTS equipment, researchers are able to make experimental design changes up to a couple months before a given launch, as opposed to the more than a year of lead time necessary for experiments using non-COTS hardware. This flexibility provides a timeline that fits more appropriately within the requirements of many structural biology groups. Highlighting this topic were two speakers who discussed the use of COTS hardware in their ISS National Laboratory research focused on cancer-related targets. **Jose Martin-Garcia** of Arizona State University spoke about his team's research on Taspase1, and **Albert Chan** of the Frederick National Laboratory for Cancer Research discussed his team's work with RAS. Additionally, **Kristofer Gonzalez-DeWhitt** of The Bionetics Corporation described how ISS crew members were able to set up counter diffusion experiments on the space station utilizing COTS pipettes and plates.

Ken Savin and Marc Giulianotti

3.1.1: Symposium on Structure in Cancer Biology II

The second session was focused on DNA repair and synthesis. **Michal Hammel** showcased the power of X-ray scattering for examining the assembly and functional conformations for a DNA double-strand break repair machine. **Sylvie Doublie** from the University of Vermont used structures to understand cancer-associated mutations in DNA repair enzymes. **Walter Chazin** from Vanderbilt used NMR, X-ray scattering and crystallography to examine protein-DNA interactions for cut and patch DNA repair. **Chi-Lin Tsai** presented a novel 4Fe-4S containing nuclease structure needed for replication restart. **Dong Wang** from the University of California San Diego unveiled structural views of transcription-couple damage recognition. The power of combined crystallography and EM to understand individual reaction steps and the effects of cancer mutants in complex molecules was nicely shown when **Lorena Beese** from Duke examined repair nucleases and **John Tainer** from MD Anderson described a large helicase complex. The combined set of talks gave us an important glimpse into the dramatic progress being made on large and dynamic molecules involved in DNA remodeling and cancer biology.

Betsy Goldsmith and John Tainer

3.1.3 Structural Biology Combining Solution SAS and High Resolution Methods (cryoEM, MX, NMR)

L to R: Jesse Hopkins, William Thomas, Aparna Annamraju, Miljan Simonovic, Melissa Gildenberg, Kushol Gupta

Small angle scattering (SAS) of both X-rays and Neutrons is a valuable biophysical tool that provides powerful complementary information to high resolution structural techniques like cryoEM, crystallography, and NMR. This session focused on projects that combined the high resolution methods with SAS to yield information beyond what either technique would provide on its own.

The session started with a talk by **Miljan Simonovic,** University of Illinois at Chicago, on his work studying enzymes responsible for accurate synthesis of human selenoproteins. Here he detailed work where high resolution structures could be obtained for both native and ligand bound states, but questions remained about whether the crystal structure was changing the observed conformation or inhibiting flexibility. Here SAXS proved critical in showing that what was observed in the crystal did exist in solution, a conclusion that was contrary to the predicted 'canonical' model of enzyme activity.

Melissa Gildenberg, University of Iowa, gave the next talk which focused on modeling conformationally flexible proteins using SAXS and molecular simulations. She described how she uses a coarse grained Brownian Dynamics simulation to generate ensembles of flexible states in solution. The coarse-grained approach allows this to be used on larger systems that are intractable by all-atom MD. These full ensembles are then fit the scattering data measured in solution, yielding much better results than conventional minimal ensemble searches for systems with a wide range of conformation states.

The next talk was from **Aparna Annamraju**, University of Tennessee at Knoxville, and focused on studies of the interactions between ionic liquids and cellulose using NMR, MD, and SAXS. Cellulose is an abundant biopolymer that has a wide range of possible applications industrial. However, it is not soluble in water and common organic solvents. Her work focused on understanding why imidazolium based ionic liquids were able to fully dissociate cellulose strands from microfibrils into individual strands. Solution scattering data provided information on overall size and conformation while NMR and MD provided insight into the dissolution mechanism.

Kushol Gupta, University of Pennsylvania, discussed his work studying drug-induced aggregation in HIV integrase. Combining high resolution structures from crystallography, solution scattering data, and other biophysical methods he was able to characterize the aggregation mechanism of allosteric inhibitors of integrase (ALLINIs) from early order oligomers all the way up to a weak 3D gel. Understanding these mechanisms and resulting escape mutants provides useful data for optimizing ALLINI drug design and understanding mechanisms of resistance.

The final talk of the session was by **William Thomas**, Cornell University, who discussed his work studying allosteric transitions in a ribonucleotide reductase enzyme. His work used SAXS to reveal reversible interconversion between six unique oligomeric struc-

tures. Using the SAXS data as a guide he was able to determine high resolution structures from crystallography and cryoEM for a catalytically important intermediate and two novel inhibited helical filaments. This work provided insight into the molecular basis for the enzymes control of de novo conversion of ribonucleotides to deoxyribonucleotides.

Jesse Hopkins

3.1.4: Solid State Supramolecular Chemistry and Crystal Engineering Part I

L to R: Max Hützler, Alexander Pöthig, Grigorii Skorupskii (at rear), Rajni Bhardwaj, Dmitriy Soldatov (at rear), Yael Diskin-Posner, Christer Aakeröy (at rear), Kraig Wheeler

This session, Part I of a full day symposium on Solid State Supramolecular Chemistry and Crystal Engineering (see 3.2.4 for Part II), brought back this important topic to the ACA Annual Meetings agenda. The topic covers a very intense area of research, where crystal structure analysis is a primary experimental tool virtually of any study. The symposium was co-organized by **Wilhelm Maximilian ("Max") Hützler**, UCLouvain, Belgium and Dmitriy Soldatov, U Guelph, Canada, and was generously supported by STOE, DECTRIS and PROTO Manufacturing.

After a short introduction by the session co-chair Max Hützler, six speakers representing all generations highlighted research on a variety of subjects in academia and industry. **Christer Aakeröy**, Kansas State U, illustrated strategies in the design of functional materials through co-crystallization of judiciously selected molecules and thorough understanding of intermolecular forces governing the self-assembly process. **Kraig Wheeler**, Whitworth U, presented a series of studies focused on the formation of quasiracemate bimolecular crystals. After the coffee break, **Alexander Pöthig**, Technical U Munich (Germany), gave a lecture on pillarplexes, a new class of organometallic cavitands that can act as "molecular pores" in solution. **Grigorii Skorupskii**, MIT, presented work on conductive MOF (metal-organic framework) materials. **Yael Diskin-Posner**, Weizmann Institute of Science (Israel), introduced new inclusion complexes of metal-organic molecular capsules with photoswitching molecules. Finally, **Rajni Bhardwaj**, Eli Lilly & Co, showed how the problem of polymorphism in their pharmaceutical company was addressed using a combination of experimental techniques and computational modeling.

Dmitriy Soldatov and Wilhelm Maximilian Hützler

3.1.5: Functional Sustainable Materials

L to R: Craig Bridges, Jung-Hyun Kim, Kamila Wiaderek, Claudia Rawn, Margit Fabian, Fernando Uribe-Romo, Matthew Logan, Valeri Petkov

This session covered recent work on functional materials from a range of technological and scientific backgrounds, ranging from battery electrodes and solid electrolytes, to metal-organic framework compounds, cage structures and in-situ synthesis studies, with the talks generally having a connection to the sustainability of materials. Participants included chemists, physicists and engineers from universities and national research centers, and the session was well attended. **Jung-Hyun Kim** (The Ohio State University) began the session with a talk about the phase evolution in cathode materials, and in particular on the mixture of electrodes with solid electrolytes. The challenges and opportunities of working with LATP were presented, and how incorrect reaction time and temperature can lead to impurities that influence performance. **Kamila Wiaderek** (Argonne National Laboratory) discussed the current understanding on the structure of ε-$VOPO_4$. We learned how the water:alcohol ratio influences particle growth under hydrothermal conditions, and how the type of carbon used for electrical contact in the electrode has an important impact on the

performance - graphene shows better performance that typical conducting carbon fillers. **Margit Fabian** (Center for Energy Research) then discussed lithium and sodium oxide-halides used in solid state batteries, for studies conducted at the Budapest Neutron Center. These are challenging materials to synthesize, and Ba or Ca doping could potentially lead to the formation of various impurities, possibly due to cation size differences. **Fernando Uribe-Romo** (University of Central Florida) presented work on metal-organic frameworks (MOFs) as matrices for organic-based substitutional solid solutions. These included porous interweaved zirconia-organic frameworks and redox active MOFs. He described the fascinating result of adding ferrocene to MOFs, which influences electron hopping and thereby the conductivity. Moreover, multifluorophore MOFs could be constructed by using mixture of red, green and blue fluorophores to create white light emission. **Claudia Rawn** (University of Tennessee, Knoxville) described the successful synthesis of the compound $Ca_{12}Ga_{14}O_{33}$ (or C12G7) through a wet chemical method. The compound consists of a positively charged cage-like structure balanced by occluded anions that sit on a partially occupied site to charge balance the positively charged framework. **Craig Bridges** (Oak Ridge National Laboratory) presented work on operando neutron scattering of batteries, to look at both the microstructure and surface passivation reactions that occur in high concentration electrolytes during cycling versus a model mesoporous carbon anode. This shows that electrolyte concentration can influence the voltage at which chemical processes occur, and change the composition of the passivation layer on the electrode. **Rebecca McClain** (Northwestern University) provided insight into the mechanism of $ABiQ_2$ (A = alkali metal, Q = S, Se) formation using panoramic synthesis involving high temperature X-ray diffraction. Her work showed the presence of various intermediates and polymorphs as a function of temperature, time and composition, including ordered and disordered rock salt structures. Rebecca was the recipient of the 2019 Margaret C. Etter Student Lecturer Award from the Materials SIG in this session. The session concluded with a talk by **Valeri Petkov** (Central Michigan University) on the structural dynamics of nanoalloy catalysts in fuel cells. We learned about in-situ diffraction studies that provide compositional mapping over the membrane of a PEM fuel cell (PEMFC) during operation. In-situ PDF reveals changes in the particle size, the presence of a mixture of FCC/HCP, and the existence of a phase transition.

Craig A. Bridges and Matthew Logan

3.2.1: Application of anomalous techniques in macromolecular crystallography

L to R: Kamel el Omari, Toshiya Senda, Leighton Coates, Naohiro Matsugaki, Vincent Olieric, Wayne Hendrickson, Sarah Barwell, Armin Wagner, Elspeth Garman and Derek Mendez
Top inserts: Yasufumi Umena and Sabine Botha

The session was opened by **Wayne Hendrickson**, Columbia University. He introduced the concepts of anomalous diffraction for experimental phasing and to identify elements based on the refinement of the anomalous scattering factor f". He presented recent results obtained at NSLS-II for native SAD phasing from multiple microcrystals at longer wavelengths. **Kamel el Omari**, Diamond Light Source, UK, described how the challenges for crystallography at wavelengths longer than 2.7 Å can be overcome and presented recent highlights from the in-vacuum long-wavelength MX beamline at Diamond. **Naohiro Matsugaki**, KEK, Japan, introduced beamline BL1A at the Photon Factory. He described how a deep UV laser system can be used to shape crystals into spheres to improve data quality at long wavelengths. Laser shaping also featured prominently in the fourth presentation, given by **Vincent Olieric** from the Paul Scherrer Institute in Switzerland, to prepare crystals for fast native SAD phasing at 3.75 keV with the new JUNGFRAU detector. This detector will allow exploiting long wavelengths more efficiently compared to existing technology.

Sarah Barwell receiving the Margaret C Etter Student Lecturer Award from Toshiya Senda (Photograph by Richard Bromund)

In the second half of the session, practical aspects of phasing and element identification were presented. **Elspeth Garman**, Oxford University, UK, presented how the combination of anomalous diffraction and proton induced X-ray emission (PIXE) can be applied to gain further insight into the biochemistry of metalloproteins. **Leighton Coates**, Oak Ridge National Laboratory, studied potassium binding in the selectivity filter of a potassium channel with long wavelength X-rays close to the potassium absorption edge. **Sarah Barwell**, University of Waterloo, Canada, presented a very elegant way to study an inhibition mechanism based on anomalous scattering from iodine. Sarah was awarded the Margaret C Etter Student Lecturer Award for her beautiful work. **Yasufumi Umena**, Okayama University, Japan, demonstrated how anomalous diffraction can be used to give insight into the valence state of the four manganese atoms in the oxygen-evolving complex of photosystem II. The last two presentations covered data processing aspects for serial crystallography experiments. **Sabine Botha**, Arizona State University, presented her work towards SAD phasing for serial millisecond crystallography at the synchrotron. **Derek Mendez**, Lawrence Berkeley National Laboratory, concluded the session with his talk about data processing of two-colour experiments at X-ray free electron lasers.

Toshiya Senda & Armin Wagner

3.2.2 SAS Contrast Methods in Biology and Soft Matter

★No report submitted★

Volker Urban and Kushol Gupta

3.2.3: Home-Built Software and Hardware

The "Home-Built Software" session that debuted at the 2017 ACA meeting was reprised this year before a near-capacity audience as the augmented "Home-Built Software and Hardware" session.

The long history of home-built software and hardware has seen small and large applications from the simplest routines -- format-conversion software, for example, to link the output of one specialized program to the input of another -- to more extensive applications, including widely distributed programs for a more complete set of crystallographic calculations. Home-built hardware may be less famous on the whole, but a wide array of gadgets of varying degrees of sophistication have been made or adapted in the crystallographic laboratory. The evolving niche of home-built software and hardware was the topic of this half-day session.

Large facilities are the quintessential example of sites that by their nature need specialized software, mostly home-built. This year's session opened with a talk by **Frank Murphy**, Assistant Director of NE-CAT / Cornell University (Northeastern Collaborative Access Team at the APS at Argonne National Laboratory), funded principally by NIH. The focus of Frank's talk was v2 of RAPD, a package of programs for automated macromolecular diffraction data processing. This open-source package analyzes NE-CAT data in real time. Complete information on NE-CAT and RAPD can be found here: https://lilith.nec.aps.anl.gov/newsite/

Large facilities are also playing an increasingly important role in small-molecule crystallography, with NSF's ChemMatCARS holding a leading position as a third-generation synchrotron user facility for chemical and materials crystallography. In addition to small molecule crystallography, ChemMatCARS, which is at the Advanced Photon Source (APS) at Argonne National Laboratory, also has leading-edge instrumentation for anomalous small-angle scattering and liquid-surface scattering. **Yu-Sheng Chen**, Beamline Operations Manager and lead scientist in the advanced chemistry program at ChemMatCARS, described the current status and future plans for ChemMatCARS, including the possibilities that the anticipated APS upgrade and resulting enhanced beam will provide to the small-molecule crystallography community. As described by Yu-Sheng, current and future projects include new leading-edge developments, such as better diffuse scattering measurements than previously possible, or perhaps serial crystallography, as well as enhanced access for chemical crystallography. Full information on NSF's ChemMatCARS can be found at https://chemmatcars.uchicago.edu/ .

Aimed principally at macromolecular structure, **Blaine Mooers** contributed a talk on a library of tools for improving the efficiency of image making using PyMOL. PyMOL (see pymol.org) is an advanced molecular visualization system especially suited to macromolecular structure. Blaine presented tools that ease the user's task, akin to software ergonomics. For

example, interactive quizzes can be used to refresh a user's knowledge about commands for tasks that the user does not use frequently. You can find more about the Mooers lab's snips, clips, and shortcuts at github. https://github.com/MooersLab

Two software tools that are widely used in small-molecule crystallography were featured in the session. CRYSTALS, software for single-crystal structure refinement and analysis, was the subject of **Richard Cooper's** presentation. Based on Fortran code with some C++ wrappings, CRYSTALS also features scripting code that allows users to automate tasks, but which will be replaced by Python scripting code in the future. In a development known as "Hug and Squeeze," CRYSTALS is able to apply resonant scattering to the SQUEEZE procedure (calling out to Platon for SQUEEZE). In the context of SQUEEZE, it was noted that CRYSTALS has long had the ability to store and use precomputed additions to the structure factors. For more on Hug & Squeeze, see Cooper, Flack & Watkin, Acta C, 2017, c73, 845-853. Richard's presentation included a particularly instructive discussion of restraints, especially restraints on ADP's. The question of the relevance of a restraint was also addressed in terms of leverage, which in this presentation was defined as the influence of an observation on its own calculated value. The leverage of a restraint is the relative influence that the restraint has on the calculated value of the restrained quantity.
CRYSTALS can be found here:
Download www.xtl.ox.ac.uk
Code: https://github.com/ChemCryst/crystals

ShelXle, another program that is in widespread use in small-molecule crystallography, was featured in a presentation by author **Christian Hübschle**. This very useful graphical user interface for SHELXL has among its design criteria, as described by Christian, that "the user keeps 100% control over the input file." There is no hidden processing, no black box. This program is loaded with useful features. It can shred a CIF and load its embedded .res file. It can load other programs, as defined by the user. It has advanced features such as Henn-Meindl plots. The integrated editor includes syntax highlighting and features code completion for Shelx instructions. ShelXle is freely available under the GNU Lesser GPL, from the ShelXle download page or from SourceForge.
https://www.shelxle.org/shelx/eingabe.php
https://sourceforge.net/projects/shelxle/

Paul Boyle used his program COSET as a platform for exploring the methods and reasoning used in preparing home-built software. COSET resides in the Linux world and is written in standard C99. Details of COSET, including references and test data, are freely available at http://xray.chem.uwo.ca/COSET/index.html

The program derives possible merohedral and pseudo-merohedral twin laws. A reference paper describing COSET was published in J. Appl Cryst. (2014) 47, 467-470. The theoretical basis of the program is described in Flack (1987) Acta Cryst. A43, 564-568.

It goes without saying that crystal growth must precede crystal structure analysis. **Steven Kelley**, Director of the X-Ray Diffraction facility in the Chemistry Department at the University of Missouri, Columbia, described his method for lab-scale growth of organic crystals from the melt, including his equipment and potential hazards. He reviewed current melt-based methods in crystallography, and compared melt growth and solution growth. Steven also had some nice comments on his impression of his first ACA meeting.

And following crystal growth there's crystal mounting. **Joe Reibenspies** treated the audience to a tour through a large cornucopia of tools for crystal handling. Joe displayed a countless number of aids for the three main steps in getting a crystal from where it formed to the diffractometer – namely sample retrieval from vial to slide, specimen selection and specimen mounting. Picks, probes, pipettes, greases, STP oil treatment, slides, a microtorch and other useful tools including a yoga block all figured in the lively presentation. Joe maintains an excellent web site with a "Tools of the Trade" section that is sure to include whatever you are looking for, including web references to primary sources: https://xray.chem.tamu.edu/tool.php

Victor Young, Oleg Mikhailovskii and Larry Falvello (Photograph by Richard Bromund)

The "Home-Built" session closed with a special presentation by Etter Student Lecturer Award Winner

Oleg Mikhailovskii, on a new software solution that refines macromolecular structures to diffraction data alongside a modern molecular dynamics protocol. As described by Oleg, the incorporation of structure factor calculations into a popular biomolecular simulation package permits restraints based on structure factors to be incorporated as a maximum likelihood potential in conjunction with the usual force field. Oleg presented a performance evaluation for this new protocol based on some 84 structures, comparing the results with results obtained using conventional refinement.

This second installment of the Home-Built session again treated the audience to a selection of the broad line of topics being covered by home-built solutions. Macromolecular and small-molecule crystallographic tools were represented, as were labs of all dimensions, from home labs to national facilities with international user bases. The interest displayed by speakers and by the audience reflects the continuing viability of in-house software and hardware developments.

Victor Young and Larry Falvello

3.2.4: Solid State Supramolecular Chemistry and Crystal Engineering Part II

L to R: Raúl Castañeda, Max Hützler (at rear), Gabriel Valdivia, Wesley Newsome (at rear), Nicholas Blagden, Dmitriy Soldatov (at rear), Tomislav Friščić (at rear), Hamilton Napolitano, Martin Ward (at rear)

This session, Part II of a full day symposium on Solid State Supramolecular Chemistry and Crystal Engineering (see 3.1.4 for Part I) continued with seven more presentations in the afternoon. **Nicholas Blagden**, U Lincoln (UK), presented his perspective on the problem of crystal growth of polymorphs and co-crystalline solids. **Phillip Fanwick**, Purdue U, shared his experience as a co-editor of Acta Cryst C with the quantity and quality of submitted data, refinement of H-atoms and the overall scope of the journal. **Hamilton Napolitano**, State U Goias (Brazil) introduced the crystal structure and properties of a new chalcone, one in a class of biologically active molecules. **Gabriel Valdivia**, Brigham Young U, highlighted studies on the design of molecular terahertz generation crystals. After the coffee break, **Tomislav Friščić**, McGill U, gave an overview of how their recent studies revealed surprising relationship between solvent-free chemistry of MOFs (metal-organic frameworks) and mineralogy. **Martin Ward**, U Strathclyde (UK), described sophisticated experiments that made it possible to recover high-pressure forms of solids to ambient conditions. **Wesley Newsome**, U Central Florida, reported on the creation of solids with unique photophysical properties due to the incorporation of excimers (excited dimers) in the solid state structure of MOFs. Finally, **Raúl Castañeda**, U Ottawa, reported on the synthesis and solid state structure of heterometallic complexes with interesting physical properties.

Dmitriy Soldatov and Wilhelm Maximilian Hützler

3.3.1: Would You Publish This?

L to R: Danielle Gray, Brandon Mercado, Stacey Smith, Michael Ruf, Richard Staples, Joe Reibenspies, Jeff Bertke, Carla Slebodnick

This year more than 75 scientists attended the less formal and ever popular evening session, Would You Publish This? Presenters came with their questions and the audiences debated and provided advice. **Joe Reibenspies**, Texas A&M, started the night out by asking "Where would you publish this?" Other highlights from the session included a discussion of fun with messy twins from **Stacey Smith**, Brigham Young University, as well as a discussion about a reticular twin from **Michael Ruf**, Bruker. **Richard Staples**, Michigan State University, asked how one would go about refining small molecule structure models using datasets with multiple wavelengths so he could refine chiral structures using data collected at a synchrotron set up for protein data collection. **Jeff Bertke**, Georgetown University, tried to understand

the oxidation state of Ce in his nanocluster structures, while **Brandon Mercado**, Yale University, questioned pseudo symmetry in his structure.

Danielle Gray

4.1.1 Central Dogma in 3D: The Legacy of Tom Steitz

L to R: David Jeruzalmi, Satwik Kamtekar, Phoebe Rice, Miljan Simonovic, Robin Stanley and Martin Schmeing. Photo courtesy of David Jeruzalmi

This session was to honor many contributions to the field of structural biology and macromolecular X-ray crystallography of late Tom Steitz, the 2009 Nobel laureate in Chemistry. Speakers included former doctoral students and post-doctoral associates spanning several decades of research in the Steitz laboratory, who showcased research inspired by their training with Tom. Dr. **Phoebe Rice**, The University of Chicago, gave a brief introduction about Tom's contributions and then presented a multi-decade compendium of research from the Steitz lab and later from her own group that explains how serine-family DNA recombinases facilitate DNA rearrangements and are regulated by DNA topology. The session continued with a seminar by Dr. **Martin Schmeing**, McGill University (Montreal, Quebec Canada). Martin talked about non-ribosomal peptide synthesis and showed remarkable progress on structural characterization of elusive, multicomponent enzymatic systems that link amino acids without the assistance of the ribosomal nanomachine. Dr. **Robin Stanley**, National Institutes of Health, described how non-ribosomal biogenesis factors help the assembly of the ribosomal particle. Robin presented cryo-EM and X-ray crystal structures of AAA-ATPase Rix7 and related factors that were solved by her research group and contextualized structural and functional data. Dr. **Satwik Kamtekar**, Pacific Biosciences, summarized briefly years of research on Phi29 DNA Polymerase during his postdoc in the Steitz laboratory. Then, he shifted gears and elegantly explained how high-resolution structural results on this enzyme are guiding the development of cutting-edge DNA sequencing technologies. Dr. **David Jeruzalmi**, The City College of New York, continued the session with a seminar on replicative helicases. David showcased several decades of research, spanning his doctoral studies to the present day, and provided compelling insights about these remarkable enzymes that are required during DNA replication. Dr. **Miljan Simonović**, The University of Illinois at Chicago, closed the session with his overview seminar on how human selenoproteins are synthesized. Miljan presented structural studies on a series of human enzymes that facilitate selenoprotein synthesis that his research group has completed over the last decade. Each of the participants provided personal stories about Tom Steitz and insights into their relationship with a remarkable scientist and mentor and emphasized Tom's impact on their scientific careers and lives.

Phoebe Rice and Miljan Simonović

Session 4.1.2: Radiation damage in X-ray crystallography and cryo-EM

This session consisted of five talks on the challenges and opportunities generated in structural biology by radiation induced reactions. **Dr. Corie Ralston**, an invited speaker from Lawrence Berkeley National Laboratory, described an X-ray-mediated in situ hydroxyl radical labeling method and beamline 3.2.1 at the Advanced Light Source which can facilitate a broader use of this powerful technique. She then presented time-resolved and steady-state hydroxyl radical labeling studies, which mapped structural rearrangements of the orange carotenoid protein (OCP) and fluorescence recovery protein (FRP) so that their interactions in response to light changes can be understood at the molecular level. **Dr. Edward Snell** from the Hauptman-Woodward Medical Research Institute presented next and described a series of experiments on xylose isomerase crystals that revealed a motion of a metal cation in the active site of the enzyme attributed to mechanism, could be explained by unit cell expansion induced by X-ray radiation. **Dr. Robert Thorne** from Cornell University demonstrated through very systematic research how diffraction intensities decay with X-ray dose. His studies reconciled two long-standing controversies: (1) whether the underlying model for atomic displacements due to X-ray exposure should

use the Lorentz distribution rather than the Gaussian distribution, and (2) what are the doses that cause the decay to one-half of the initial intensity. **Dr. James Holton** from the Advanced Light Source presented a set of simulations describing how to shape a sequence of illuminating specific crystal volumes, given a particular X-ray beam profile, in order to achieve optimal diffraction data quality. The session was concluded by a talk by **Dr. Dominika Borek** from the University of Texas Southwestern Medical Center who presented comparison of radiation damage induced processes in X-ray crystallography and cryo-EM, and used a set of data from thaumatin crystals to show how one can decompose specific radiation induced changes with independent component analysis so that radiation-induced reactions proceeding with different rates can be separated.

Dominika Borek and Gerd Rosenbaum

4.1.3 and 4.2.3: Cool Structures: Important Science from Small Molecule Crystallography

Cool Structures, which has been a staple in the Small Molecule program at ACA meetings, returned in 2019 as a full-day session with ten presenters. As in the past, there was a strong emphasis in this session to showcase the science done by, or in collaboration with, emerging researchers, and two Etter Student Lecture Awards were presented.

R. Lee Ayscue and Karah Knope (Photograph by Richard Bromund)

Matthew Brown and Louise Dawe (Photograph by Richard Bromund)

These were awarded to **R. Lee Ayscue**, who presented his work from the Knope lab at Georgetown University on "Structural variability and luminescence color tuning in lanthanide-organic hybrid materials", and to **Matthew Brown** who was awarded the Canadian Division award for his work on "3D printing crystallographic data for post-printing construction" which he carried out independent from his graduate studies in chemistry at Simon Fraser University. Other presented showcased work that ranged from "Hydrogen bond nets in dithionate metal salt crystals" (**Robert Burrow**) to "Single Crystal Neutron Diffuse Scattering of Layered Ferromagnet Fe3-xGeTe2" (**Yaohua Liu**), and the variety of works presented by "Unique/Problem Structures in the Daily Life of a Staff Crystallographer" (**Michael Gau**). The variety of small molecule research made for a dynamic session by all presenters.

Karah Knope, Louise Dawe, Jeffrey Bacon and Stacey Smith

4.1.4 In situ and in Operando Characterization of Functional Films

The session on in situ and in operando techniques for characterizing functional thin films gathered participants from the community of synchrotron, free electron laser and neutron source users into a discussion of cutting edge characterization of thin films, an increasingly common part of applications in energy harvesting, energy storage, catalysis, and microelectronics. **Christin-Ann Dippel** (DESY) started the session describing the development of grazing incidence pair distribution function (GIPDF) analysis and its application to study the growth of sputtered platinum layers. This new approach enables the structural characterization of even amorphous ultrathin films in situ and operando. Several participants presented work characterizing organohalide perovskite thin films.

Uta Ruett and Joseph Strzalka

L to R: Christin-Ann Dippel (DESY), Uta Ruett (ANL), Shambhavi Pratap (TU München), Hua Zhou (ANL), Jacob Jones (NC State), Hsinhan Tsai (LANL), Wanyi Nie (LANL), Joseph Strzalka (ANL), Alamgir Karim (U Houston) and Stephen Rankin (U Kentucky)

Wanyi Nie (LANL) reported about grazing incidence wide-angle x-ray scattering (GIWAXS) studies of perovskite thin films under simulated solar illumination, revealing light-induced lattice expansion. **Hsinhan Tsai** (LANL) discussed in situ functional characterization of x-ray induced photocurrent in perovskite thin films that establishes these materials as excellent candidates for next-generation x-ray detectors. **Shambhavi Pratap** (TU München) focused on the formation of perovskite thin films during spin casting enabled by an innovative multimodal measurement chamber supporting simultaneous GIWAXS and photoluminescence measurements. The fabrication of other thin film material systems was also presented. **Alamgir Karim** (U Houston) spoke about high-throughput fabrication of ordered block-copolymer thin films via dynamic zone annealing as studied in situ with grazing incidence small angle scattering (GISAXS). **Jacob Jones** (North Carolina State University) complemented the experimental talks with a discussion on developing analytical tools. He spotlighted the role of Bayesian inference in improving the quantification of the results of structural analysis, especially the handling of uncertainties and the comparison of structural parameters, as illustrated with his own experimental work on ferroelectric thin films. **Stephen Rankin** (U Kentucky) presented GISAXS and GIWAXS studies of surfactant-templated mesoporous metal oxide thin films. **Hua Zhou** (Argonne) wrapped up the session with a look forward to frontier methods in the application of nanometer size and coherent synchrotron x-ray beams, and free electron lasers. His work extends the use of surface scattering techniques to mesoscale applications and transient phenomena.

4.1.5 Diversity and Inclusion - Diverse Teams Perform Better

Prof. **Benny Chan** led an exciting and challenging mini-workshop about identity and intersectionality. He also spoke about the pipeline model of minorities in STEM and contrasted that with an "obstacle course" model.

Prof. **Laura McCullough** presented her talk by video connection. She provided statistics and definitions on gender representation in chemistry and physics, and demonstrated the malleability of biases.

Dr. **William Bauer** presented a model for interactions with minority-serving institutions.

Dr. **Tsehai Grell** spoke about the distinction between diversity and inclusion, and about implicit biases. At an audience question, she also spoke about how to support grad students with families.

Prof. **Bernie Santarsiero** spoke about the elements of student success, emphasizing community support and cultural dialogs.

co-chairs Anna Gardberg (Industrial) and Rebecca McAuliffe (YSIG). Supporting SIGS: Industrial, YSIG
Presented With Support from Constellation Pharmaceuticals

4.1.6: General Interest II

In the second half of the full day session, the focus shifted to protein crystallography. **Chelsy Chesterman** (GSK Vaccines) opened the session by showing

everyone the library of Dab antibodies they have created and how they can be used to create synthetic symmetry to aid crystallization. **George Lountos** (Frederick National Laboratory for Cancer Research) then presented the crystal structure of part of the Y.pestis bacteria (the plague, Black Death) and how it shows a potential for new anti-plague agents to be developed to overcome antibiotic resistant plague strains and avoid side effects to the host. **Zhen Huang** (SeNA Research Institute, GSU) then explained how to use selenium-atom-specifically-derivatized nucleic acids to the benefit of protein crystallography. **Miki Senda** (High Energy Accelerator Organization [KEK]) elucidated a protocol for creating well-diffracting protein crystals based on their high-throughput experience. **David Moreau** (Cornell University) showed how traditional assumptions of uniform solvent throughout the crystal are incorrect, with the solvent composition inside a protein often being different from the crystallization solvent. He then showed methods for measuring the composition and density of the solvent inside the protein. **Nicholas Noinaj** (Purdue University) informed the session of the latest work into the structures of Beta-barrel outer membrane proteins and the biological implications of these structural revelations. **Bi-Cheng Wang** (University of Georgia) then provided the session with an overview of the upgrade plans at the Advanced Photon Source and informed us what user services will be available during the planned two year shutdown. Finally, **Diana Tomchick** (UT Southwestern Medical Center) closed out the session by revealing how the selenoprotein-O pseudokinase transfers AMP from ATP to certain residues on protein substrates, showing formerly unrecognized activity. They also showed the interesting structural data behind this discovery, and the implications it has for other pseudokinases.

Matthew L. Brown, Joe Tanski, Brandon Mercado

4.2.1: What is the Meaning of Resolution?

Session 4.2.1 included four talks discussing how different problems in data collection and analysis may complicate assessment of resolution limits. In the first presentation, Dr. **Greg Pintilie** from Stanford University and SLAC Cryo-EM Facility discussed the advantage of using Z-scores to assess how a model correlates with a cryo-EM map. He used as an example a recent Electron Microscopy Data Bank (EMDB) map challenge, in which assessment of model quality with Z-scores allowed the identification of regions in the models that required further refinement. The next speaker was Dr. **Scott Stagg** from Florida State University, who presented his experience in the EMDB map challenge with the use of global quality indicators (such as the Fourier Shell Coefficient) vs. local quality indicators (RMSD-based fit of the model to cryo-EM density). He also discussed the impact of data quality and quantity, as well as detector performance on these indicators. Dr. **Zbyszek Otwinowski** from the University of Texas Southwestern Medical Center discussed how resolution is a measure of data information content both in cryo-EM and X-ray crystallography, and how criteria defining resolution limits should take it into account. He also described limitations of using global quality indicators. The concluding talk, delivered by Dr. **Clemens Vonrhein** from Global Phasing, focused on challenges of dealing with highly anisotropic diffraction data and the best strategies of using them in structural analysis. He also discussed the STARANISO server that presents data information content to users with a reciprocal space viewer and also in the form of .log files so that users can analyze both their own data and also assess quality of data sets deposited into the Protein Data Bank.

Raquel Bromberg and Zbyszek Otwinowski

4.2.2: Structure Based Drug Design

Session 4.2.2 was organized to highlight examples and methods of crystallography in drug discovery efforts. **Seungil Han**, Pfizer, presented the fragment based discovery story of PF-06650833, detailing structures of the protein kinase IRAK4 in complexes with small molecules to rapidly optimize an inhibitor from early hit to lead in a successful program that yielded the advancing clinical candidate for immunology. He addressed aspects common to drug discovery efforts, including compound evaluation with efficiency indices and chemical properties for appropriate ADME behavior in addition to improving affinity and selectivity for the target.

L - R: Nina Wolf, Clarissa Jakob, Debanu Das, Seungil Han, Stephen Burley, Leah Frye, Michael Martynowycz and David Dranow

Clarissa Jakob, AbbVie, described an interesting study for oncology targeting the wild-type IDH1 rather than the more heavily studied mutant forms, using X-ray crystallography to elucidate structure-activity relationships of initial screening hits and optimizing novel binding modes for inhibitor designs of useful tool compounds. **David Dranow**, UCB, outlined efforts on malaria and cryptosporidiosis and presented structures of lysyl-tRNA and prolyl-tRNA with early screening hits to rationalize and design selective inhibitors with promising proof of concept compounds exhibiting oral efficacy in mouse models. **Michael Martynowycz**, UCLA, introduced the MicroED technique with the exciting possibilities that electron diffraction studies provide for both small-molecule and macromolecular structure determination. He reviewed developing methods and discussed results on several disease relevant applications including alpha-synuclein and Tau peptides.

After the coffee break, **Stephen Burley**, RCSB, spoke about the contributions of structural biologists to 210 new drug approvals between 2010 and 2016 as captured in the PDB, and noted new analysis underlining the importance of the public database in the scientific ecosystem of drug discovery and development. **Leah Frye**, Schrodinger, talked about computational advances in structure-based design strategies and featured tools in the Maestro system to address applications such as target druggability, core hopping, and the energetics of water and ligand binding for prospective design. **Debanu Das**, Accelero Biostructures, highlighted methods of fragment-based drug discovery and the crucial role of structure determination for efficient progression of chemical matter. Finally, **Nina Wolf**, UIC, presented structures of ClpC1 with Rufomycin and Ecumicin, and noted implications for anti-TB agents with new evidence of a covalent bond for the one heptapeptide complex. I'd like to thank **Thierry Fischmann**, Merck, for help in planning the interesting session with the speakers.

Kenton Longenecker

4.2.4: In situ and in Operando Measurements

★No report submitted★

Andrey A. Yakovenko and Sanjit Ghosa

4.2.5: Sustaining Crystallography Education and Training

This half-day session included an engaging group of speakers who highlighted unique ways in which they involve students in crystallography at their institutions. **Dean Johnston** (Otterbein University) discussed incorporating single crystal and powder diffraction into synthesis projects for undergraduates in short-term research experiences. **Suzanna Ward** (CCDC) described how their Database has been building the future of crystallography with their international outreach projects. **Lauren DePue** (UT Austin) described how she engages undergraduates in the structure determination of compounds synthesized from an array of amines and carboxylic acids. **Shao-Liang Zheng** (Harvard University) told us about how he enhances crystallographic education by hosting student-centered guest lectures by experts in different areas of crystallography. **Sandy Eagle** (East Tennessee State University) spoke about her experience teaching crystallography across the undergraduate curriculum using a small desktop diffractometer, such as a Rigaku XtaLAB Mini. **Marvin Hackert** (UT Austin) gave a talk about carrying out 3D printing of molecular models to support both undergraduate and graduate teaching and research, which included a review of the types of printers and their advantages and weaknesses. **Michael Ruf** (Bruker AXS) spoke about being "hooked on crystallography" with a story of identifying minerals in grains of sand collected at the beach, and discussed details of shutter-less data collection of a weakly diffracting sample. **Mark Whitener** (Montclair State University) ended the session with a talk that described his adventures doing coordination chemistry and crystallography with limited research funding. The session generated considerable discussion and interest from the audience and contributors. The future of the ACA is very much related to the educational experiences of today's students.

Joe Tanski and Brian Toby

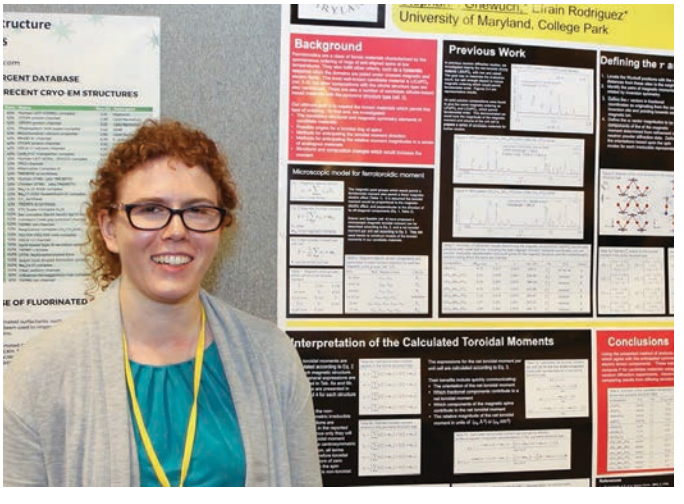
Poster Sessions

(Photographs by Richard Bromund)

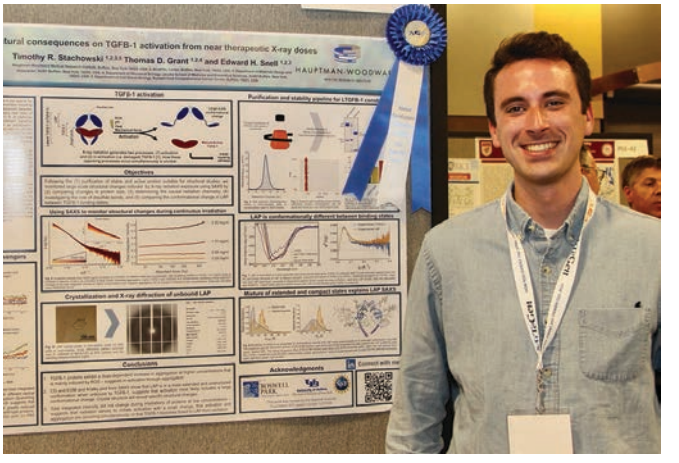
Poster sessions are the key component of the meeting for social and scientific interactions, as they bring everyone together into one venue, including vendors. The poster sessions at ACA2019 featured the usual very high quality presentations from attendees at all career levels and diverse institutions. Focusing on the poster prizes, the judges were challenged to identify the awardees, with much discussion and debate about the top posters in each category. The awards were announced at the banquet, where the winners received their prizes.

Pauling Prize winners:

Ravi Yadav, Purdue, Noinaj lab, "Structural basis for iron piracy by Neisserial lactoferrin binding protein B"



Stephanie Gnewuch, U. Maryland, Rodriguez lab, "Symmetry Analysis of the Toroidal Moment in Magnetoelectric Crystalline Materials"

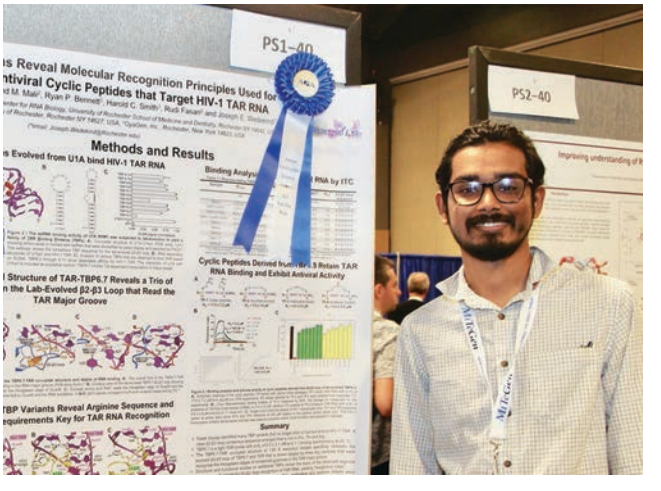


Timothy Stachowski, HWI Buffalo, Snell lab, "Structural consequences on TGFB-1 activation from near therapeutic X-ray doses"

IUCr Pauling Prize:

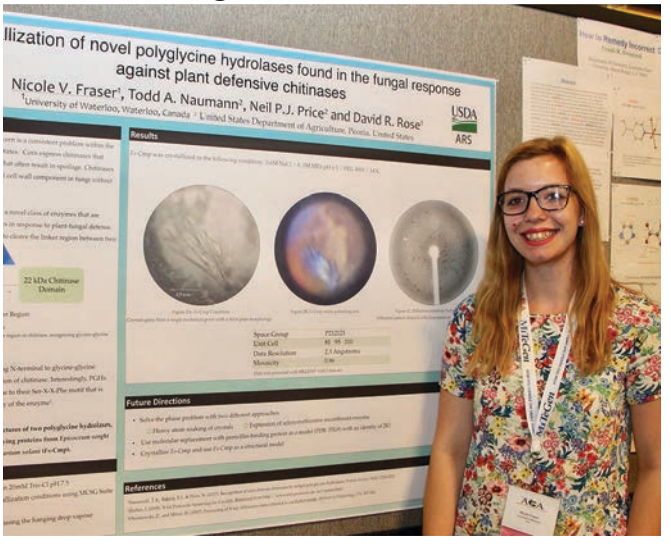
Veronica Carta, Indiana U, Sneddon lab, "Hydrogen Bonding in High-Z' Molecular Structures"

Sundaralingam Pauling Prize:



Sai Shashank Chavali, U Rochester, Wedekind lab, "Lab-Evolved Proteins Reveal Molecular Recognition Principles Used for Development of Antiviral Cyclic Peptides that Target HIV-1 TAR RNA"

Delbaere Pauling Prize:

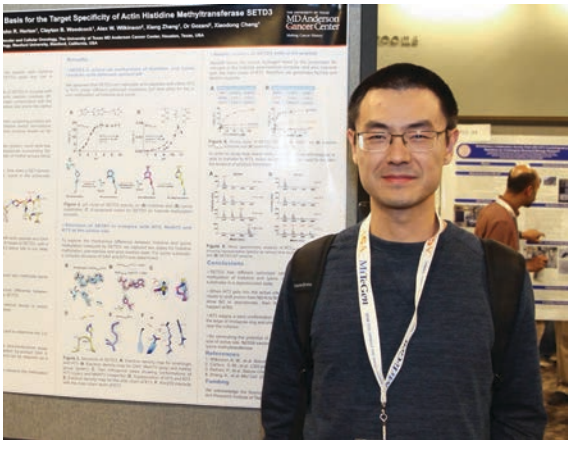


Nicole Fraser, U Waterloo, Rose lab, "Crystallization of novel polyglycine hydrolases found in the fungal response against flat defensive chitinases"

Oxford Cryosystems Low Temperature Prize:

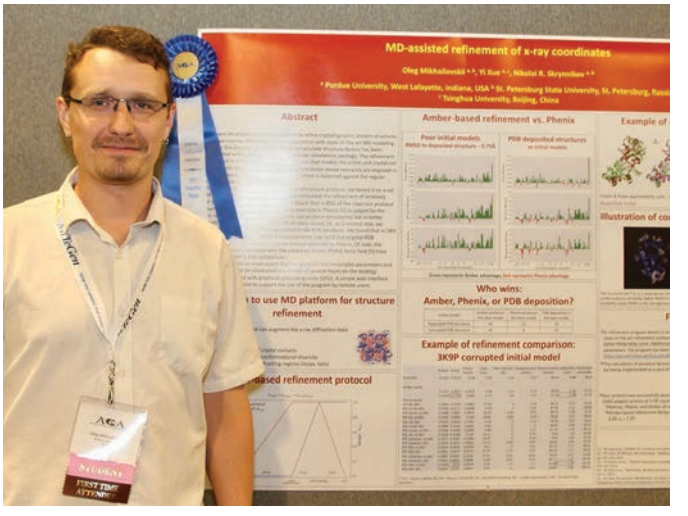
Yimin Mao, U Maryland, Zavalij lab, "Furan-2,5-dicarboxylic acid, a promising platform molecule: polymer, monomer, and MOFs"

RCSB Protein Data Base Prize:



Shaobo Dai, MD Anderson, Cheng lab, "Structural Basis for the Target Specificity of Actin Histidine Methyltransferase SETD3"

Taylor & Francis Biomolecular Crystallography Poster Prize:



Oleg Mikhailovskii, Purdue, Skrynnikov lab, "MD-assisted refinement of x-ray coordinates"

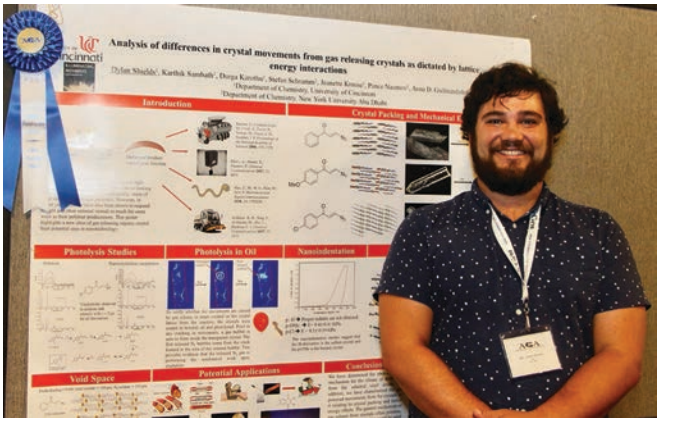
Journal of Structural Dynamics Poster Prize:

Bhupendra Karki, U Louisville, Freelon lab, "Local structural study of novel mott-insulating cousins of the iron pnictides"

Journal of Chemical Crystallography Poster Prize:

Amelia Wheaton, U Wisconsin Madison, Berry lab, "Polymorphic transformations of [Co(μ-OOCtBu)2py]2.0.5(C7H8)"

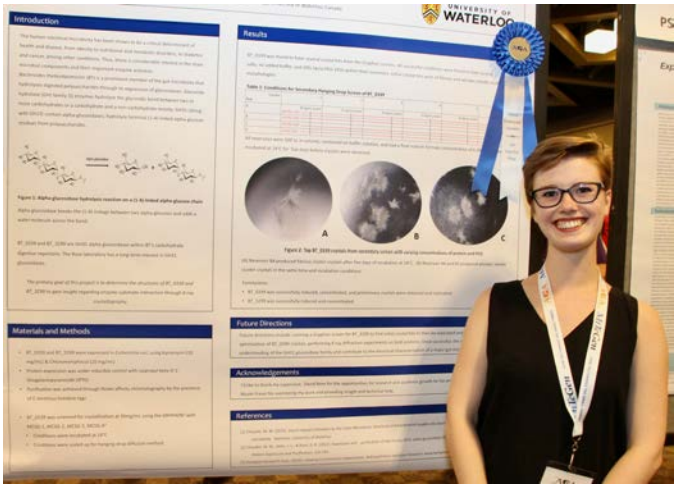
CrystEngComm Poster Prize:



Dylan Shields, U Cincinnati, Gudmundsdottir lab, "Analysis of differences in crystal movements from gas releasing crystals as dictated by lattice energy

interactions"

MiTeGen-Society of Physics Students Undergraduate Poster Prize:



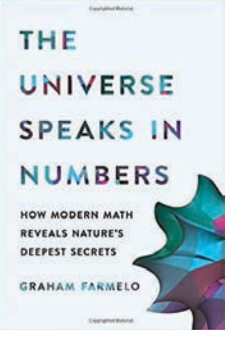
Clarisse Reid, U Waterloo, Rose lab, "Crystallization of two alpha-glucosidases found in Bacteroides thetaiotaomicron"

The number of attendees volunteering to act as judges was extremely gratifying – there were actually more volunteers than were needed. In fact, some were kind enough to step in at the last minute when necessary. Sincere thanks go out to the judges:
George Lountos, Thomas Proffen, Sandy Eagle, Effrain Rodriguez, Lauren DuPue, Alex Filatov, Matthias Zeller, Kraig Wheeler, Carrie Wilmot, Louise LaSalle, Tiffany Kinnibrugh, Korey Carter, Robert Burrow, Patrick Loll, Miljan Simonovic, Marian Szebenyi, Eric Montemayor, Catherine Lawson, John Helliwell, Jim Fettinger, Andrew Howard, Andrey Yakovenko, Christine Beavers, Edwin Stevens, Martin Schmeing, Brian Patrick

The co-Chairs would like to express our appreciation to all the prize sponsors and to the ACA staff for their expert assistance.

Co-Chairs: Louise Dawe (Wilfrid Laurier University), David Rose (University of Waterloo)

Book Reviews



The Universe Speaks in Numbers: How Modern Math Reveals Nature's Deepest Secrets
By Graham Farmelo
ISBN 978-0-465-05665-1

In The Universe Speaks in Numbers, Graham Farmelo presents a concise version of the history of the relationship between mathematics and physics. As Farmelo explains in his book, the relationship, though perhaps a natural one, has not always been an easy one. He even goes so far as to describe it as one that has gone through a long divorce and subsequent reconciliation.

Farmelo begins by describing Einstein's philosophy, that a purely mathematical and theoretical approach to the study of physics could wield meaningful insights into the natural world, as opposed to a purely experimental one. Even though Einstein's genius was celebrated in his own time as it is now, such an approach was considered laughable by many of his peers and fellow physicists. A young Robert Oppenheimer once described Einstein as "completely cuckoo," Farmelo explains. And Oppenheimer wasn't the only one.

But, as with many great minds, Einstein was simply ahead of his time. A significant amount of scientific research up to that point was observation and experiment-based. Now, the use of mathematics to study and describe physics on a theoretical level is widely practiced--string theory comes to mind as perhaps the most famous example of theoretical physics in the forefront of the zeitgeist.

After beginning with Einstein, Farmelo goes back to the basics--classical physics. It's a field that Isaac Newton--a mathematician by practice and title--helped describe. Newton, despite being well-known in high school and college physics courses today for his Laws of Motion, would not have considered himself as a physicist in his own time. Newton described his use of mathematics to explain what he saw in nature in his Principia--now considered a foundational text of calculus. Today, calculus and physics are essentially married subjects--but in Newton's time, the idea of wedding mathematical calculations with experimental insights to support theoretical observations was revolutionary, to say the least. His work catalyzed the integrated study of mathematics and science in an unprecedented way that would culminate in the invention of modern physics in the twentieth century.

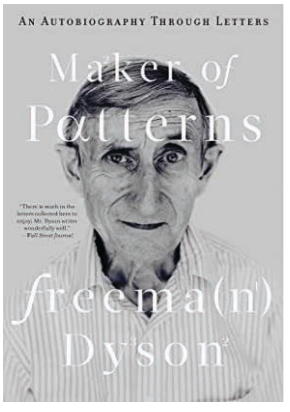
Farmelo makes sure to pay his respects to some of Newton's "giant" predecessors, upon whose shoulders Newton stood to see further. These include Aristotle and Galileo, amongst others. But the main focus of Farmelo's first chapter is Newton. After Newton, he details James Clerk Maxwell's mathematical investigations into electromagnetism--the culmination of which is a series of equations that bear his name. From there, Farmelo moves on to the two revolutionary discoveries that define modern physics: basic relativity and quantum mechanics.

Then, Farmelo comes to the aforementioned long divorce. In the mid-twentieth century, many physicists, Freeman Dyson among them, felt physics stood alone from mathematics. Experimentation and observation were the foundations of the field. Dyson and his fellow physicists viewed the mathematical foundations of theoretical physics with skepticism. Now 92, Dyson--along with others in the field--have changed their tune. It's intriguing to read The Universe Speaks in Numbers not long after reading Dyson's memoir Maker of Patterns: An Autobiography Through Letters. He's gone from being the narrator to the narrated, so to speak--from the director of the show to an actor in it, and it's an interesting transition. If you want more on Dyson after reading The Universe Speaks in Numbers, or even if you want a scientist's immediate perspective on the events Farmelo describes in his own book, I recommend checking out Dyson's memoir.

It's humbling to note, as Farmelo does, that it took three centuries to get from Newton to the Standard Model of particle physics, and only four decades to get from the Standard Model to where we are today. The last four decades occupy the second half of The Universe Speaks in Numbers, and as you might expect, more modern characters like Stephen Hawking make an appearance, while Dyson continues to pop up as the fields of theoretical physics and mathematics begin to repair their relationship and reconcile. If you want to learn how, you'll have to read it for yourself.

Farmelo is both a professor of physics and a skilled science writer--and it shows. He demonstrates a firm command of the subject matter, which coupled with his accessible language and writing style makes The Universe Speaks in Numbers a delightful and insightful read.

Jeanette S. Ferrara, MA



Maker of Patterns: An Autobiography Through Letters
By Freeman Dyson
ISBN: 978-0871403865

Freeman Dyson's Maker of Patterns is an intimate, interesting self-portrait. It covers the years of his life from 1941 to 1978. Unlike most autobiographers, whose self-histories are inherently tinted by the lens of hindsight, Dyson tells his life story through letters written to his family in this 37-year period.

The epistolary narrative is one-sided, as Dyson only provides his letters to his family, but not their responses to him. However, modern-day Dyson does make an appearance, so to speak, in the form of contextual notes, always in italics. These notes introduce main characters, and fill in narrative holes that the reader might otherwise find confusing.

For example, upon the birth of several of Dyson's children, he stopped writing letters for a while. He explains that by the time his later children came along, he used the telephone to call his parents across the pond and share the good news, rather than wait for a letter to be delivered.

Dyson begins with letters he wrote home to his parents as a young student at Cambridge University. In 1941, World War II had been raging in Europe for quite some time. Dyson admits in a note that it was a great time for a young man like himself to seek an education, as there was a plethora of prestigious professors and dearth of students. His letters describes the depth of conversations had with noted figures such as mathematician Godfrey Hardy--all around a billiard table.

From Cambridge, Dyson's letters take us to Cornell University, where he began pursuing a doctoral degree in 1947 and met Richard Feynman, the noted physicist. From there, Dyson went to the Institute for Advanced Study in Princeton, New Jersey from 1948-1949, then to Birmingham, England for fellowship from 1949-1951. In 1951, Dyson returned to Cornell University as a physics professor--even though he still had not earned his doctorate (and lacks one to this day). In 1953, the Institute for Advanced Study offered him a permanent position--and he has stayed in Princeton ever since.

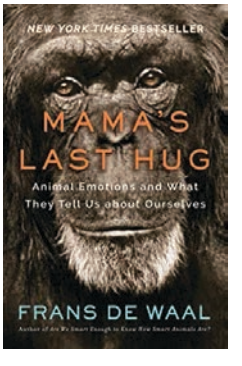
Dyson's detailed interpersonal relationships with renowned characters such as Robert Oppenheimer and Richard Feynman were certainly enough to keep the pages turning. But perhaps the most powerful narrative was his familial one. Once Dyson started growing his family, his children make regular appearances in the letters, often more fleshed out as characters than the celebrities of academia running in the Institute's social circles.

And those children have grown up to be quite impressive themselves. His oldest daughter, Esther, is widely regarded as one of the most influential women in technology. And his son George, who helped Dyson digitize the letters for ease of reading, is a noted historian.

Assuming that the letters have been transcribed in their entirety and not edited unnecessarily, the effect is one of a unique personal history told when the past was still present.

Fair warning: this book is less about Dyson's academic achievements in the fields of theoretical physics and mathematics and more about his personal life and relationships. If you are looking for a more technical book, I recommend reading one of Dyson's many earlier works.

Jeanette S. Ferrara, MA



Mama's Last Hug: Animal Emotions and What They Tell Us About Ourselves
By Frans de Waal
ISBN 9780393635065

Frans de Waal's latest book, Mama's Last Hug, derives its name from a singular event. In 2016, an elderly professor named Jan van Hoof visited a dying female chimpanzee named Mama at the Burgers Zoo in the Netherlands. Van Hoof had known Mama for over forty years, having spent many of them studying her behavior and the behavior of her fellow chimpanzees in the zoo's colony.

Van Hoof entered her evening enclosure, known as a night cage, and as soon as Mama recognized him her face burst into a wide grin and she started to make vocalizations indicating she was happy to see him. When van Hoof got close enough, she

wrapped her arms around him in a warm embrace.

Even though van Hoof had known Mama for over four decades, he had never interacted with her without being safely behind bars. Any grooming sessions or conversations had taken place with a physical barrier between them. Despite any cute or cuddly appearances, an adult chimpanzee can and will kill a human without hesitation. However, Mama's deteriorating condition facilitated extenuating circumstances, and van Hoof was able to enter her enclosure--still only with her permission. The event was unprecedented--and the video footage went viral.

Despite choosing the Mama's Last Hug as the title of his book, de Waal only covers the titular event in-depth in the first chapter of the book. The aging Mama's final hug serves as an entry point and later, a touchstone, for a larger narrative regarding expressions of animal emotions, not only of primates but other mammals as well--including humans. The following six chapters cover a broad variety of topics, from anthropomorphism to bartering to alpha male bullying. De Waal occasionally relates the current topic of discussion back to Mama and her role in the Burgers Zoo chimpanzee colony.

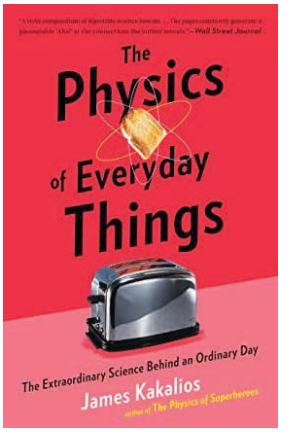
One interesting social behavior de Waal covers--which directly pertains to the title of the book--is the alpha female. Mama was a matriarchal figure in her colony. If Mama liked you, you were going to be just fine, and if Mama did not like you, you were not. Even in patriarchal societies, alpha females can and do wield a tremendous amount of social-emotional power.

De Waal illustrates the concept of the alpha female by directly referencing a passage from Bruce Springsteen's 2016 autobiography Born to Run. When Springsteen was an up-and-coming musician, he used to play at a club in New Jersey. The success of the band's performance was determined by one young woman in the audience--Kathy. If Kathy liked the music, she would get up to dance and everyone else would follow suit. If Kathy didn't like the music, the night was a bust. But even so, they didn't want Kathy to like them too much--that would cause tension and foster a detrimental rivalry with the alpha males who hung around the club vying for Kathy's attention.

After describing Springsteen's youthful experience with alpha female control, De Waal brings the narrative back to Mama and the Burgers Zoo chimpanzee colony, likening Mama's control over the colony's social hierarchy to Kathy's control over the success of a band's evening performance at a hole-in-the-wall club.

Passages like this one in Mama's Last Hug serve to provide helpful context for the reader regarding the social and behavioral phenomenons de Waal describes. They also underscore several of de Waal's key points about animal emotions, human emotions, and humans as social animals with emotions. De Waal has a unique gift for condensing decades of his own scientific research into a concise, digestible format that flows naturally and is easy to read with little to no background in behavioral studies.

Jeanette S. Ferrara, MA



The Physics of Everyday Things: The Extraordinary Science Behind an Ordinary Day
James Kakalios
978-0-7704-3775-6

James Kakalios' newest book is a delightful endeavor into the physics of everyday life. Kakalios does not take the time to explain the basic concepts of physics, but rather the basic physics (or not-so-basic physics) of mundane mechanisms. These range from alarm clocks and toasters to car engines and airplanes--all things that we largely take for granted in our everyday lives. At times, Kalakios leans towards oversimplification of certain concepts, but as he himself admits in the chapter where he explains how an MRI machine works, "if you know all this--why are you reading this book?"

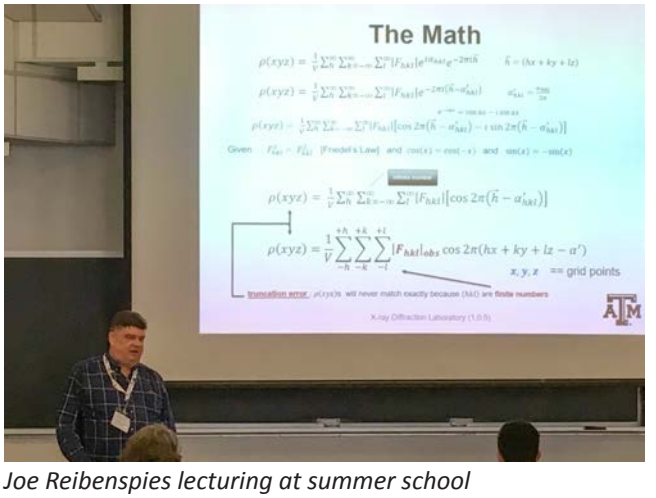
The Physics of Everyday Things is not geared towards physicists or engineers, but rather physics enthusiasts.The ideal audience for this book might be a younger student of physics--perhaps a high schooler or college freshman--or someone who hasn't studied physics since their earlier days in academia. In order to enjoy the book and thoroughly appreciate it, the reader must have some knowledge of physics fundamentals. But someone who lives and breathes physics for a living might find it a little too trite to be entertaining.

Jeanette S. Ferrara, MA

ACA Summer School 2019

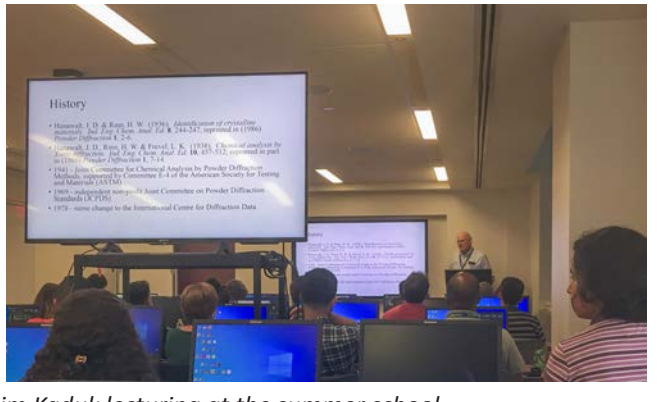
L to R: Amy Sarjeant, Charlotte Stern, Allen Oliver and Christos Malliakas

For eight years the ACA Summer Course in Chemical Crystallography had been co-hosted by Northwestern University and the University of Notre Dame. The most recent course at Northwestern University, from June 23rd-30th, will be the last time it will be co-hosted with Notre Dame University. Course organizers were: Charlotte Stern (Northwestern U) and Christos Malliakas (Northwestern U), Allen Oliver (U Notre Dame), and Amy Sarjeant (CCDC). The program opened with a welcoming reception for the 31 attendees and 15 faculty in the Institute for Technology at Northwestern. Attendees were from across the globe including: Venezuela, Brazil, Uruguay, New Zealand and the United States. Academic, National Laboratory and Industrial attendees were on the course roster.



Joe Reibenspies lecturing at summer school

The ACA Summer Course in Chemical Crystallography is a week long program that is now well into its third decade of instruction here in the United States. The course is directed towards Single-Crystal Chemical Crystallography and Powder Diffraction techniques, as applicable to small molecule studies and is designed to instruct attendees in the theory and practice of these two aspects of crystallography. Mornings were comprised of lectures on the theory of the experiment and the afternoons and early evenings covered hands-on workshops. Workshop material included interpretation of the International Tables, Symmetry and Space group analysis, and practical work on sample preparation for both single crystal and powder diffraction experiments. Later in the week this practical work moved to hands-on use of single crystal software such as SHELX and OLEX2, the CSD and ICDD databases, and powder XRD applications such as GSAS and FOX. Students worked with their own data that they brought with them or that we collected on one of our own single crystal or powder instruments, but also used canned data provided by the instructors. We have noticed that students over the years bring more basic knowledge than they did in the past, so we have divided them into groups depending on their ability. We have also incorporated some challenging problems that crystallographers might encounter so that when they see them in their own labs they might know where to go or whom to ask. Most importantly with the ratio of attendees and faculty there is time for one-on-one instruction. The networking from these close interactions is invaluable.



Jim Kaduk lecturing at the summer school

Attendees were encouraged to submit samples. There were about 50 samples submitted both for powder and single crystal data collections. As in past years, we (organizers) encouraged publication of these data with the request that an acknowledgment to the course be added. We have had a number of publications that we are aware of from previous courses.

Three vendors, Bruker, Stoe and Rigaku, kindly donated time and expertise from their applications specialists towards the program. This enabled direct instruction of the various software packages by experts. This was appreciated by the course

attendees. Generous sponsorship was provided by The American Crystallographic Association, The US National Committee for Crystallography, Bruker AXS, The International Center for Diffraction Data, The Cambridge Crystallographic Data Centre, The Pittsburgh Diffraction Society, MiTeGen, Stoe and Rigaku Americas. The International Center for Diffraction Data (ICDD) kindly provided temporary licenses for the Powder Diffraction File to allow instruction of this software. Northwestern owns a site-license to the Cambridge Structural Database and the Inorganic Crystal Structure Database. Other software used and made available to students included: OLEX2, Platon, SHELX, GSAS2, APEX3, CrysAlisPro, FOX, Avogadro, WinPloTR, OpenBabel, PreDICT and FullProf. Lecture rooms, conference rooms, computer rooms and facility space for data collection were kindly donated by Northwestern University. Instrumentation accessible to the attendees included four single-crystal and three powder diffractometers.

Feedback from the attendees was very positive and it was clear that this experience was extremely valuable to them. This was especially highlighted on the final day when the attendees were requested to give a short presentation on their experience. We would also like to thank our faculty for their donation of time, energy, enthusiasm and knowledge to this course. Finally, our thanks go out to the attendees, without whom we would not have the course.

Collecting single crystal data at the summer school

We are looking forward to our new venue for the course at Purdue University, which will rotate with Northwestern University hosting the course.

Charlotte Stern

Back: R. Papoular, J. Ferrara, P. Le Magueres, E. Reinheimer, L. Treadwell, A. Sarjeant, M. Del Campo, M. Zeller, B. O'Neal, J. Kaduk, A. Kalamarides, J. Reibenspies, R. Fortney-Zirker, R. VonDreele, M. Tuck, R. Sommer, C. Malliakas, J. Custodio, T. Boyle, A. Sanni, A. Tripithani. A Sakthivel, T. Higaki, D. Lesse

Middle: J. Lassa, D. Gray, G. Diaz Delgado, C. Ward, W. Ferriera, M. Silva, S. Urcia, M. De Souza, Z. Schulte, C. Posner, M.-C. Davilia Miliani, S. Shaner, M. Jones, J. Herder, D. Krvchuk, B. Wulsiak, N. Di Benedetto, L. Applegate, M. Shohel, B. Menefee

Front: M. Ringgold, B. Hernandez-Sanchez, G. Ludovico, R. Al-Sayyad, B. Noll, A. Oliver, C. Stern

Puzzle Corner

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

Solution to Crystal Connections #16: All relate to Cincinnati/ Northern Kentucky, site of this year's ACA meeting

1) Year in which space shuttle Columbia crashed: 2003, the same year as the last Cincinnati/Northern KY meeting

2) Recipient of the Buerger Award in that year: Jim Ibers gave the Buerger Award address at that meeting

3) Originally the Red Stockings (not to be confused with the Red Sox), later the Big Red Machine: The Cincinnati Reds

4) 1965 movie starring Steve McQueen as a poker player: The Cincinnati Kid

5) Her wedding ceremony was held at an ACA meeting: Jeanette Krause (Univ. of Cincinnati) married Allen Oliver at the 2017 New Orleans meeting

6) The only person to be both president of the USA and the Chief Justice of the Supreme Court: William Howard Taft, born in Cincinnati in 1857

7) Opened in 1866, crossing the Ohio River: The John A. Roebling Suspension Bridge, linking Cincinnati and Covington

8) "Happy Trails" singing cowboy: Roy Rogers, born in Cincinnati in 1911, at the approximate current location of 2nd base, Riverfront Stadium

9) A good method for eating ice-cream cones: The Licking River joins the Ohio at Covington

Marian Szebenyi (MacCHESS) provided the solution to Crystoquote #4. She also identified the beamline picture in the "Cereal Crystallography" DISORDERED puzzle as the CHESS G3 serial crystallography setup at beamline ID7B2. No complete solution to Crystal Connections #16 was submitted, the licking ice cream cones clue being problematic.

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

Frank Fronczek – ffroncz@lsu.edu

Crystoquote #5:

Letter substitution reveals a quote by a well-known crystallographer

CITAT HDE DGHDZE CIT JKEELMLGLCZ CIDC ODCPAT HKPGQ JAKRLQT D EPAJALET CK CIT LORTECLBDCKA.
- GLOPE JDPGLOB

Solution to Crystoquote #4:

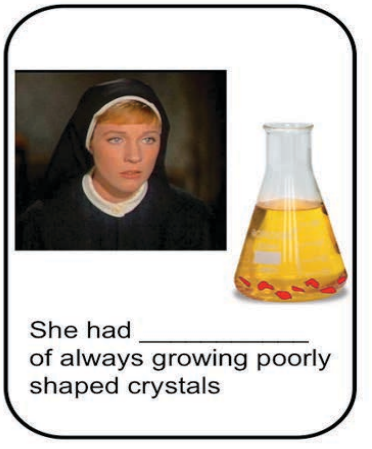
I then acquired a chemistry set that was stored under my bed and was able to mix chemicals and make wonderfully colored solutions and evil-smelling products.
Jenny Glusker

Fall 2019 DISORDERED Puzzle

DISORDERED

Recrystallize these distorted words into nicer forms

SIMPR	○
HALTS	○○○
BULODIAC	○ ○
ELENDE	○
KBOCL	○
DELAB	○



She had _____
of always growing poorly shaped crystals

Answer:

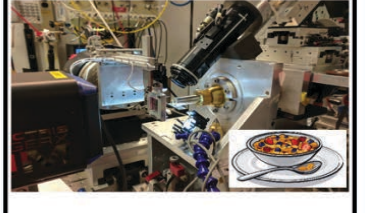
□ □□□ □□□□□

Solution to Summer 2019 DISORDERED Puzzle

DISORDERED

Shoot at these random words sequentially to make the full pattern

GASLINC	SCALING
RTCLASSY	CRYSTALS
GILYOOB	BIOLOGY
SHAPING	PHASING
CROTLENE	ELECTRON
AGREES	GREASE



Have breakfast at the beamline and do…

Answer:

"CEREAL" CRYSTALLOGRAPHY

OCTOBER 2019

10-12 **Latin American Crystallographic Association,** Valparaíso, Chile
https://www.cristalografia.cl/3rdlacameeting

15-30 **X-Ray Methods in Structural Biology,** Cold Springs Harbor Laboratory, NY
https://meetings.cshl.edu/courses.aspx?course=C-CRYS&year=19

24-26 **Pittsburgh Diffraction Conference,** Oak Ridge National Laboratory, TN
https://conference.sns.gov/event/78/

DECEMBER 2019

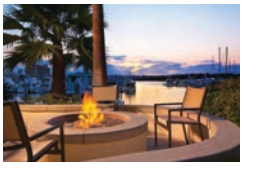
17 - 20 **AsCA, 16th Conference of the Asian Crystallographic Association**, Singapore
https://asca2019.org

April 2020

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

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

We gratefully acknowledge the continued support of our CORPORATE MEMBERS and welcome new members

Diamond Level: $2,200

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STOE SINCE 1887

Rigaku oxford diffraction

anatrace | Molecular Dimensions

BRUKER

MiTeGen

ttplabtech

ARI Art Robbins Instruments

Ruby Level: $1,800

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DECTRIS detecting the future

Anton Paar

ThermoFisher SCIENTIFIC

Emerald Level: $900

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- Acknowledgment in the Annual Program Book
- Be seen with your logo and link on our web site

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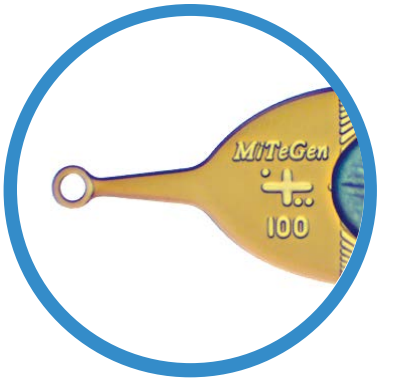

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