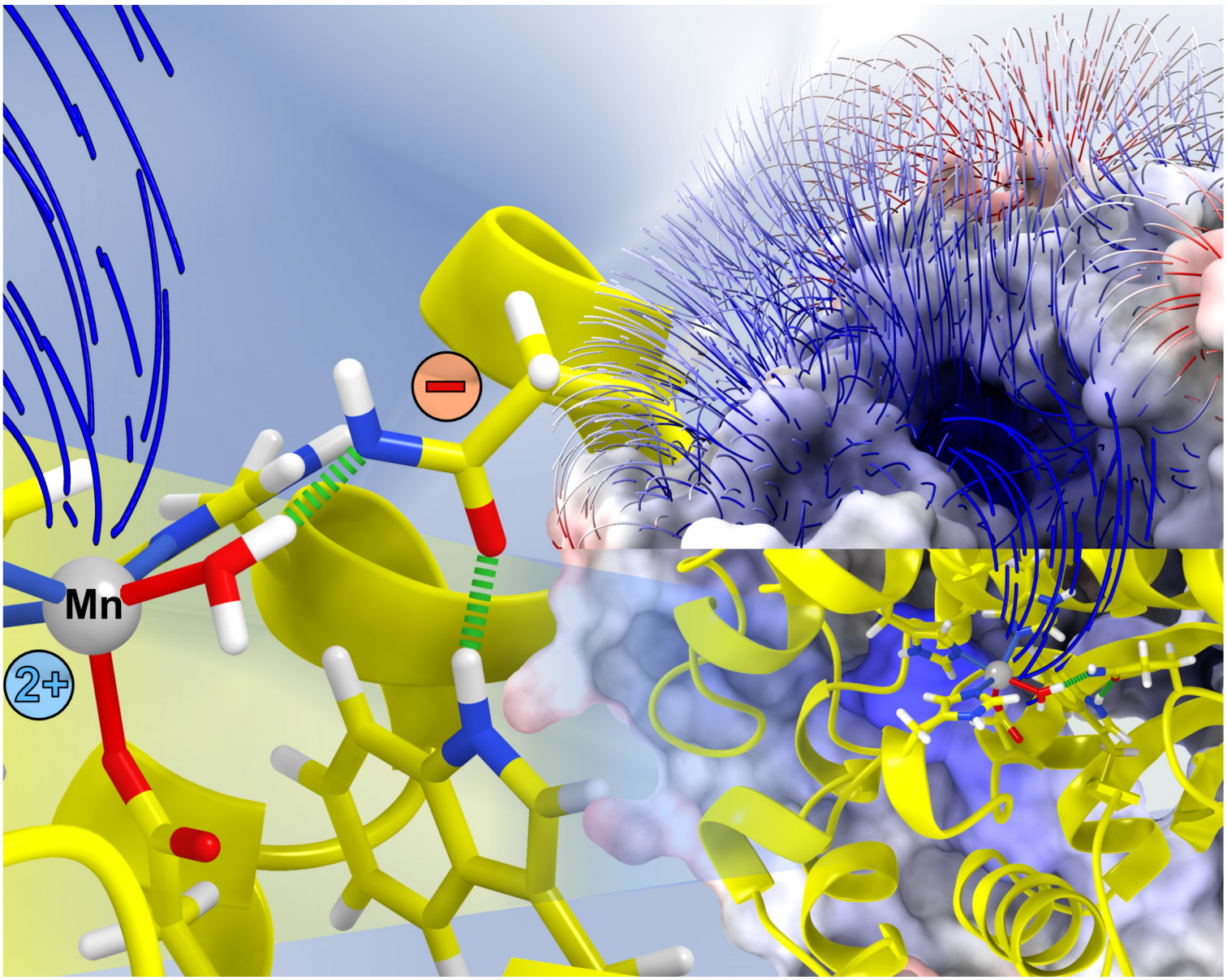
ACA RefleXions

American Crystallographic Association

Structure Matters

Number 3

Fall 2021



how a mitochondrial enzyme rapidly protects us from oxidative damage

The Borgstahl Group at the Eppley Institute for Research in Cancer

A REVOLUTION IN STRUCTURAL ANALYSIS
XtaLAB Synergy-ED AND XtaLAB Synergy-DW VHF

- **The combination of X-ray diffraction and electron diffraction broadens the range of single crystal sample size from nanometers to microns**

XtaLAB Synergy-DW VHF: The ultimate X-ray diffractometer with a powerful rotating anode source and two selectable wavelengths.

XtaLAB Synergy-ED: The world's first electron diffractometer designed to be used by crystallographers.

Rigaku oxford diffraction

CrysAlis Pro

All Synergy Diffractometers are operated by our popular CrysAlis Pro software.

The development of MicroED or 3DED has ushered in a new era of structural science. No longer constrained by the lower limit of sample size imposed by X-ray diffraction, structural scientists can now investigate nano-sized crystals using electron diffraction while still using X-ray diffraction to investigate micron-sized samples. Rigaku makes this easy to do as both X-ray and ED instruments are operated using our user-friendly end-to-end CrysAlis Pro software package.

Rigaku®

Rigaku Americas Corporation | 9009 New Trails Drive | The Woodlands, TX 77381 USA | rigaku.com | info@rigaku.com

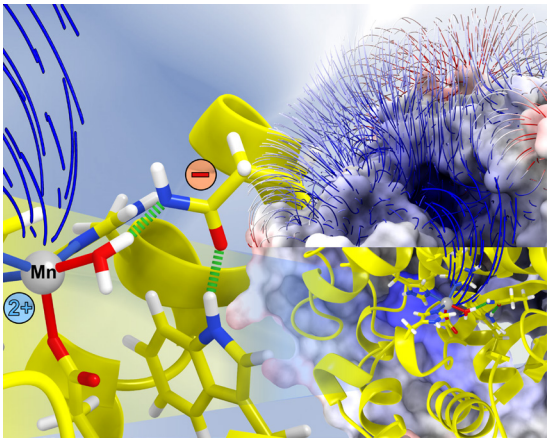
ACA RefleXions

ACA – Structure Matters

www.AmerCrystalAssn.org

Table of Contents

Index of Advertisers 1
President's Column 2
Canadian RefleXions 4
Amzel, Dunitz, and Johnson call for memorials 6
ACA 72nd Annual Meeting 7
Annual Elections 2021 8
ACA 2021 Candidates 9
ACA Awards and Fellows 25
Marilyn M. Olmstead Memorial Session 34
2021 ACA Meeting Report 35
Marek Grabowski Remembrance 37
Alan Mighell Remembrance 38
YSIG Speed Mentoring Session 40
Transactions Sessions T1 and T2 41
2021 Session Reports 44
Workshops 64
ACA Living History Project - Update 67
Book Reviews 68
Puzzle Corner 71
Corporate Sponsor News 73
Corporate Sponsor Members 76



About the Cover:
The Borgstahl Group at the Eppley Institute for Research in Cancer

Like a vacuum cleaner, electrostatic forces found on the surface of the human manganese superoxide dismutase active site funnel (blue positively charged vectors) draw in the negatively charged superoxide ($O2^{\bullet-}$) to the manganese metal. The superoxide is destroyed and the oxidative damage associated with aging and disease is prevented. The Borgstahl group at UNMC has revealed the unusual biochemistry that make this happen.

The lab of Eppley Institute professor Gloria Borgstahl, with scientists at Oak Ridge National Laboratory (ORNL), have published a landmark discovery on how a mitochondrial enzyme rapidly protects us from oxidative damage. This type of damage is responsible for all aspects of aging and disease.

The enzyme, manganese superoxide dismutase (MnSOD) uses concerted proton and electron transfers, or CPETs, for the destruction of superoxide. CPETs are a type of chemical reaction used by over a quarter of human enzymes and this discovery contributes to their understanding. The transfer of protons and electrons are key to biological life and are involved in processes like generating cellular energy and protecting cells from DNA damage.

This work has been published by ***Nature Communications****.*

Index of Advertisers

Rigaku	Inside Front
Proto	3
Dectris	24
Bruker	27
Cryo Industries of America	61
ATPS	62
Anton Parr	Back Cover

Contributions to ***ACA RefleXions*** may be sent to *Editor*:

Paul Swepston.....paulswepston@me.com

Cover:	Paul Swepston	Book Reviews:	Joseph Ferrara
Historian:	Virginia Pett	News & Awards:	Kay Onan
Photographer:	Richard Bromund	Puzzle Corner:	Frank Fronczek
Copy Editor:	Sue Byram	Spotlight on Stamps:	Daniel Rabinovich

Please address matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:

Kristin Stevens, Executive Director of the ACA
American Crystallographic Association
P. O. Box 96, Ellicott Station
Buffalo, NY 14205
tel: 716-898-8692; fax: 716-898-8695
kstevens@hwi.buffalo.edu

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

ACA RefleXions (ISSN 1058-9945) Number 3, 2021. Published four times per year in the spring, summer, fall, and winter for the membership of the American Crystallographic Association, P. O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to *ACA RefleXions*. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P. O.Box 96, Ellicott Station, Buffalo, NY, 14205-0096.

David Rose
ACA President

President's Column
Fall 2021

The dictionary defines "slack" as "characterized by a lack of work or activity". I started using the Slack app to follow the organization of our annual meeting, first in 2020 and again this year. I can tell you that the activity on the ACA Slack channels has been anything but slack!

At the time of writing, we have just completed our 2021 Annual Meeting. I'm more than confident you will agree it was a success; you will read about highlights in this issue of *RefleXions*. However, this meeting did not happen overnight. As soon as the dust settled from the 2020 conference, our Meeting Committee of Carla Slebodnick, Nozomi Ando, Brandon Mercado, Anna Gardberg, Kristin Stevens and Kristina Vitale, with input from SIG Chairs and you, our members, had already assembled a program outline and identified session topics and Chairs. However, as I have learned following Slack, that is only the first step.

We made the decision early in the year to focus on a virtual meeting, and it seems that, indeed, a large, in-person gathering would have been, if not impossible, at least inadvisable. While that eliminated the need for parallel in-person planning, one thing that we have learned is that planning a virtual conference is at least as complex (and expensive) as in-person. In addition to chasing down session Chairs, arrangements have to be in place for appropriate software versions and licenses, prerecorded talks and/or practice sessions, organizing 'Zoom facilitators', and many other details. The meeting relies on not just one internet system, but 1000 or more, one each for every presenter and attendee; the potential for a weak link is always there. The fact that attendees were likely unaware of the facilitators, all the other background and the 'Backstage' chatter, again on Slack, speaks to the thoroughness of the preparation. The success of the meeting is completely due to the contributions of the Meeting Committee, the SIG and Session Chairs, and the Poster Chairs, Tiffany Kinnibrugh and Sara Andres, our industrial sponsors, and, of course, Kristin and Kristina 'picking up the slack'.

Now our attention turns to the exciting prospect of getting together in person next year in Portland on July 29-August 3rd, 2022. What a delight it will be to chat with long-time friends, meet new members serendipitously over coffee, leisurely stroll through the vendors exhibits, and spend time with early-career scientists discussing their posters and presentations, their career plans and aspirations. Successful as our virtual meetings have been, there's nothing like being there. Having said that, we understand that some of our members, or prospective members, have difficulty with in-person travel for any number of legitimate reasons. Council and the Meeting Committee will continue to discuss ways to offer opportunities for these individuals to be included in meetings and other activities as much as possible. A reminder that Council is always open to receiving hardship requests for support to attend the meeting. Finally, it is especially important in 2022 to take advantage of the ACA room block at the meeting hotel. With the struggles of the travel industry, we expect that the hotel will not be forgiving if we do not meet our agreed (3+ years ago) target, and that would incur a significant financial hardship on our society. Headquarters will always be interested to hear of any 'bargains' that are identified close to or at the meeting site, so we can consider attempts to mitigate them. However, let's all stay together as much as possible, to maximize social interactions.

Meeting again in person will allow us to celebrate the accomplishments of our 2022 Award winners and 2021 class of ACA Fellows. In Portland, we will recognize the 2022 Bau Neutron

Diffraction Awardee, Arthur Schultz, of Argonne National Laboratory, our 2022 Fankuchen Awardee, David Goodsell, from Scripps Research Institute, the 2022 Trueblood Awardee, Airlie McCoy, of Cambridge University, and our 2022 Etter Early Career Awardee, Brent Nannenga, Arizona State University. All these individuals have been invited to present lectures at the Portland meeting and we look forward to hearing first-hand of their amazing contributions; our colleagues are, indeed, inspiring. More details on the Awardees, as well as information on our terrific new Fellows can be found on the ACA Website. The success of our meetings depends ultimately on us as members submitting, through our SIGs, ideas for scientific sessions featuring cutting-edge developments in our field and important new results. Our science has been instrumental in overcoming the pandemic and needs to continue to be in the consciousness of policymakers and the general public; we can't slack off now!

In the heat of our current optimism, it is easy to forget that this disease is still very much with us. The pandemic does not end locally until it ends globally. Large unvaccinated populations will continue to give rise to variants, which will spread quickly as travel restrictions ease and good public health practices are forgotten. Those of us who are fortunate to live in countries that are well-served with vaccine supplies must press for fair and free distribution of vaccines to all parts of the world. The momentum that our science has gained during this experience must be maintained to the benefit of our future health and economy. We have not seen the last of SARS-CoV-2 nor of future serious infectious diseases. This is an exciting time for Structural Science, especially for our trainees and early-career scientists. The future is bright! Structural Science Awakens!

David Rose

Canadian Reflexions

Gerald Audette
Canadian
Representative

September and Fall is, to me, always a fresh start. A new academic year is upon us with lots to look forward to and reflect on the conference season that is just past. With that in mind, I would like to take a quick moment to thank my colleagues on Council, and of course David Rose for his year of leadership at ACA President. David has been a great leader for our Association during the second "phase" of the altered landscape that resulted from the COVID-19 pandemic. It is great working with such an enthusiastic group, and I look forward to continuing to work with everyone into 2022 and looking froward to our next meeting in Portland.

The 2021 ACA meeting, Structure Science Awakens, was again a success. The Canadian Division, as always, co-sponsored sessions, including the very popular session "Getting that First Crystal". We had many Canadian colleagues, both established and trainees, presenting talks in various sessions, and of course posters. A big congratulations to Dean Lang, a PhD candidate at the University of Calgary in the lab of Dr. Ken Ng, who won the Louis Delbaere Pauling Poster Prize from his poster "Structural insights into the mechanisms of substrate recognition and catalysis for the N-methyltransferases involved in benzylisoquinoline alkaloid metabolism." Dean's poster explained a large body of very detailed work in a clear and well-laid out fashion – Congratulations!

I am delighted to announce that three of the seven ACA Fellows inducted at the 2021 annual meeting are Canadian. These incredibly well deserving members of our community are Hanna Dabkowska (Brockhouse Institute for Materials Research, McMaster University), P. Lynne Howell (The Hospital for Sick Children and the University of Toronto), and Frank Hawthorne (University of Manitoba). The profiles of the 2021 ACA Fellows can be found at https://www.amercrystalassn.org/fellows. If you've not already done so, pass on a congratulations to the very well deserving ACA Fellows.

This past August 13-20, 2021, saw the 104th Canadian Chemistry Conference and Exhibition (CCCE) / 51st IUPAC General Assembly and 48th World Chemistry Congress (IUPAC | CCCE 2021; https://www.cheminst.ca/conference/ccce2021/) as a virtual event. As in previous years, the Canadian Chemical Crystallography Workshop (CCCW) was held prior to the CCCE, from Aug. 8 – 11, 2021. As in past years, the CCCW was a successful event, and led once again by Louise Dawe. The Canadian Materials Diffraction Workshop (CDMW) was also a virtual workshop. Held July 26-29, 2021, and led by Valerie Jarvis from McMaster University, the CDMW was another success. The third annual Canadian diffraction workshop is the Canadian Powder Diffraction Workshop (CPDW). The CPDW, being co-organized by Jim Britten (McMaster) and Roberta L. Flemming (Western University) is scheduled for Saturday October 30 - Tuesday November 2, 2021, ahead of the 2021 Geological Association of Canada - Mineralogical Association of Canada Joint Annual Meeting (GAC-MAC; https://gacmac2021.ca/) in London, Ontario and it is hoped that it will be an in-person event, although a virtual format will be implemented if required.

This past August saw the 25th IUCr Congress and General Assembly in Prague, Czech Republic, which was delayed from 2020 due to the pandemic, and was held as hybrid event. A big congratulations must go out to the organizers and local co-chairs for getting the Congress off under such trying circumstances. Though many of us are now very used to remote "Zoom" (or other platform)

meetings, to organize and deliver a hybrid event is no small undertaking. Congratulations to all involved, and I hope that those of us that did get a chance to attend found something worthwhile and enlightening.

Speaking of the IUCr congress, there are a few bits of "Canadian Content" of note. The first item of note from the IUCr congress is that the next IUCr President will be none other than Hanna Dabkowska of the Brockhouse Institute for Materials Research at McMaster University. Hanna, who has been the IUCr Vice President since the 2017 Congress in Hyderabad, India, was elected at the General Assembly in Prague and will take over the leadership of the IUCr from Sven Lind for the next triennium until the Melbourne Congress in 2023. Congratulations to Hanna! For those who might want to know a bit more about Hanna, she was highlighted in the "News from Canada" column in the Spring 2019 edition of Reflexions. Congratulations Hanna! We know that you will be a fantastic leader of the IUCr and incredible advocate for crystallography in Canada and the World.

The second item of note arising from the 2021 IUCr congress is the determination of who will be hosting the 2026 Congress. I am excited to report that the IUCr Congress and General Assembly will be coming back to Canada in 2026, and will be held in Calgary, Alberta. The bid for the 2026 IUCr congress was a about a year in the making and is a combined effort of the Canadian National Committee for Crystallography (CNCC), the US National Committee for Crystallography (USNCCr) and the ACA. The CNCC-USNCCr-ACA combined bid's organizing committee was led by Louise Dawe (Wilfred Laurier) and Joe Ferrara (Rigaku), with membership spanning both national committees. The members of the organizing committee for the bid were Kristin Stevens, Gerald Audette, Branton J. Campbell, Cora Lind-Kovacs, Tomislav Friščić, David Rose, Dianna Tomchick, Brian Toby. We presented our combined bid at the General Assembly of the IUCr congress in Prague – the video for the bid is here (https://www.youtube.com/watch?v=DVWbGhLY_sk) – and we were successful! Now the work begins to welcome our international colleagues to Canada, and Calgary in particular, in 2026. We are being led by our local co-Chairs for the 2026 IUCr Congress, Marie Fraser (U. Calgary) and M. Joanne Lemieux (U. Alberta). Please join me in thanking them both for agreeing to take on this significant and important role.

Previous columns highlighted Canadian researchers and their groups. I thought to take this opportunity to briefly introduce our IUCr 2026 Local Co-Chairs, Marie Fraser and M. Joanne Lemiuex. Marie Fraser, a Professor of Biochemistry at the University of Calgary, and was highlighted in the Summer 2016 issue of Reflexions (https://acas.memberclicks.net/assets/RefleXions/SUMMER2016.pdf); I'll therefore take the time to introduce Joanne Lemieux.

Joanne Lemieux is a Professor of Biochemistry and Director of the Membrane Protein Disease Research Group at the University of Alberta. Joanne completed her BSc (with Catherine Mezei) and MSc (with Carl Breckenridge) at Dalhousie University in Halifax, Nova Scotia. She completed her PhD at New York University School of Medicine with Da-Nang Wang, where she solved one of the first X-ray crystal structures of a gradient driven transporter, GlpT (Huang, Lemieux et al. Science 301, 616-620, 2003). Following a postdoctoral fellowship with Michael James, Joanne joined the faculty in the Dept. of Biochemistry at the University of Alberta in 2007. Her research focuses on the structure and function of enzymes and membrane proteins including gradient-driven transporters,

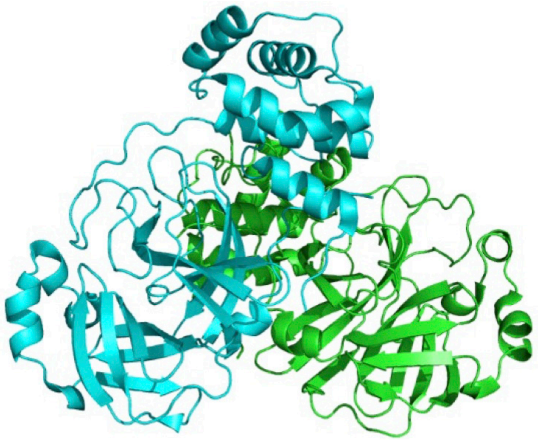


Figure 1. The crystal structure of the dimeric apo-form of the SARS-CoV-2 main protease (Mpro) (PDB ID 6WTM). From Vuong et al. Nat. Commun 11, 4282 (2020).

immune checkpoint receptors, intermembrane proteases and viral proteases.

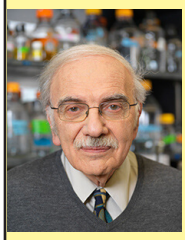
Recently, Joanne has led a team with the research groups of University of Alberta medicinal chemists (James Nieman and John Vederas) and virologists (Lorne Tyrrell) and biochemists (Howard Young), to develop antiviral inhibitors that target the main protease of SARS-CoV-2. The team initially demonstrated that a feline Mpro inhibitor, GC376, was effective at inhibiting the protease both in vitro and in cell culture (Figure 1; Vuong et al., 2020 Nat Comm). Next crystallographic studies demonstrated the importance of dimerization in organizing the substrate binding pocket (Arutyunova et al, 2021 J Mol Bio). Since the feline drug would require a large dosage in human, more effective antivirals were needed, and therefore derivatives were optimised with higher selectivity (Vuong et al., Eur J Med Chem). Working with the Nieman team, peptidomimetic based on early Pfizer compounds were optimised (Bai et al, 2021 J Med Chem). In this paper an irreversible acyloxymethylketone (AMK) warhead was used, which showed a selective index well above the feline drug. In more recent work, the team demonstrated the use of a nitrile warhead in enhancing specificity over other cellular cysteine proteases (Bia et al, 2021 RCS Med Chem). Protein crystallography was essential in assisting with structure guided drug design, and this was accomplished from teamwork between Joanne Lemieux's and Howard Young's labs. In vivo efficacy studies are in progress. With all work being done at the University of Alberta, except for remote data collection at CLS and SSRL, it has been a productive 1.5 years for Joanne and her team, especially during the challenging times of the pandemic.

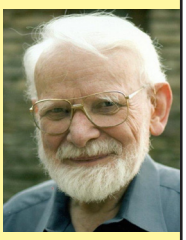
Gerald Audette

Dear ACA members:

It is with sadness that we report the recent passing of three distinguished scholars who each made major contributions to our field:

Mario Amzel
Jack Dunitz
Carroll Johnson





We would like to feature memorials to all three in the Winter edition of RefleXions and are inviting any contributions.
Please submit your memories or testimonials to Paul Swepston <paulswepston@me.com> or to ACA headquarters <aca@hwi.buffalo.edu> by December 1st.

Thanks for helping us remember these valued colleagues. More formal celebrations of their contributions will follow.

American Crystallographic Association 72nd Annual Meeting

Portland, Oregon 2022

Tentative Schedule (Subject to Change):
Workshops & Opening Reception: Friday, July 29, 2022
Sessions Day One: Saturday, July 30, 2022
Sessions Day Two: Sunday, July 31, 2022
Sessions Day Three: Monday, August 1, 2022
Sessions Day Four & Banquet: Tuesday, August 2, 2022

ACA Meeting Committee

Nozomi Ando

Carla Slebodnick

Anna Gardberg (21-24)

Brandon Mercado (20-23)

Stay Tuned! More Details Coming Soon!

www.acameeting.com

Annual Elections 2021

The American Crystallographic Association

Candidates for ACA Offices in 2021

The Nominating Committee (Lisa Keefe (Chair) / Joe Ferrara / Daniel Decato) proposes the following candidates for the 2021 ACA Election:

Vice President:
Sarah Bowman & Cora Lind-Kovacs

Treasurer:
Bo Liang & Steve Ginell

Education Committee:
Cassandra Eagle & Dean Johnston & Silvina Pagola

Communicatons:
Veronica Carta & Aviv Paz

Meeting Committee:
John Horton & Samantha Powell

To nominate write-in candidates for any office, write to the ACA Secretary:

Kushol Gupta, Ph.D.
kgupta@pennmedicine.upenn.edu
Biochemistry & Biophysics, Univ of Pennsylvania
242 Anat Chem Bldg
Philadelphia, PA 19104

Letters must be received by October 15, 2021 and must be signed by five ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in October 2021.

Sarah EJ Bowman - Vice President

Director, National Crystallization Center, & Associate Research Scientist at Hauptman-Woodward Medical Research Institute Associate Research Professor, University at Buffalo Department of Biochemistry

Education/Career:

- Bachelor's English Literature & Women's Studies (Cornell College 1996)
- BS Chemistry (Metropolitan State College of Denver 2005)
- PhD Chemistry (University of Rochester 2010), advisor Kara Bren
- NIH NRSA Postdoctoral Fellow (Massachusetts Institute of Technology 2010-2016), advisors Catherine Drennan and Collin Stultz
- Postdoctoral Fellow (Los Alamos National Laboratory 2016-2017), advisors Bob Williams and Michelle Espy
- Director of the Crystallization Center (Hauptman-Woodward Medical Research Institute 2017-present)

Statement:

I am thrilled and honored to have been nominated as a candidate for Vice-President of the ACA. The ACA is such an important professional home to me, and I am sure that many others feel this way; I would love to be involved with moving the organization forward.

I am relative newcomer to the field of crystallography. My first trip to a synchrotron was to beamline 3-ID at APS for Nuclear Resonance Vibrational Spectroscopy experiments on the metalloprotein that I studied as a graduate student. It was so exciting to be doing work at a synchrotron that I resolved to pursue X-ray crystallography in my postdoctoral studies (this was before remote date collection became more standard). I began a joint postdoctoral position with Catherine Drennan (X-ray crystallography) and Collin Stultz (molecular dynamics) at MIT, where I started my work in structural science (and got to visit synchrotrons a lot!). Thus began my deep love and fascination with crystallography, which forms the center of my current work. As the Director of the National Crystallization Center at HWI, I am now fortunate to be associated with an enormous spectrum of structural studies and to be very engaged with crystallographers and structural scientists from academia, industry and government laboratories.

I bring this enthusiasm for the field and my organizational leadership skills to my participation in the ACA. I joined ACA when I began my independent position at HWI, just a few years ago. When I attended my first ACA meeting in Toronto (2018), I felt like I had finally found my professional home. In large part because of this, I have continued to become more and more involved in the ACA. I have participated as a speaker and as a session chair at ACA meetings, and am currently the BioMac SIG Chair Elect. The more I experience participation with the organization, the more I want to contribute my time and effort to the ACA.

The ACA is a unique professional organization in that it serves the entire structural sciences community. The enormous strengths of the ACA include 1) the incredible diversity of topics embraced, from materials science and biological molecules to light source operations, 2) the size of the target molecules being studied, from small molecules to massive macromolecular machinery, and 3) the techniques used, from crystal-based methods like X-ray crystallography, neutron diffraction and microED to powder diffraction, cryoEM and small angle scattering. At the core of the work we all do as members of ACA is the focus on using structural science to probe fundamental questions in each of our fields. The organization is in a position to bring people working in structural science together and to foster interdisciplinary conversations and interactions. We all bring our distinctive specialties into the ACA, and we all benefit from the presence of the breadth of methods and application areas.

Bowman...cont.

I was very happy to see the organization embrace its role as the Structural Science Society, as it is really the premier professional organization that comfortably houses this breadth of science. In addition, the broad participation of scientists from industry, academia, non-profit, and government institutes further strengthens the membership of the ACA.

As Vice-President of ACA, one of my goals would be to work to increase the membership, with specific focus on increasing the diversity of our membership. Organizationally, there have been actions to expand our DEI efforts, including the Diversity Task Force ad hoc committee and the Angles of Difference facilitator training in Diversity Equity and Inclusion in Crystallography. These are critical steps to take as an organization and I will continue to engage in and expand these efforts.

We are all aware of what the organization and its members have weathered over the past two years – a global pandemic, two virtual meetings, and disruptions to every facet of our personal and professional lives. During this time the ACA has stood strong as a meaningful and rewarding organization. In spite of the extremely trying circumstances, there have been valuable lessons learned that can help the organization in ongoing outreach, in inclusivity, and in its ability to meet the needs of its members. The creative responses in the face of the challenges we've all faced can inform new directions. I would plan to leverage information we've gained from the virtual meetings, the coffee hours, and the other ways we've learned to interact with one another remotely to further increase the welcoming nature of the ACA and engagement of the organizational membership. I feel that these things can also contribute strongly to bringing students, postdocs and early career researchers into involvement in the ACA. We know a lot more about how to reach out remotely, and this should be viewed as an opportunity to enrich student engagement in the organization. As we look to the future, even as we return in person to the ACA Annual Meeting, we could also continue periodic remote seminars, coffee breaks and interactions, which would help keep members engaged and interactive, and enable broader participation. These types of activities could also be opportunities to showcase particular focus areas of ACA SIGs, which are a vital part of the organization.

I am passionate about structural science and excited about the future of the ACA. I would be thrilled to participate in helping to shape that future as the next ACA Vice-President.

Research Interests:

My research interests include developing new methods for crystallization, for detection of micro- and nanocrystals, and for in situ X-ray data collection. I am also focused on ways to combine crystallographic and spectroscopic approaches to answer fundamental questions about protein biochemistry, especially in proteins that contain metals, using spectroscopic methods for single crystals (EPR, UV-vis, and EDX methods) in parallel with crystallography.

Professional Activities and Honors:

2021 Chair-Elect /2022 Chair ACA Biological Macromolecules Special Interest Group; 2021 Session Chair Crystallography against Corona 25th IUCr Congress; 2021 Session Chair Getting the First Crystal ACA Annual Meeting; 2018-2021 Organizer, Metals in Structural Biology Workshop SSRL/LCLS Users' Meeting; 2020/2021 NIH Study Section Reviewer MSFA, MSFB (Temporary Member, Early Career Reviewer); 2018-2021 participant in New Technologies Working Group (IMCA-CAT, Sector 17, APS); Ruth L Kirschstein National Research Service Award F32 Postdoc Fellowship; 2009 NIH Sponsored Delegate to 59th Lindau Meeting of Nobel Laureates & Young Researchers

Cora Lind-Kovacs - Vice President

Education:
Pre-Diploma Chemistry, University of Wuppertal, Germany (1996); M.S. Chemistry, Ph.D. Chemistry, Georgia Institute of Technology (1999, 2001); Post-doctoral Associate, Cornell University (2001-2003)

Professional Activities:
Professor, The University of Toledo; ACA Member since 1999; Etter Award 2007; US National Committee for Crystallography Member 2007-2009, Secretary 2010-2012, Vice Chair 2015-2017, Chair 2018-2020; ACA Powder SIG Chair 2008; Transactions Symposium Organizer 2015; IUCr Bragg Prize Selection Committee 2019/2020; American Association to Advance Powder Diffraction 2021; IUCr Commission on Powder Diffraction 2021-2023; ACA representative for IYCr planning and legacy conferences 2013, 2015; instructor in summer schools (ACA Summer School, Modern Methods in Rietveld Refinement and Structural Analysis, Duquesne/PANalytical Powder Workshop, National School on Neutron and X-ray Scattering); reviewer for APS, SNS, HFIR, NIST, ANSTO.

Research Interests:
Structure-property relationships in solid-state materials, X-ray and neutron powder diffraction, Rietveld analysis, structure determination from powder data, non-ambient diffraction (low+high temperature, high pressure), phase transformations as a function of temperature, pressure and composition.

Statement:
I am honored to have been asked to run for Vice President of the American Crystallographic Association. I joined the ACA as a graduate student, and started to attend ACA meetings as an assistant professor – ironically one year after two of my graduate students got to attend the 2006 Honolulu meeting while I had other obligations! I remember well how exciting it was to attend that first meeting, to be surrounded by people who love reciprocal space and everything related to crystallography as much as I do. Discovering how many people in the ACA are just as passionate as I am about education, outreach and training only made me feel more at home. It was an almost instant transition from being a "newbie" to being connected enough that I would run into people that I wanted to greet and chat with wherever I went. Finding opportunities to get involved and stay involved – as SIG chair, session chair, workshop and symposium organizer, summer school teacher, on the IYCr task force – was easy and natural, because I felt welcomed and encouraged to do so. ACA is a great place for anyone, well established crystallographers, early career scientists, and even students, to take on tasks and contribute.

I know quite a few people who had a very similar experience in getting connected with the ACA – but I also know others who did not, who felt like ACA had established "cliques" that were hard to get into. And maybe the difference is that I am very much an extrovert – I love meeting people, I love talking about pretty much anything crystallography related, and I don't have a problem starting such conversations. So people like myself are likely to join ACA, attend that first meeting – and stay with ACA. But what about the others?

ACA, like many other organizations, has been struggling with a decline in membership. This of course forces us to think about how we can recruit new members. But the flip side of that coin is of course keeping members who joined! If we could simply have 25 new members join each year – not a huge number – and keep them all, our membership could grow by 250 in 10 years. If we can recruit 50, that number could be 500. So what can we do to help with that? One option may be to establish "meeting pals", where any first time attendee could be paired with someone who is more familiar with ACA meetings already, so that they have someone to have lunch with, who can probably answer simple questions, and who can take the initiative to introduce them to others. The YSSIG may be a great starting point for putting something like this together, as many first time attendees will be students. But there are enough of us who are still YSSIG members who are only "young at heart" who could serve as contacts for more senior first time attendees. ACA already recognizes first time attendees with

Lind-Kovacs cont...
their badges, but this could be an additional opportunity to help them get connected and feel welcomed and at home. Of course, to make this work, we also have to devise strategies to recruit those 25, 50 or more new members.

Covid has been bad in many respects, but it also has taught all of us, or at least all of us "digital migrants", way more about using virtual systems and online resources than most of us ever bargained for. I would love to see us put this knowledge to good use. Can we maybe create a monthly or bimonthly virtual crystallography seminar series? The ACS Inorganic Division has started to offer monthly Periodic Table Talks of their sub divisions, and these have been extremely well attended. I don't know about you – but only a small number of the seminars in our department involve crystallography, so having something to attend throughout the year would be great. Similarly, can we create a platform for young crystallographers to practice their thesis defense, or their job interview talk? These would definitely be initiatives that add value to ACA memberships. If this is successful, we could even take it further, and have a student or postdoc talk competition. This would of course take more resources, both in terms of volunteer time commitment and monetary.

Another important question that ACA will need to address over the next couple of years is the format of the annual meeting. In 2020, most of us had a love-hate relationship with the virtual meeting format that was forced upon us. Love because we actually did get to have a meeting, and any meeting format was better than none. Hate because we would so have preferred to meet in person, have that cup of coffee or glass of wine while chatting with new and old friends. As Covid stretched into 2021, we attended more fully virtual meetings and maybe also hybrid meetings, saw more different styles and platforms. Some we may still hate, but others actually did a good job. Clearly, we want to hold in-person meetings again, and benefit from the networking, the friendships, the conversations that can only happen at such meetings. But there will likely be a growing expectation to make some kind of virtual participation possible. Virtual participation is inherently inclusive as it eliminates the need to travel, which can be difficult for some members with medical conditions, family obligations or disabilities. I don't know the answer to "what will ACA meetings look like over the next few years?", and I am painfully aware that running a hybrid meeting that allows full live participation in all sessions is the most cumbersome in terms of logistics, and also considerably more expensive than either in-person or fully virtual meetings. But I believe that we need to take a good, honest look at all the different options, and discuss the financial and logistical feasibility, to determine a path forward that will benefit the widest possible membership base.

Lastly, the ACA will also be involved in planning the 27th IUCr Congress, which will be held in Calgary AB August 11-18, 2026, together with the US and Canadian National Committees for Crystallography. The current plan for this meeting is to run in hybrid format, with the majority of attendees participating in-person, but also allowing virtual attendance. Any considerations that apply to near-future ACA meetings will provide valuable insights for planning this congress as well.

Steve Ginell - Treasurer

Current positions: Consultant and Visiting Scientist Hauptman-Woodward Research Institute

Education:
A.B., Physics, Kansas Wesleyan University (1971); M.S., Natural Sciences, Roswell Park Memorial Institute, SUNY at Buffalo (1975); Ph.D., Biophysics, Roswell Park Memorial Institute, SUNY at Buffalo (1980)

Professional Activities:
ACA Meeting Committee (2019-present); Program Co-Chair, ACA Annual Meeting Covington, KY (2019); Co-Chair and Organizer Transaction Symposium, ACA Annual Meeting Albuquerque, NM

Ginell cont...
(2014); Co-Chair and Organizer for sessions at ACA Annual Meetings (2016, 2014, 2013, 2012), ACA Communications Committee (2011-2014), ACA Nomination Committee (2009-2011), Chair/Chair-elect ACA BioMac SIG (2004-2007), Advanced Photon Source (APS) User Organization Steering Committee (2003-2005); Organizing Committee, APS Users Meeting, (2005); Co-Organizer, workshops at APS Users Meeting, (2004, 2005).

Research Interests:
Structural biology, macromolecular crystallography, radiation damage in macromolecular crystals, development of techniques and methods for structural biology research using synchrotron radiation with an emphasis of pushing the limits of the experimental envelope at ultra-high resolution and cryo-temperatures to 10K.

Statement:
I have the time. I have the experience. I have the passion. I would be honored to serve ACA as treasurer.

At this point in my career, I have the time to devote to what I find interesting and rewarding. One passion is ensuring that future generations of structural scientists have a vibrant professional society.

My first several ACA meetings introduced me to an engaging and involved community of crystallographers who were dedicated to their science as well as their professional society. I concur that service to the community and one's professional society is vitally important for the growth of science and education. During the past several years as SIG chair, Communications Committee member, session chair, Transactions Symposium organizer, and most recently as Annual Meeting Program co-chair have provided me insight into the diversity of the ACA and the need for the ACA to be financially secure. To be financially secure, the ACA needs an involved membership that is diverse and that brings together both the traditional fields of crystallography as well as the newer related areas of structural science. As a member of the ACA Council, I will work to maintain the vitality of the ACA and reach out to structural scientists in varied relevant disciplines to engage with ACA.

While my expertise is in crystallography, I am knowledgeable of the financial challenges that face not-for-profit organizations, from my service as treasurer of my community homeowner's association, fund raising for numerous ACA meeting sessions and other scientific programs, to fund raising for non-science community organizations.

If elected treasurer, I will carry out the duties of ACA treasurer and work collaboratively with the ACA staff, members of ACA Council, committees, and the SIGs to ensure that the ACA supports all facets of structural science, increases membership, and builds upon the current financial foundation for a fiscally sound future.

Bo Liang - Treasurer

Assistant Professor
Department of Biochemistry
Emory University School of Medicine

Co-Scientific Director
Robert P. Apkarian Integrated Electron Microscopy Core
Emory University

Education & Training:
2000 - 2004 B.S. in Biological Science & B.E. in Computer Science, University of Science and Technology of China (USTC)
2004 - 2009 Ph.D. in Molecular Biophysics, Mentor: Prof. Hong Li, Florida State University (FSU)
2009 - 2016 Postdoctoral Fellow in Biological Chemistry and Molecular Pharmacology (BCMP), and Microbiology and Immunobiology

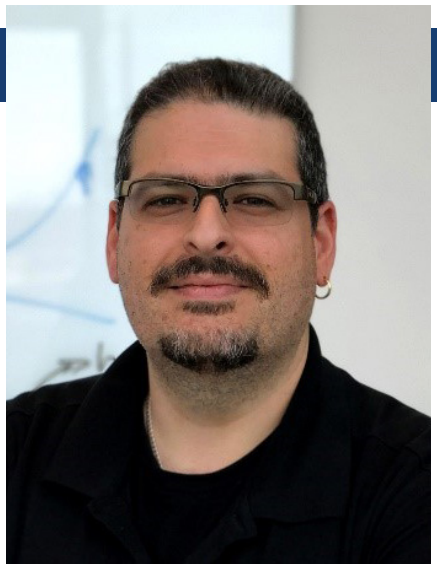
Liang cont...
(MBIB), Mentors: Profs. Stephen Harrison and Sean Whelan, Harvard Medical School (HMS)

Research Interests:
I am broadly interested in the structural basis and physiological function of biologically important complexes in space and time. I am particularly interested in interdisciplinary research in biochemistry, structural biology, molecular cell biology, microbiology, and neurobiology. The principal goal of our research is to scrutinize high-resolution structural details and understand the molecular mechanisms of large assemblies, including ribonucleoprotein complexes and membrane proteins, using integrated cryo-electron microscopy (cryo-EM) and x-ray crystallography.

Statement:
I joined the Biochemistry faculty as a tenure-track Assistant Professor in October 2016. I was the first faculty recruit to spearhead the efforts to bring single-particle cryo-EM to Emory after extensive training as a post-doctoral fellow with Drs. Stephen Harrison and Sean Whelan at Harvard Medical School. Emory purchased two electron microscopes along with my start-up package to be used for single particle analysis, including an FEI 120 kV Talos L120C TEM and an FEI 200 kV Talos Arctica TEM. I am also the Co-Scientific Director of the Robert P. Apkarian Integrated Electron Microscopy Core at Emory. My research involving single-particle cryo-electron microscopy (cryo-EM) falls under one of the top University-wide priority research areas, ensuring continued institutional commitment to my and others' research programs. Currently, the entire community of structural biologists at Emory is now performing state-of-the-art cryo-EM experiments and pushing the boundaries of knowledge in biochemical and biomedical research. Importantly, as a structural biologist, I have extensive crystallography experiences since 2004 and continues to use x-ray crystallography as one of the main tools for the ongoing projects and programs in my research laboratory. I enjoyed the excitement of both cryo-EM and crystallization and model building.

Throughout my career, I have participated in many critical services aside from my scientific research. For example, (A) I served as the Vice President, President, and Senior Consultant (a total of 3 years) of a student organization as a graduate student at Florida State University. (B) I have also been a Trainee Committee member (3 years) of Biological Chemistry and Molecular Pharmacology (BCMP) at Harvard Medical School. (C) I have served as a Board Member (1 year), Co-Chair (3 years), and Secretary (2 years) of the Harvard Medical Postdoctoral Association. After I became a PI, I have also engaged as (D) the Co-Director of the Biochemistry Departmental Seminar Program and the Executive Committee of the MMG Graduate Program at Emory University. Those experiences greatly enrich my service portfolio and motivate me to give back and serve the community.
In summary, I understand the importance and have the motivation and expertise to support the structural biology community. It would be a great honor for me to serve as the treasurer of the ACA Council and contribute to the growth and sustainment of the ACA society. Thank you!

Tamir Gonan - USND President



Investigator Howard Hughes Medical Institute
Professor of Biological Chemistry and Physiology
University of California Los Angeles
Los Angeles, California

Education:
BSc (First Class Honors) University of Auckland, New Zealand 1999
PhD University of Auckland, New Zealand 2002
Postdoctoral Fellow Harvard Medical School 2002-2005

Professional Activities:
HHMI Early Career Scientist 2009; HHMI Group Leader 2011-2017; HHMI Investigator 2017 – current; Chair Elect, Biophysical Society CryoEM

Gonan cont...

subgroup 2018; Chair/Co-chair ACA-MicroED session 2019, 2020, 2021; ACA- Complementary Methods Co Chair; ACA-membership experience committee 2018; Member, Royal Society of New Zealand 2012-current; Reviewer for several Journals and major finding agencies nationally and internationally; Organizer of an annual MicroED course and summit; Director MicroED Imaging Center at UCLA.

Research Interests:

Membrane biophysics, mechanisms of membrane transport, homeostasis, amino acid uptake, cryoEM, MicroED method development, instrumentation, algorithms, crystallography (X-ray and electron).

Statement:

I am a membrane biophysicist and an expert in cryoEM and X-ray crystallography. My research focuses on the application of cutting-edge structural biology techniques to understanding the function of membrane channels and transporters that are important for cellular homeostasis. In 2011 we began developing a new method for structural biology called MicroED, or Microcrystal Electron Diffraction. With this method, we pushed the boundaries of cryoEM and determined several previously unknown structures at resolutions better than 1Å. Because MicroED is a hybrid method between X-ray crystallography and cryoEM we are faced with the same challenges and opportunities as both fields.

Ii would be an honor to continue serving as the president of the USND. I believe that outreach and education are critical and are some of the most important activities that we should engage in and in my capacity as president of the USND I already initiated several programs. The environment at the ACA meetings is second to none and I see this as a prime location for both outreach and education. The conference size is perfect to allow students, postdocs, professionals and professors to interact, exchange ideas and make new long lasting connections in a somewhat informal and welcoming atmosphere. I attended the ACA meetings many times in different capacity and it is always an event I look forward to. I have organized several conferences, workshops and courses focusing on Challenges in structural biology, MicroED and membrane proteins in the past and have been organizing and chairing sessions at the biophysical society and the ACA several times. This experience taught me that planning is critical for a successful meeting.

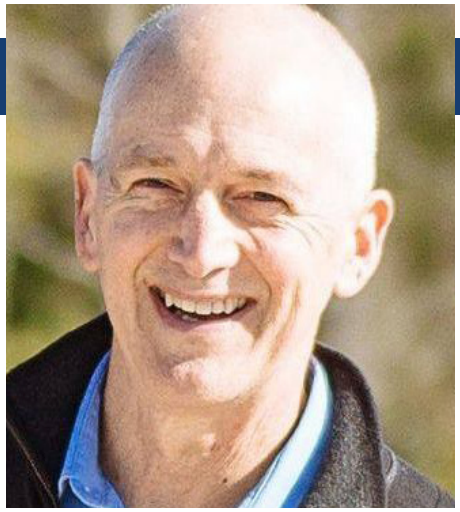
I believe that we have exciting opportunities for merging seminars and workshops from various fields of structural biology such as cryoEM, MicroED and X-ray crystallography in upcoming meetings of the ACA in biological structure, small molecule and inorganic materials research. If selected, I will work to help change mindsets in funding agencies so that funding would become available specifically for outreach and education purposes which can be secured from several federal funding agencies including the NIH, NSF, DOE and DOD although a concerted effort must be made.

There are many ways to get involved with the ACA, from attending the annual meeting to participating in workshops and taking leadership roles.

The ACA offers a number of unique opportunities for those in the structural sciences and crystallographic communities to do what you love, build your resume and network among new scientists as well as established professionals.

For more information go to: https://acas.memberclicks.net/get-involved

Lee Daniels - USND President



Many of us welcomed the relatively recent approval of a US National Division of the ACA, and I now thank the division for giving me a chance to serve in a leadership role. While I have served a number of SIGs and committees, given talks and chaired sessions, and attended nearly every meeting for the past 34 years, the real service has been what the ACA provided to me professionally. A chance to serve the US National Division is another way I hope to give back.

Yes, a majority of ACA members reside in the US, but the US National division gives us an opportunity represent the ACA specifically in situations where the ACA, as a broad "American" (i.e. Western Hemisphere) organization cannot be active. The US National Division provides a platform for the concerns and plans of US scientists, much like our honorable Canadian division does for their regional interests.

The ACA is a powerful source of ideas and education in the structural sciences, and I look forward to a chance to continue to work with all of you.

Veronica Carta - Communications Committee

Indiana University, Department of Chemistry.
Research Crystallographer with the rank of Assistant Scientist at the Indiana University Molecular Structure Center (IUMSC), Department of Chemistry, Indiana University, Bloomington, IN, USA.

Education:
PhD in Inorganic Chemistry, University of British Columbia, Vancouver, BC, Canada (2018). MSc and BSc in Chemistry, La Sapienza University of Rome, Rome, Italy.

Professional Activities:
Member of the American Crystallography Association (2018-present). Referee for Acta Crystallographica (IUCr) and Journal of Chemical Crystallography (Springer).

Research Interest:
Small molecule X-ray diffraction analysis, powder x-ray diffraction, polymorphism, weak non-covalent interactions.

Statement:
It is an honor to receive a nomination to serve on the ACA's Communication Committee. Crystallography has been key to my research during my doctoral degree in supramolecular chemistry. The mentorship I received from members of the crystallographic community contributed to my education in structural chemistry and to my decision to undertake a career in small molecule service crystallography. I am thankful to the ACA for creating a community that promotes research, education, and professional development in crystallography, as well as the opportunity to create connections among scientists, and mentoring relationships.
Science communication and outreach are becoming more and more crucial in our society, as they play a key role in dismantling misconceptions and misinformation. Without a science background, it can be challenging to interpret data presented by the media, to discern objective facts from non-substantiated statements, and to

Carta cont...
recognize misleading news and conspiracy theories. A scientific approach helps people navigating the myriad of information they are exposed to on the Web, on social media, and in their everyday life. Science communication and outreach also contribute to making science more inclusive, encouraging more people of different backgrounds to pursue higher education or a career in STEM and improving science literacy within the general public.

As a member of the Communication Committee I would be enthusiastic about engaging in outreach activities and promoting them through our social media platforms (Twitter, Facebook, and Instagram). Social media platforms are a resource that the ACA can use to promote initiatives and make announcements, thereby facilitating communication to both ACA members and the public and increasing public knowledge about the ACA and structural science.

Aviv Paz - Communications Committee

Associate Research Scientist Hauptman-Woodward Medical Research Institute, Buffalo NY
Adjunct Associate Professor of Oncology Roswell Park Comprehensive Cancer Center, Buffalo NY

Education:
B.Med.Sc, Sackler School of Medicine, Tel-Aviv University, Ramat-Aviv, Israel (1999); M.Sc. in Biotechnology (with honors), The Mina & Everard Goodman Faculty of Life Sciences, Bar Ilan University, Ramat-Gan, Israel (2003); Ph.D. Feinberg Graduate School, Weizmann Institute of Science, Rehovot, Israel (2009); Postdoctoral Researcher, David-Geffen School of Medicine, University of California Los-Angeles, Los-Angeles CA (2010-2014).

Professional activities:
Instructor at the international "New Strategies for Cloning and Expression of Protein Complexes in E. coli and Insect Cells" workshop, Rehovot, Israel (2009), American Association for the Advancement of Science member (2012-2014), Instructor at the Membrane Protein Crystallization Workshop, InStem, Bengaluru, India (2013), ACA member (2019 to present), Secretary of the HWI Scientific Governance Council (2020-present), Head of the HWI seminar committee (2021-present).

Research Interest:
The everchanging shapes and conformations of proteins (excluding rare static proteins) have always fascinated me. I studied the structure, function, and dynamics of various enzymes, membrane transporters, channels, and intrinsically disordered proteins with a focus on membrane proteins in recent years. To do so, I used biophysical, biochemical, structural, computational, and functional assays; always striving to give a structural description to the function studied, be it ligand/drug binding to an enzyme, or a series of structural fluctuations that enable the transport of cargo from one side of the membrane to the other.

Statement:
I would like to be more involved and give back to the ACA, an organization that is important to us all. As such, I am delighted to be nominated to serve on the Communication Committee.

Although some experiments and data collections are better performed under vacuum, Science should not be performed in vacuum. In my opinion, the ACA should reach out and convey our vision, findings, and their importance with four principal groups: 1. Students and trainees; The ACA has many offers for the professional development of students and trainees. Advertising them would benefit these students and our community as a whole. 2. Existing members and non-crystallographers who practice structural studies; In the last few years, we have witnessed experimental and computational advances that are redefining structural biology. We should

Paz cont...
embrace these fields and keep an open line of communication between us and the scientists that practice these alternatives since our global aims are identical. 3. Scientists from other disciplines; Some of the most challenging and groundbreaking structures were the results of close collaborations between scientists from other fields with structural biologists. Communicating with scientists from other disciplines, highlighting the merits and importance of structural biology could foster interdisciplinary collaborations and even help in increasing the odds of obtaining grants when the referees are not structural biologists. 4. The general public and policymakers; Paradoxically, the horrible COVID-19 pandemic has made it easier to explain the importance of structural biology to non-scientists. I do not think it is a stretch to estimate that most people on earth have seen the structure of the virus and heard something regarding proteins, vaccines, and antibodies that target specific regions of proteins. We should strike while the iron is hot and continue to explain the importance of structural biology to leverage this exposure and emerging understanding of the public and policymakers to the importance of what we passionately study on a daily basis.

Cassandra Eagle - Education Committee

East Tennessee State University (ETSU)
Professor, Department of Chemistry, East Tennessee State University

Education:
B. Sc. Chemistry, Pfeiffer College (1984); Ph. D. Chemistry, University of Toledo (1986);

Employment:
Postdoctoral Research Fellow, Texas A&M University (1987 – 1988); Camille and Henry Dreyfus Foundation Teaching and Research Fellow, Trinity University (1988 – 1989); Assistant Professor of Chemistry, Williams College (1989 – 1992); Assistant Professor of Chemistry, Appalachian State University (1992 – 1995); Associate Professor of Chemistry, Appalachian State University (1995 – 2000); Professor of Chemistry, Appalachian State University (2000 – 2010); Chair and Professor of Chemistry, East Tennessee State University (2010 – 2016); Professor of Chemistry, East Tennessee State University (2016 – present)

Professional Activities, Honors & Awards:
Dean's List, Pfeiffer College; Who's Who Among American Colleges and Universities (1984); Sigma Xi Graduate Research Symposium Award (1986); Camille and Henry Dreyfus Foundation Teaching and Research Fellow (1988); ASU Faculty Advisor Award (1994 and 2001); University of Toledo Distinguished Alumni Lecturer (1995); College of Arts & Sciences Academy of Outstanding Teachers (1997); North Carolina Board of Governors Excellence in Teaching Award for Appalachian State University (2002); National Science Foundation Solid State Chemistry Summer Research Award (2005); ETSU Jewell Friend Award (2014), American Chemical Society Member (1986 – present); American Crystallographic Association Member (2019 -); ACA Poster Prize Judge (2019); ACA Transactions Committee (2020).

Statement:
Since my days as an undergraduate, I have been dedicated to becoming the best teacher I can be by using models, concepts and analogies. I am not interested in "dumbing down" chemistry (or crystallography) to make it easier to understand; I am interested in helping people understand at a high level by connecting them with a concept they already understand. This is particularly important now when there are so many people skeptical and/or afraid of science. Thus, when I teach chemistry, I use analogies that reach people at their level of understanding and bring them to the next level (or hopefully, higher) of understanding. For example; when teaching General Chemistry, I start with; if two people want to have a non-virtual, face-to-face conversation, they need to be on the same floor of a building and in the same room. Then, I relate this to the quantum numbers n and l. Once I have made a connection, I move forward to explain the context in the sense of electrons. This style of teaching has afforded me awards for teaching excellence through the years (see above).

Eagle cont...
When I moved to ETSU in 2010, part of my start up package was a Single Crystal X-ray Diffractometer (Rigaku XtaLab Mini). For the last 11 years, I have thoroughly enjoyed teaching crystallography to my students. In that time, I mentored 9 undergraduate and 8 graduate students in crystallography. I enjoy it most when I see their eyes light up when they realize that they independently solve a structure.

I am now working to popularize crystallography in undergraduate and graduate schools. It is my goal to have a diffractometer be as important as an nmr spectrometer in colleges and universities.

I am honored to be nominated and it is my goal, if elected, to use what I have learned through the years to reach the general public and help them understand that crystallography has a plethora of gifts when the mind is opened to education.

Dean Johnston - Education Committee

Education Professor Department of Chemistry, Otterbein University

Education:
BA in Chemistry (1988) The College of Wooster (OH); PhD in Inorganic Chemistry (1993) Northwestern University, advisor: Dr. Duward Shriver; Post-doctoral work at the University of North Carolina, Chapel Hill with Dr. Holden Thorp

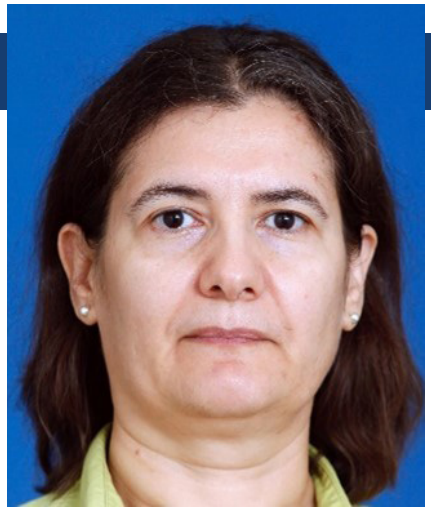
Professional Activities:
Member, American Crystallographic Association; Member, American Chemical Society, Inorganic Chemistry division and Chemical Education division; Member and contributor, IONiC VIPEr (Virtual Inorganic Pedagogical Electronic Resource); VIPEr Fellow (2020 cohort), an NSF-sponsored Inorganic Chemistry education research project.

Research Interests:
Synthetic inorganic chemistry, metal cluster chemistry, development of online materials for teaching chemistry and crystallography.

Statement:
I am honored to be nominated to serve on the Education Committee. I have personally benefited from the ACA's education efforts as a participant in the 2010 Summer Course in Chemical Crystallography. I have also enjoyed the opportunity to learn from workshops held at annual ACA meetings as path to expand my expertise and incorporate new topics into my courses. As a faculty member, my teaching responsibilities range from first-year chemistry courses to special-topics courses on crystallography and structural methods. At all levels I strive to highlight the many contributions of crystallography.

My career choice to be a faculty member at a small liberal arts college reflects my personal focus and passion for chemical education. In addition to incorporating crystallography in many of my courses, I have secured grant funding to support the development of curricular materials, including online tutorials for teaching aspects of symmetry and crystallography. I have always appreciated the ACA's strong support of crystallographic education and I hope that my service to this committee can help continue that tradition.

Silvina Pagola - Education Committee



Research Assistant Professor, Department of Chemistry & Biochemistry, Old Dominion University, and X-ray diffraction specialist at the College of Sciences Major Instrumentation Cluster (COSMIC) https://www.odu.edu/sci/research/cosmic

My professional training is in synchrotron and laboratory X-ray powder diffraction, crystal structure determination from powders using direct-space methods (winPSSP software at http://users.uoi.gr/nkourkou/winpssp/), Rietveld analysis using free-distribution software, and in mechanochemistry (as a synthetic chemist).

Statement:

Most of us would probably agree on the existence of a current need to improve crystallography education in the USA at the undergraduate level (four-year colleges and universities). As a chemist by training and frequent undergraduate research advisor, I am concerned about the lack of undergraduate training in single crystal and powder X-ray diffraction in many higher-education institutions with chemistry programs approved by the American Chemical Society (ACS), which currently does not require X-ray diffraction instrumentation as mandatory, for the over-690 accredited programs[1], as per 2015 ACS "Guidelines and Evaluation Procedures for Bachelor's Degree Programs". I see this as a significant obstacle toward achieving a comprehensive, versatile education in chemistry. Probably most of our X-ray diffraction "end users" are chemists, sometimes working with or as X-ray crystallographers applying automated software and methods to solve crystal structures, essentially within all chemistry sub-disciplines. Understanding the structures and chemical bonding of substances is after all, one the most fundamental objectives of chemistry, necessary to understand how substances react.

Toward improving this situation in the near future, I plan to work in collaboration with the ACS Approval Office and the ACA Education Committee, to initiate administrative procedures, provide justification and research (if needed), planification of available resources, costs and schedule of changes, etc. for the American Chemical Society to update the current guidelines as deemed feasible. This could involve several stages, initially requesting specified obligatory minimal instruction in X-ray diffraction methods in the undergraduate chemistry and biochemistry curricula for the accredited programs to remain as such, or to strongly encourage accredited programs to provide students access to X-ray instrumentation onsite (such as affordable benchtop diffractometers) or at institutions close by, or implementing undergraduate laboratories or undergraduate research projects using diffraction data collected elsewhere. This could be supported by enabling instructional workshops for faculty (including online participation), regional X-ray diffraction and crystallography schools, and the availability of educational materials and resources through the ACA website.

Once these changes start and continue, provided resources and instrumentation become available, we could expect X-ray diffraction (single crystal, powder, thin-films and macromolecular) to recruit new practitioners every year from more than 690 accredited chemistry and biochemistry programs in the USA!!!!

[1]https://www.acs.org/content/acs/en/education/policies/acs-approval-program.html

John Horton - Meeting Committee

Associate Professor
MD Anderson Cancer Center-The University of Texas
Department of Epigenetics and Molecular Carcinogenesis

Education:
BA (Major: Chemistry), Cornell University (1984); PhD, Biochemistry and Molecular Biophysics, Columbia University (1992); Postdoctoral research, Cold Spring Harbor Laboratory (1992-1996).

Professional Activities:
Damon Runyon Fellow (1992-1995). Synchrotron Beamline Coordinator, Beamline X26C, National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (BNL) (1995-1997). Southeast Regional Collaborative Access Team (SER-CAT) Planning Committee (1997-2001). SER-CAT Executive Board, State of Georgia Representative (2001-2004, 2008-2010). Co-Chair and Organizer, "New Structures" session ACA 2007 meeting. Vice-chair of the ACA BioMAC SIG for the Knoxville meeting in 2008 and Chair of the BioMAC SIG of the Toronto meeting in 2009. SER-CAT Executive Board, State of Texas Representative (2018-present). Regular reviewer of manuscripts for several journals as well as a reviewer of Macromolecular Crystallography General User Proposals for the APS.

Research Interests:
Our laboratory is focused on increasing our understanding of the macromolecular machinery of epigenetics in normal and cancer cells and how this machinery regulates gene expression using biophysical techniques. Beyond determination of the macromolecular structures of this machinery, our laboratory is screening libraries of compounds with the hope of developing inhibitory compounds for use as effective drug treatments for various cancers. While my expertise is in X-ray crystallography, I am enlarging my structural science repertoire by incorporating complementary methods such as cryo-EM as the proteins of epigenetic control are usually part of larger macromolecular complexes which cannot be easily crystallized. My interests also include understanding macromolecular structure/function in neural cellular development and differentiation.

Statement:
I am honored to be nominated by the ACA for the Meeting Committee. If selected I hope to bring my varied experiences in structural biology to the planning of the meeting. My Ph.D. dissertation work in Wayne Hendrickson's lab at Columbia University laid the groundwork for the application of selenomethionine as a direct phasing vehicle for macromolecular crystallography. Since then, I have done research at Cold Spring Harbor Laboratory, Emory University, and presently, I am Associate Professor at the MD Anderson Cancer Center of The University of Texas. Much of my structural work involves study of protein-DNA interactions as well as understanding the recognition and catalysis of methyltransferases and demethylases. Recently, I utilized my expertise for drug discovery, particularly for discovery of inhibitor compounds of lysine demethylases involved in epigenetic changes in chromatin. Aberrant expression of these enzymes can be involved in "misinformation" in a cell that can cause it to become malignant.

In addition to my scientific pursuits, I was involved in the initial planning stages and realization of the SER-CAT organization and synchrotron facility at the APS and have participated as the State of Georgia's and Texas' representative at SER-CAT Executive Board meetings as SER-CAT matured. In addition, I teach and mentor undergraduate students, graduate students and postdoctoral scientists in protein science, crystallographic methods, and structural biology, and endeavor to expose them to and excite them about ACA activities whenever possible.

My past experiences with the ACA include being the Vice-chair of the SIG for the 2008 Knoxville meeting and Chair of the SIG of the 2009 Toronto meeting. I have also chaired several BioMac sessions as well as given

Horton cont...

talks in many sessions over the years. I believe the ACA should have a strong presence within the small molecule and macromolecular structure communities. The ACA annual meeting should be a 'destination meeting' for everyone in structural fields and the annual meeting should offer innovative and timely sessions that are interesting and exciting to all members.

To be honest, I stepped away from the ACA for many years as I felt the organization offered few growth opportunities for its members. I was not alone as I know of many colleagues in academia and industry that have done the same. It is time to entice and encourage these older colleagues to return and younger colleagues to join. Today, I believe the ACA is in a rejuvenation phase and at an exciting crossroads…and it's a great time to be a member! I think the theme of the 2021 ACA Annual Meeting says it all: "Structural Science Awakens" indeed! One exciting recent development is utilizing artificial intelligence to tackle the protein folding problem. Some believe that Deepmind's AlphaFold or RoseATAFold closes doors; however, as we look to the history of science, we know that new knowledge opens more doors of exploration than it closes. The annual ACA meeting should be a time and place where all members are excited to assemble and mingle, to discover, examine, and open those doors. The lines between our SIGs are blurring and, while past co-sponsored sessions have been adequate, I anticipate a future where there are opportunities for more interaction between members of the different SIGs in our workshops and sessions.

One thing that COVID has reinforced is the need, a requirement really, to improve communication with our local communities who are not as enthralled with science as we are. As structural scientists, we are in a unique position to communicate and educate with our 'pictures' and we can do a better job. To this end, we should encourage teachers, journalists, undergraduates, and other nonscientists to join us at our annual ACA meetings to publicize our science and aid us in becoming better communicators to scientists and nonscientists alike. They can be included in sessions on better ways of sharing our science in classrooms and boardrooms as well as with the general public.

Our science is inspiring…our annual meeting should also inspire, educate, and rejuvenate. If elected to the Meetings Committee, I hope to help plan future meetings where every attendee departs feeling informed, inspired and excited.

Samantha Powell - Meeting Committee

Pacific Northwest National Laboratory
Postdoctoral Researcher, Biological Sciences Division, Pacific Northwest National Laboratory

Education:
BS Chemistry, Colorado School of Mines (2014); PhD Chemistry & Biochemistry (2019); NASEM RAP Postdoctoral Fellow, Air Force Research Lab, Ft. Sam Houston (2019-2020); Postdoctoral Researcher, PNNL (2020-Present)

Professional Activities:
Member, ACA; Member, American Chemistry Society; Member, American Association for the Advancement of Science; Mentor, Washington State Opportunity Scholarship

Research Interests:
Macromolecular Crystallography, X-ray Crystallography, Cryo-EM, MicroED, Proteomics, Method Development

Powell cont...

Statement:

I'm honored that the ACA Nominating Committee has asked me to run for the Meeting Committee, especially being a new member of ACA and an early career scientist. Although I've only attended one ACA meeting (2021) thus far and it was held virtually, I intend to continue attending for many years to come. It was clear to me early on that ACA is a very exciting, supportive, and collaborative community that I wanted to be a part of in a larger capacity.

My previous research focused on the structural determination of protein-ligand complexes using X-ray Crystallography. And in my current position, I utilize Cryo-EM (SPA and MicroED) for structure elucidation as well as work at the interface of structural biology and proteomics. As a member of the meeting committee, it is important to be able to put together a meeting program that consists of interesting, cutting-edge, and relevant topics. I believe that my broad research background in structural biology will help me in doing just that.

Additionally, ACA is currently a relatively small association. This presents a great opportunity for students and early career scientists, like me, to quickly get acquainted with experts in the field, to learn about leading science, and to get involved with ACA. If nominated, a priority of mine is to make sure that early career scientists have ample chances for events such as networking and opportunities for oral presentations at the meeting. This requires also recruiting more young scientists to attend our meetings.

My experience with planning large events, such as banquets, has been on smaller scale as president of the chemistry graduate student society at my graduate university. However, I am very organized and efficient and am a fast learner. I'm prepared, ready to contribute, and excited to learn from the others on the Meeting Committee as we put together another awesome ACA meeting!

REMINDER

The ACA's 2022 Membership Opens November 1st!

Just a reminder that invoices for 2022 membership dues will be sent out on October 31, 2021.

If you chose to auto renew, your credit card will automatically be charged on December 31, 2021.

If you are unsure if you are on auto renew or if you wish to stop auto renew, please contact Kristina Vitale, ACA Membership Coordinator (kvitale@hwi.buffalo.edu).

DECTRIS
detecting the future

EIGER2 R 4M

Macromolecular crystallography from synchrotrons to your LAB

Pixel size
75 x 75 µm²

Two thresholds

large active area of
155 x 163 mm²

«More than 70% of the protein crystallography structures released in the PDB in 2020 are based on data collected with DECTRIS HPC detectors. The EIGER2 R 4M brings everything that makes our detectors so successful to your lab.»

Dr. Marcus Müller
Product Manager XRD at DECTRIS

Read more about our EIGER2 R series

Read our application note!

Take a look at our webinars

dectris.com

David S. Goodsell Selected to Receive the 2022 I. Fankuchen Award

David Goodsell is the recipient of the 2022 I. Fankuchen Award, an honor that is "To recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography." He is Professor of Computational Biology in the Department of Integrative Structural and Computational Biology at the Scripps Research Institute and Research Professor at Rutgers University, The State University of New Jersey, who is known for his extraordinary skills as a communicator of science.

David started his work in structural biology with Richard Dickinson at UCLA. During his postdoctoral appointment with Arthur Olson, David developed the automated docking method known as AutoDock, the most widely-used computational docking program in the scientific community. His studies now center on methods for computational structural biology especially their application to drug design, protein function prediction, and modeling of the molecular structure of entire cells. In support of this research, David developed CellPack, a new method for creating three-dimensional atomic models of large portions of cells.

David has succeeded admirably in a dual career in research and in scientific outreach and education. It was in graduate school, while writing molecular graphics programs to visualize protein and DNA structures, that David became interested in scientific illustration. He developed his own signature style of watercolor painting that incorporates scientific rigor while creating easily interpretable illustrations of molecules and the structure of living cells. He has elaborated complicated biological assemblies in profoundly accurate, artistic and informative ways to aid in the realization of their complexity and functionalities in ways that would not be appreciated without his contribution.

For the last two decades, David has worked with the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) writing and illustrating a monthly column – Molecule of the Month - that tells stories about molecular structure and function. These columns have introduced students, teachers and researchers around the globe to the science of structural biology using three-dimensional structures. The success of these columns inspired development of a much larger public outreach effort by the RCSB PDB, much of it in collaboration with David. He has made his extraordinary, iconic educational materials and paintings freely available to the public.

Throughout his unique and impressive career, David has promoted and enabled effective teaching and learning of biochemistry and molecular biology and has inspired the public with his vision, his creativity, and his artistic genius.

Brent Nannenga Selected to Receive the 2022 Margaret C. Etter Early Career Award

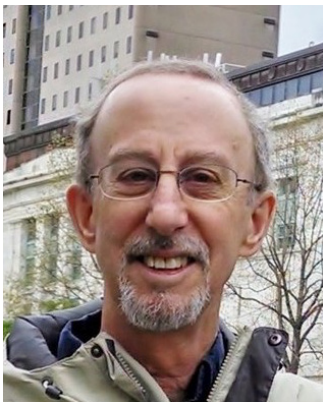
Brent Nannenga is the recipient of the 2022 Margaret Etter Early Career Award, an award "To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career." Brent is an Assistant Professor of Chemical Engineering in the School for Engineering of Matter, Transport and Energy as well as an affiliate of the Biodesign Center for Applied Structural Discovery at the Biodesign Institute at Arizona State University (ASU). His research focuses on protein engineering and

studying the structure-function relationships of these designed proteins. His work also includes developing and improving new techniques for structural biology, specifically using cryo-electron microscopy and he has already made considerable impact on the field.

After earning his PhD in Chemical Engineering at the University of Washington in Seattle, Brent went to the Janelia Research Campus of the Howard Hughes Medical Institute to work with Professor Tamir Gonen. Here he learned and excelled in a variety of techniques including cryo-electron microscopy (cryo-EM), diffraction data analysis, protein purification and protein crystallography (both electron and x-ray) which are areas with which few engineers have direct experience. In this laboratory, Brent was a key player in the development of a new technique for structural biology called micro-electron diffraction (microED) This is a technique that allows high resolution structures to be produced from vanishingly small crystals that would not be usable by other methods. This work – determining protein structures by electron diffraction of three-dimensional (3D) crystals – was thought to be futile but Brent and colleagues were undeterred. Brent grew nanocrystals of lysozyme only a billionth the size of what is required for x-ray crystallography and demonstrated that he could record electron diffraction data. He collected an entire data set from a single nano crystal and, with other team members, indexed, integrated and solved the structure. This was unprecedented work; the very first time that a protein structure was determined by electron diffraction from 3D crystals. Brent had helped pioneer a new field of research in cryoEM called MicroED.

At ASU Brent has developed a large, active, creative, independent, and original research program that is very well-funded, focused on the ultimate goal of building biomolecules to fabricate specific nanomaterials. He has succeeded because of his creativity and energy, willingness to try out new ideas and because of his personal experimental skill and hard work. He has been awarded the prestigious Burton Medal of the Microscopy Society of America (for young scientists), an Air Force Office of Scientific Research Young Investigator Award, and an NSF CAREER award from the Division of Materials Research- Biomaterials.

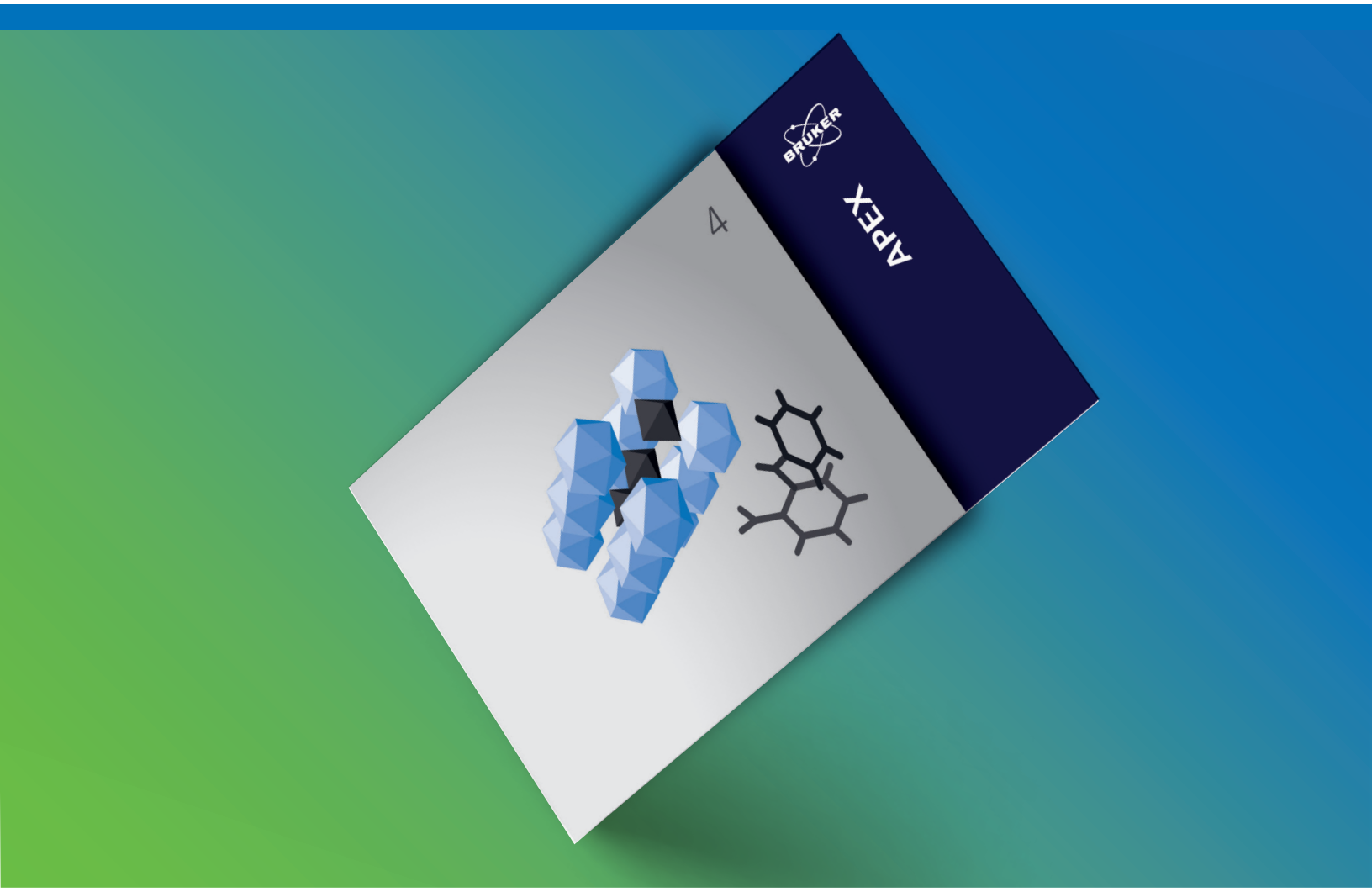
Art J. Schultz Selected to Receive the 2022 Robert Bau Neutron Diffraction Award



Art J. Schultz, Emeritus Scientist at Argonne National Laboratory and Scientific R&D Services and Consultant, Spallation Neutron Source, Oak Ridge National laboratory, is the recipient of the ACA's 2022 Robert Bau Neutron Diffraction Award. This award recognizes "exceptional research achievement in neutron diffraction." Art is unique in his ability to bring together the strong chemical and x-ray structural determination background that originated in his Ph.D studies with Richard Eisenberg and the evolution of this into all aspects of neutron scattering and instrumentation.

Art spent essentially his entire career at Argonne National Laboratory. Some of Art's earliest work centered on continuing Robert Bau's pioneering work on describing the M-H bond by studying transition metal hydrides, primarily with neutron diffraction. He extended this work in a number of seminal publications on activated sigma complexes. He has also contributed significantly by describing temperature and pressure effects on cooperative Jahn-Teller distortions and by studies of organic and high Tc superconductors and other magnetic materials.

In the early 1980s, under Art's able leadership, the Single Crystal Diffractometer (SCD) at the Intense



APEX4 – Software Without Compromise

- Automation or manual control, your choice.
- Fastest processing and improved GUI feedback.
- Greatly improved twin handling.
- Database search powered by *Structurefinder*.

For more information please visit bruker.com/apex4

Innovation with Integrity

SC-XRD

Pulsed Neutron Source (IPNS) at Argonne was developed. This was the first of its kind, a single-crystal diffractometer based on time-of-flight (ToF) neutron diffraction. For many years it was one of only two single-crystal neutron diffraction facilities in the U.S. that were generally available to the scientific community. And, for much of its lifetime at IPNS, this instrument was the only reliably available single-crystal ToF diffractometer in North America. By paying extreme attention to detail in experiments, Art firmly established that the ToF Laue technique could match monochromatic measurements in accuracy and still have the tremendous advantage of speed and resolution.

Developing a first-of-its-kind, principle-establishing diffractometer could have been a career-defining achievement for many scientists but Art did much more, nurturing the applications of SCD in frontier research. He proposed many of the collaborative research projects that were undertaken using SCD, extending the neutron user community to include many researcher who would not otherwise have found their way to the technique. He has been an effective mentor to many scientists and has been an organizer or co-organizer of sessions at ACA meetings, of Transactions Symposia, and of workshops and been a lecturer in many of the National Schools on Neutron and X-Ray Scattering.

Just before and after the IPNS shutdown in 2008, Art continued his work in instrument development at the Spallation Neutron Source (SNS). He led an Argonne National Laboratory (ANL) team that cooperated with SNS instrument scientist to develop TOPAZ, a single-crystal diffractometer, and to conceive of and develop funding for another SNS instrument, MaNDi, a macromolecular single-crystal diffractometer. MaNDi is currently the world's most capable macromolecular neutron diffractometer.

Over the course of his illustrious career, Art has pioneered the development of time-of-flight (ToF) single-crystal neutron diffraction methods, has made numerous seminal discoveries exploiting the powerful ToF technique and has helped develop the worldwide neutron diffraction community.

Airlie J. McCoy Selected to Receive 2022 Kenneth N. Trueblood Award

The Kenneth N. Trueblood award is presented "To recognize exceptional achievement in computational or chemical crystallography." This award is given in recognition of Airlie's key contributions to the tools that could not be imagined not so long ago and which now are routinely used to solve crystal structures of very complex and difficult structures. Airlie has been, for over 20 years, one of the key architects of the most important software package for solving the phase problem in macromolecular crystallography, PHASER.

Airlie's background is unusual; she pursued multiple majors for her B.Sc. degree: Applied Mathematics, Mathematical Physics, Physics and Biochemistry (with first class honors) and studied protein structure for her PhD. Ultimately, she moved to the Cambridge Institute for Medical Research (CIMR), joining the Randy Read group, where she has worked ever since. It is here where Airlie's talents really came to the fore. Her strong mathematical background and excellent crystallographic intuition, as well as her insight into the needs of macromolecular crystallography for new methods, spurred her to develop the most impactful concept introduced into PHASER: the maximum likelihood methods and true multivariate statistics to broaden the range of convergence of the search methods of molecular replacement. Her sophisticated algorithm limits the number of solutions that need to be considered. She has the rare capacity to make theory work in practice.

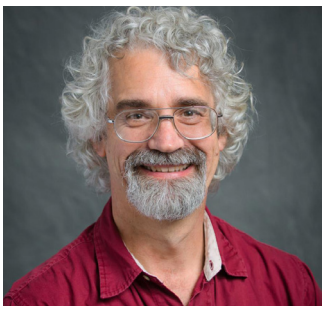
The design and coding of the automation of these methods is Airlie's particular achievement: the success of the automation strategy, even

for difficult cases, and its ease of use has resulted in PHASER essentially becoming the default software for structure solution by MR in macromolecular crystallography. Roughly half of the structures in the protein databank since 2010 have been solved using PHASER. Therefore, not only has Airlie contributed to the canon of software for macromolecular crystallography but has also contributed significantly to the advancement of macromolecular crystallography itself.

Her abilities do not only include implementing state-of-the-art concepts into PHASER code but also her superb ability to explain these in a clear and accessible manner using comprehensive and beautifully presented teaching materials and legendary patience. She is a role model for a whole generation of methods and software developers in the field, not just by her teaching but also by her mentoring of more junior researchers in the field. The award of two distinctions have already honored Airlie's contributions. In 2013, she was invited to be one of the special Bragg Lecturers at a celebration of the Braggs and in 2016 she was presented with a Suffrage Science award recognizing "scientific achievements and ability to inspire others."

Airlie embodies a truly exceptional level of achievement in computational crystallography. She is a truly inspirational leader in the style of so many great crystallographers before her: she shares her knowledge and experience generously, she is a great mentor, and she is a trusted, respected and admired collaborator.

ACA Fellows



Richard Gillilan, Staff Scientist at the macromolecular diffraction facility at the Cornell High Energy Synchrotron Source (MacCHESS), has been instrumental to the growth of biological small-angle X-ray scattering (BioSAXS) in the US and beyond. He is a highly productive and innovative scientist whose professional career has moved him from theoretical chemistry, to molecular dynamics, to scientific visualization with an emphasis on virtual reality, to his current work using X-ray scattering to address biological questions. After notable contributions in the area of microcrystallography he turned to biological small-angle X-ray scattering.

Richard was responsible for developing a beamline at CHESS into a state-of-the-art BioSAXS facility. He started with a feasibility study using PVC pipes and wooden blocks and built a world-class facility. Richard has been the central driving force for the many advances of macromolecular SAXS at MacCHESS. His deep appreciation for basic physics and optics has led him to successfully develop many effective beamline arrangements with appropriate detection technology for highly accurate and diverse SAXS experiments with widely varying samples. When Richard first introduced BioSAXS to users at CHESS, he provided an end-to-end approach that has driven the success of users and the community worldwide. This approach included the advancement of automation, the creation of user-friendly open-source software, equipping of wet lab facilities, and community outreach. More recently Richard has become one of the leading pioneers of high-pressure studies and the BioSAXS station now boasts both a high-pressure static cell and a high-pressure chromatography system. This facility provides the only high-pressure BioSAXS beamline in the Western Hemisphere.

Richard's dedication to education and training has had an enormous impact on individuals who spend time with him at CHESS, on the ACA and on BioSAXS in the US. He has been Chair of the Synchrotron Scientific Interest Group (SIG) and of the Small-angle Scattering SIG. He has organized numerous workshops and sessions, has developed YouTube tutorials, and his BioSAXS Essentials

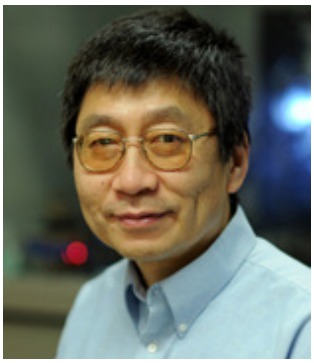
hands-on course has provided the foundational knowledge for many researchers new to SAXS.
His stated dream is to "build and support a scientific community, make exciting new experimental and computation tools accessible and enable great science." He has been successful. Richard's contributions to developing macromolecular SAXS methodology and training of a broad community of scientists to use SAXS are nothing short of spectacular.

P. Lynne Howell, Senior Scientist in the Program in Molecular Medicine at The Hospital for Sick Children and Professor of Biochemistry at the University of Toronto, has made seminal contributions to the understanding of the molecular mechanisms that underlie bacterial communication, bacterial adherence to solid surfaces and bacterial community formation. She has established herself as a world leader in determining x-ray crystal structures of bacterial proteins involved in surface adhesion and biofilm formation and in understanding how these processes lead to persistence and pathogenicity. Her work to uncover the structures, roles, catalytic residues and protein-protein interactions among numerous proteins in several exopolysaccharide biosynthetic clusters has been foundational to understanding the biochemistry that underpins how these microbes work.

The high caliber of Lynne's research program is apparent from the distinctions she has received throughout her career, which include a Canadian Institutes of Health Research (CIHR) Investigator Award and a Tier 1 Canada Research Chair in Structural Biology, the latter of which she has held for the maximum length of time (14 years). This latter award serves as testament to her consistent high-level productivity. She has 129 structures in the Protein Database (PDB) and has published over 170 articles, seven of which have been highlighted by the journal.

In addition to her excellence in research, Lynne has contributed service to the crystallographic community throughout her career. Among her roles have been: member of the program/organizing committee for the 1999 annual meeting of the ACA, member of the International Union of Crystallography (IUCr) Commission on Biological Macromolecules (2009-2017), member of the Board of Directors of the Canadian Light Source (2014 - present), and member of the executive board of the Canadian National Committee for Crystallography (CNCC) (2011-2019). Her service has also included leadership roles in research areas at the Hospital for Sick Children.
Above all else, Lynne's most notable achievement may be her mentoring of students, post-docs and young researchers, that is, her investment in the next generation of scientists. She takes time to truly mentor them. She is a role model and an inspiration to many young scientists and especially to women scientists.

Lynne is an exceptional scientist who has made important contributions to the field of structural biology, and to crystallography in particular; a leader in the crystallographic community; an enthusiastic mentor; and a strong proponent for young scientists and women in STEM.



Liang Tong, William R. Kenan, Jr. Professor in Biological Sciences at Columbia University, has provided unprecedented molecular insights into cellular processes, especially large molecular complexes involved in RNA processing and fatty acid metabolism, using crystallography and cryogenic electron microscopy (cryo-EM). Liang is a highly productive researcher with over 300 publications, many in the very best journals, e.g. Science and

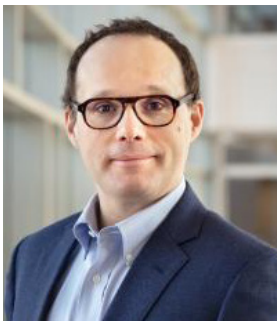
Nature. The impact of his work is reflected in an h index of 84.

Liang was the first to successfully reconstitute an active, human pre-mRNA 3'-end processing machinery, using 13 recombinant proteins and 2 synthetic RNAs. He then determined the structure of this machinery, with the pre-mRNA substrate poised for the processing reaction. This is the first structure of any active processing machinery. This work has had broad impacts on understanding other RNA 3'-end processing machineries and RNA biology in general.

His studies on yeast Rai1 and mammalian homolog DXO unexpectedly revealed novel catalytic activities and has opened a new field of research on mRNA capping surveillance and has illuminated a previously unrecognized RNA quality control mechanism. His studies on large metabolic enzymes have been equally remarkable. One highlight is the first structure of the 500kD homodimer of acetyl-CoA carboxylase, the central regulator of fatty acid metabolism. The structure reveals how the ten domains of this large enzyme work together to carry out the catalysis, as well as presenting a novel mechanism for its allosteric regulation.

Besides using crystallography and cryo-EM as tools to understanding biology, Liang has been highly productive in developing crystallographic technology and software, especially with respect to the molecular replacement method. These software packages are in use in laboratories around the world.
Liang has been an active member of the ACA and a strong advocate for crystallography throughout his career. He is currently a co-editor, with Eddy Arnold, of the Third Edition of the International Tables for Crystallography, Volume F: Crystallography Biological Macromolecules.

Liang has made landmark contributions to understanding large molecular machines, has developed software used around the world and is contributing to the knowledge of future generations by his work on Volume F.



Leighton Coates, Senior Scientist at the Oak Ridge National Laboratory (ORNL), is a leader in the development of neutron protein crystallography. After spending two years as a post-doctoral researcher at the Los Alamos Neutron Scattering Center as a beamline scientist, he moved to ORNL to work with a team of engineers, scientists, and project managers to design and construct a macromolecular neutron diffractometer (MaNDi) at the Spallation Neutron Source. This five-year project resulted in an instrument that enables neutron diffraction studies of smaller single crystals with larger unit cells. Leighton then took responsibility for the commissioning, operation and continuing improvement of MaNDI. This diffractometer has become a productive and important instrument in single crystal diffraction since it provides critical complementarity to synchrotron-based protein studies. In particular, it is capable of mapping the hydrogen atom positions of the active regions of proteins.

Leighton's research has centered on antibiotic resistance, most notably on the catalytic mechanism of class A β-lactamases using neutrons, X-rays and quantum mechanical simulations to probe proton transfer events. More recently he has collaborated on a pioneering and impressive experiment that studied an attractive coronavirus drug target, a ligand-free protease, at room temperature to compare with the structure solved at 100K. The active site cavity shows significant plasticity that indicates that the 100K ligand-free structure may not be physiologically relevant for molecular docking studies.

Leighton has grown the neutron user community in structural biology by organizing and speaking in workshops and sessions at the ACA annual

meetings and other international meetings. He has also organized and attended smaller crystallographic meetings and local workshops that are important venues for younger scientists to speak, network and present research findings. Leighton is currently President of the Pittsburgh Diffraction Society (PDS).

Leighton has made outstanding professional contributions to neutron protein diffractometry by providing leadership in the development of both diffractometers and of software and methods to support neutron crystallography. He has contributed extensively to the crystallographic community by serving as President of the PDS, by organizing scientific meetings to promote and support neutron macromolecular crystallography, and publishing extensively in the crystallographic literature.

Jan Ilavsky, Staff Scientist, X-Ray Science Division, Advanced Photon Source (APS), Argonne National Laboratory, has been a key figure in the development of small angle scattering (SAS) over the last two decades. He built and now supports the premier ultra-small-angle x-ray scattering (USAXS) facility at the APS. Under his stewardship the USAXS beamline at the APS has evolved from a niche instrument to a world-leading measurement facility. This facility enables unprecedented and accurate structure and microstructure characterization across a continuous size range from sub-Ångstrom to tens of micrometers. Under Jan's leadership, the APS USAXS facility is now one of the most robust and productive small-angle scattering instruments in the world.

Jan is deeply committed to ensuring the strength and robust analyses of scattering data. To this end, he authored the general-purpose Nika and Irena software packages. They are widely used by the international small-angle scattering community for reliable SAS data reduction and analysis for both small-angle x-ray scattering (SAXS) and small-angle neutron scattering (SANS). The user-friendly design of these software packages greatly eases what would otherwise be a steep learning curve, facilitates sound interpretation of data, and accelerates the data-to-publication process. Jan is also responsive to the SAS community and these packages, which are open source, are continually updated in response to user requests.

SAXS measurements characterize the microstructure and nanostructure of heterogeneous material systems. When intensity-calibrated, SAXS data also contain information that is key to determining a material's performance in specific applications. Seeing a need, Jan developed and distributed a glassy carbon absolute x-ray intensity standard that was used until NIST, with input from Jan, developed a standard reference material (SRM).

Jan is dedicated to educational outreach. He has been tireless in training new users in small angle scattering methods with both extensive written tutorials for his software and via many workshops and schools used to teach the methods and analysis. His interest in improving the level of crystallographic knowledge and research in developing countries has taken him to Africa to teach scientists.

Jan, probably more than any other single individual, has internationalized quantitative methodology in small-angle x-ray scattering. He has made sustained and lasting contributions to applied science through his research, his teaching in various schools and workshops, and his service to the national and international crystallographic community.

Hanna Dabkowska, Research Scientist at the Brockhouse Institute for Materials at McMaster University, has an international reputation for preparing the materials and growing the crystals essential for condensed matter research, particularly crystal growth through high-temperature melt methods. Her research into the physical properties of inorganic network materials has been published in such prestigious journals as Nature, Nature Communications and the Proceedings of the National Academy of Sciences. Besides publishing research on crystal growth, she has provided educational materials on it, for example, chapters on crystal growth in the Handbook of Crystal Growth; Springer Handbook of Crystal Growth, Defects and Characterization; and Elementary Crystal Growth. She has over 230 publications in peer-reviewed journals and they have earned her an h-index of 41.

Hanna has proven to be a valuable mentor to crystallographers, especially those in the early stages of their careers. She has provided attention and opportunities, and has given selflessly of her time and wisdom. In her lab, she has provided guidance to over 120 students in the art and science of crystal growing.

With limitless dedication, Hanna has promoted crystallographic science and worked to strengthen the organizations that support it throughout the world. This is evident from her long-standing service to the International Union of Crystallography (IUCr) and the International Organization for Crystal Growth (IOCG). On the IUCr she served on the Executive Committee (2011-2017) and was elected Vice President in 2017 and president in 2021. She was the Chair of the Commission of Crystal Growth and Characterization of Materials (2005-2011), Chair of the Calendar Committee (2013-2017), member of the Finance Committee, representative to the Committee on Space Research (2005-2019), and representative to the ACA Council since 2011. Hanna has been a member of the Executive Committee of the International Organization for Crystal Growth since 2007 and was elected vice President in 2019.

Hanna has provided abundant service to crystallography within International organizations, her work has had a significant impact in the crystal growth community and she has provided invalulable mentorship to many early career scientists.

Frank Hawthorne, Distinguished Professor Emeritus at the University of Manitoba, is arguably one of the most significant mineralogical crystallographers of our generation. He has devoted his career to developing a theoretical mathematical and chemical framework within which the structures of minerals can be understood and, more importantly, can be predicted.

Experimentally he has examined systematically the structure and properties of many different types of rock-forming minerals in particular and oxygen-based minerals in general. He has brought a wide range of diffraction, spectroscopic, and analytical techniques to bear on these systems. Minerals present complexities not normally encountered in the synthetic materials prepared in the laboratory so it is impractical to use conventional methods such as quantum mechanical and two-body potential calculations. He has shown that it is possible to predict mineral structures by analyzing the topologies of their bond networks and including the constraints described by the bond valence theory.

Frank's contributions to the scientific community

are immense in both quantity and impact. He has made 730 entries to the American Mineralogist Crystal Structure Database and 915 to the Inorganic Crystal Structure Database (ICSD); has 748 publications in the Web of Science; and has an h-index of 65. He has contributed 14 different chapters to the highly successful book series Reviews in Mineralogy and Geochemistry. He has been mentor to numerous doctoral students who have gone on to advise their own students.

Frank's distinguished career has been recognized with many awards; in fact, his honors fill an entire page in Wikipedia. Recently the American Crystallographic Association honored him with the M. J. Buerger Award (2018), an award "to recognize mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA." This was a particularly apt award since Professor Buerger was himself a mineralogist. In 2018 Canada appointed Frank a Companion of the Order of Canada, its highest award. In another arena, the mineral frankhawthorneite is named after him.

Frank has greatly advanced knowledge of the stabilities of minerals in geological processes and has benefited the crystallographic community by his many publications. The breadth of his work was captured by a colleague: "[Frank] has left few stones unturned in the mineralogical world."

Marilyn M. Olmstead Memorial Session

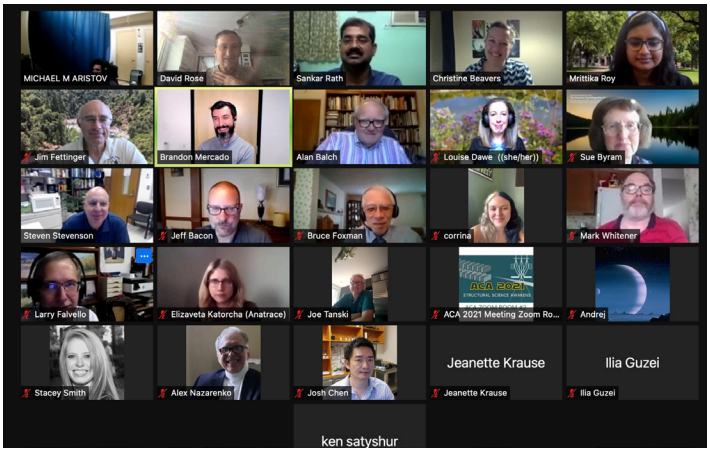
Organized by Brandon Mercado (Yale) and Christine Beavers (Diamond Light Source)

Brandon Mercado and I had the distinct honor of organizing a session in memory of our mentor, role model and academic mother, Professor Marilyn M. Olmstead, who tragically passed away September 30th, 2020. In advance of the session, we solicited video and audio contributions from her many friends, colleagues, and collaborators. Producing such a recording was sure to be a difficult and emotional task; we were very thankful to receive touching submissions from a diverse

group of chemists and crystallographers. These contributions, along with a plethora of wonderful photos, were professionally edited into memorial video by Raleigh Capozzalo (raleighcapozzalo.com), which we shared during the first half of the session. Session attendees were able to enjoy the memories shared in the video, and then for the rest of the evening, the session proceeded in an open-mic fashion.

Because of the emotional nature of this session, we hesitate to mention anyone's contribution specifically; the session was a moving recollection of treasured memories, scientific and otherwise, which would have been lesser had any of the attendees not been able to join us. Members of Marilyn's family were able to attend this virtual session and they were appreciative of the love shared for her by the crystallographic family. Brandon and I, as well as Marilyn's family, would like to encourage all ACA members to consider donating to the Marilyn M. Olmstead Inorganic Chemistry Graduate Research Fund (https://give.ucdavis.edu/CHEM/324712).

Christine Beavers



2021 ACA Meeting Report for ACA RefleXions

The 71st Annual Meeting of The American Crystallographic Association (vACA2021) Friday, July 30 – Thursday, August 5, 2021

The 71st Annual Meeting of the American Crystallographic Association was again moved from an in-person format to a virtual format (vACA2021). Following the Star Trek-inspired theme from 2020, a Star Wars-inspired meeting theme, "Structural Science Awakens," was chosen in 2021 to highlight the ACA's new tagline ACA: The Structural Science Society.

The scientific program was held July 30-Aug 5, with associated workshops August 9 – 16. With the remarkable work of many volunteers and organizers, the vACA2021 was able to offer a full scientific program in 2021, with 35 scientific sessions, 4 interactive poster sessions, 5 workshops, speed mentoring for the young scientist, and opportunities for exhibitors to interact with our members during poster sessions and/or corporate Webinars. The meeting was well attended with over 600 registrants and over 300 workshop participants (Table 1).

Table 1: 2021 Meeting Attendance

Registration Type	# Attendees	# Poster Presenters	# Oral Presenters	WS 1	WS 2	WS 3	WS 4	WS 5	WS total
HS/Undergrad	139	8	1	9	15	74	36	21	**155**
Grad		28	41						
Postdoc	109	12	36						
Regular	355	35	154	7	9	63	34	37	**150**
Retired	26	0	8						
TOTAL	**629**	**83**	**240**	**16**	**24**	**137**	**70**	**58**	**305**

Workshop 1: Characterization of Soft Materials Via Small Angle Scattering: Applications of Scattering for Polymer Systems. **Workshop 2**: Introduction to Hydroxyl Radical Footprinting Methods for Structural Analysis of Proteins and Complexes. **Workshop 3**: Fundamentals of Single Particle Cryo-EM. **Workshop 4**: Managing and using national cryoEM facilities. **Workshop 5**: MicroED of Small and Macromolecules.

The scientific program opened with the Transactions Symposium "Function Follows Form: Celebrating the 50th Anniversary of the Protein Data Bank," highlighting the establishment and importance of this database in structural biology (Fig. 1).

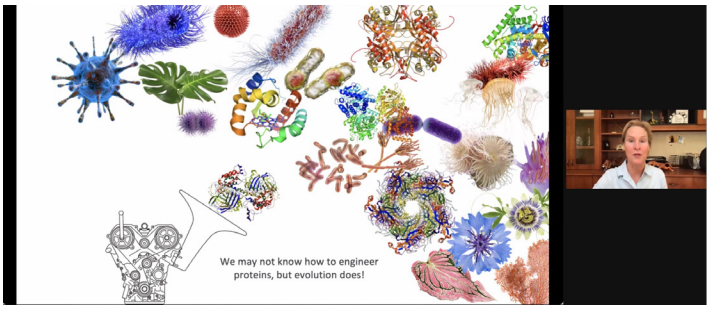


Figure 1. Day two of the PDB50 Transaction Symposium kicked off with a Nobel Lecture by Frances Arnold

The next six days were dedicated to parallel scientific sessions and poster sessions. As in previous years, presentations represented many topics in biology, chemistry, geosciences, materials science, and education and outreach. Notable highlights include the session 4.2.5 "Structure Based Drug Design," where **Rachel Palte** (Merck & Co) presented an analysis of paratopes and epitopes of 5 anti-hArg antibodies via cryo-EM structural studies of complexes consisting of antibodies bridging trimers of hArg1. The attendees and speakers in the session engaged in a lively discussion of the complementarity of multiple techniques, for example X-ray and SAXS, or X-ray and SPR. The Structural Dynamics session (1.1.2 Mapping Free Energy Landscapes of Molecular Machines), which was sponsored by the AIP journal, included a Judith Flippen-Anderson lecture by **Lewis Kay** from University of Toronto. Session 3.1.5 "What I Learned From My First Structures," was popular with multiple generations of crystallographers sharing early experiences with punch cards and Weissenberg through modern instrumentation. Among the presenters, **Bruce Foxman** shared four lessons from his early days in determining the structure of Rel3. Session 1.2.2 "Materials for Sustainability and Energy," focused on materials capable of energy storage, a critical component in renewable energy production. **Hailong Chen** described the importance of the lithium sublattice in halide superionic conductors.

Plenary lectures were given by 2018 Nobel Laureate, **Frances Arnold** (CalTech) as well as ACA Award recipients:

- Margaret C. Etter Early Career Award: Dr. Julia V. Zaikina (Iowa State), "How to Discover New Solids Containing Alkali Metals: Predictive Screening, Facile Synthesis, and In Situ Studies."
- Buerger Award: Wah Chiu (Stanford) "CryoEM Structures of Macromolecules"
- Warren Award: Jacqueline Cole (Cambridge). "Advances in Photocrystallography"

The ACA congratulates the Etter Student Lecturer awardees and poster awardees who are too numerous to mention individually.

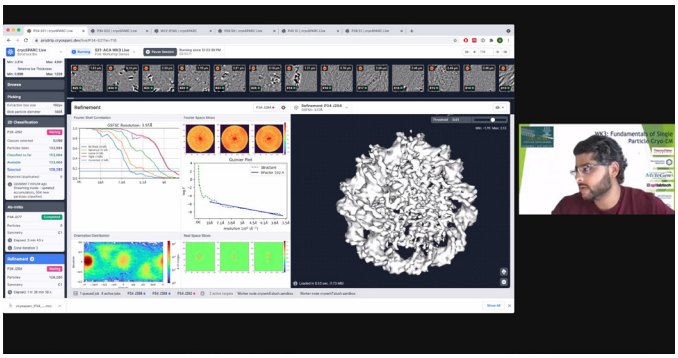


Figure 2. Ali Punjani (CEO of Structura Biotechnology Inc and a 2021 ACA Student Etter Awardee) demonstrates cryoSPARC Live during the Cryo-EM Workshop.

Five virtual workshops were offered in association with the meeting: (1) Characterization of Soft Materials Via Small Angle Scattering: Applications of Scattering for Polymer Systems, (2) Introduction to Hydroxyl Radical Footprinting Methods for Structural Analysis of Proteins and Complexes, (3) Fundamentals of Single Particle Cryo-EM, (4) Managing and using national cryoEM facilities, and (5) MicroED of Small and Macromolecules. The organizers continued the tradition of providing hands-on training through the virtual platform. The 2-day Cryo-EM Workshop, led by **Mark Herzik**, **Liz Kellogg**, and **Ed Twomey**, featured real-time

remote data collection at the NIH National Center for Cryo-EM Access and Training (NCCAT), real-time data processing in cryoSPARC Live (Fig. 2), and a quiz with a MiTeGen-sponsored gift. **Tamir Gonen** and **Brandon Mercado** led the MicroED workshop, which included fantastic tutorials on how to process electron diffraction data for macromolecular and small molecule samples, presented by **Max Clabbers** and **Jessica Bruhn**, respectively.

The meeting was made possible by generous contributions from our sponsors: Rigaku, Thermo Fisher Scientific, Structural Dynamics, DECTRIS, ELDICO Scientific, MiTeGen, Constellation Pharmaceuticals, the International Union of Crystallography, anatrace, Molecular Dimensions, Douglas Instruments, Bruker, the American Institute of Physics, IUCr Journals, SPT Labtech, NanoImaging Services, Xenocs, STOE, and Anton Paar.
In anticipation of an in-person meeting for 2022, please reserve your calendars to join us in Portland, OR, July 29 – Aug 3!

The ACA Meeting Committee

Nozomi Ando, Carla Slebodnick, Brandon Mercado, Anna Gardberg

Marek Grabowski
March 26, 1960 – August 11, 2021

Marek Grabowski, University of Virginia, passed away on August 11, 2021. He had a sudden and unexpected medical emergency.

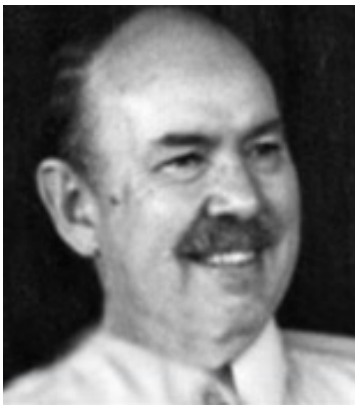
Marek was born in 1960 in Łódź, Poland. He had a passion for learning and solving problems, winning the Physics Olympiad in Lodz, Poland, in 1978. Marek attended the Łódź University of Technology (1979-1984) and later obtained a Master's degree in Physics at the University of Łódź (1985-1987). After graduation, he came to the United States, continuing his education in Theoretical Particle Physics and String Theory at the Virginia Polytechnic Institute in Blacksburg, Virginia. After earning his doctoral degree, Marek completed a postdoctoral fellowship at the Mathematical Physics Laboratory at Laval University in Quebec, Canada. He then returned to Charlottesville and joined Professor Wladek

Minor's lab at the University of Virginia in 2001 to study protein structures. Marek published many papers that attracted a significant number of citations. He was a frequent presenter at ACA, Structural Genomics, and IUCr Congress meetings.

Marek believed that structural biology provides our best glimpse into the molecular machinery responsible for life. His dedication to the integrity of experimental data influenced every project he touched. His contribution was critical for the development of data management systems used by several large-scale NIH centers. The combination of his keen insight and attention to detail was an essential contribution to the success of these large-scale endeavors. He also felt that preserving raw diffraction images was crucial to increase the reliability of molecular models. Overall, Marek's works reflect an appreciation for the value of structural biology and a desire for scientific transparency. Marek was a brilliant scientist, a great friend, and a magnificent, always smiling person. He will be missed very deeply.

Wladek Minor

Remembering Alan D. Mighell



U.S. crystallographer Alan Donald Mighell of Rockville, MD, a long-time ACA member, passed on Wednesday, April 8, 2021. He was 86 years of age.

Alan obtained his B.S. degree from George Washington University in 1957, a M.S. degree from George Washington University in 1960, and a Ph.D. degree in Chemistry from Princeton University, in 1963. After his graduation, he was a post-doctoral fellow at Princeton University from 1963-1964, followed by a prestigious NRC Postdoctoral Fellow appointment at NBS from 1964-1966. He continued to stay at NBS as a staff scientist working in Stan Block's crystallography group. From 1978 to 1996, he was a project leader of the NBS/NIST Crystallographic Data Center. NBS (National Bureau of Standards) changed its name to NIST (National Institute of Standards and Technology) in 1988 to reflect the importance of technology as part of the organization's emphasis. Alan retired from NIST in 1996 and from 1997 to 2021 he was a research associate at the Materials Measurement Science Division (formerly Ceramics Division). He worked for the federal government for a total of almost 50 years.

Alan was a member of a number of scientific organizations in addition to the American Crystallographic Association (ACA), including the International Centre for Diffraction Data (ICDD), the Microcopy Society of America (MSA), and the Materials Research Society (MRS). Alan was a member of the Phi Beta Kappa Honorary Society; he received a Silver Medal Award from the U.S. Department of Commerce in 1975.

At NBS/NIST Alan's research interests were in the areas of both single crystal and powder diffraction research. These areas included X-ray and electron diffraction, crystallographic databases, structural crystallography, symmetry determination, materials identification and characterization, powder indexing, cell reduction and matrix procedures, and Rietveld analysis. More specifically, his principal research interests encompassed the design and development of procedures for materials identification and for establishing lattice relationships.

Alan was a meticulous and hard-working scientist. He published about 100 peer-reviewed papers. Many of them are of seminal quality. His contributions to the crystallographic research community are immense. To name a few:

(1) Alan has spent a large portion of his career working on the 'reduced cells' and mathematical tools for lattice analysis with regard to crystallographic symmetry and similarities [1-3]. Symmetry determination and identification procedures based on reduction have proved invaluable in crystallography and materials science (for materials characterization applications), and thus represent some of his most significant work that has most lasting values. The reduced cell represents a unique standard cell that can be rigorously defined mathematically. Procedures based on reduction are highly reliable and are widely used in the scientific community. They have been adapted to automated diffractometry and are routinely used as an integral part of structure-determination methodology. Also, using lattice matching, one can prevent inadvertent duplicate publications of crystal structures.

(2) He was the leader of NIST Crystal Data project from 1978 to 1996 (NIST standard reference database). The NIST Crystal and Electron Diffraction Data Center built a comprehensive database with evaluated chemical, physical, and crystallographic information on all types of well-characterized substances. The data were evaluated and standardized by specially designed

computer programs as well as by experts in the field. From its master database, the Data Center produced NIST Crystal Data and an Electron Diffraction Database. These distributed databases were made available to the scientific community via CD-ROM, scientific instruments and online systems. In addition, the Data Center has developed theory and software that can be used for establishing all types of lattice relationships for the determination of symmetry, for the identification of unknowns using lattice matching techniques, and for data evaluation. This project has been successfully concluded in recent years.

(3) Alan's involvement with the computer software (called NBS*AIDS83 [4]) was significant for the crystallographic world, particularly the powder diffraction community. This program has three basic functions: 1) data evaluation and database building, 2) data transformation to standard settings (e.g., crystal data cell and space group), and 3) derivative data generation (e.g., reduced cell, Pearson's symbol). The program is used by the scientific community in several ways. Editors at NIST, ICDD, and at other data centers have used this workhorse program as a tool to create hundreds of thousands of evaluated database entries. Second, a research version of the program has been distributed to the scientific community, which has served to improve the quality of experimental data at the source.

(4) Alan's efforts of commemorating the NIST centennial should not be forgotten. He was one of the co-authors to initiate, collect and edit a special issue of NIST publications authored by NIST crystallographers [5]. This issue contains their representative important crystallographic work during their tenure at NIST. These were papers about their past accomplishments, present status, and future potential of crystallography at NBS/NIST. He was also a co-organizer of a special symposium at ACA to celebrate the NIST centennial occasion. Many talks were presented by NIST's friends, collaborators, and staff. The symposium was well-attended.

(5) Alan also spent a lot of effort disseminating and educating the public on the importance of crystallographic databases and pertinent crystallographic science by organizing workshops and short courses at various international meetings. These meetings included annual meetings of ACA, the Materials Research Society, and the Denver X-ray Conference.

(6) His continuous effort to 'clean up' crystallographic errors in reported literature structures/data was admirable. Even after retirement, he still diligently applied his metric symmetry program to work on a number of 'suspicious' reported crystal structures and determined the correctness/mistakes of the structures. As we know that correct structures are critical for understanding structure/property relationships, it is therefore important to eliminate erroneous structures.

.

In addition to Alan's major scientific contributions, he was very talented in music. He played the flute in the Maryland Montgomery County Youth Orchestra. He was in the Montgomery Blair High School Band and played at President Eisenhower's inauguration. He won a scholarship for his flute playing, but then decided to go into science instead. He was a season ticket holder at the Kennedy Center for the National Symphony performances for many years.

Alan loved nature and animals. He loved to hike the C & O Canal. He rescued several cats and dogs. He helped with the Boy Scouts and went on many camping trips. Alan was also a tennis enthusiast. He often discussed tennis technique and various famous tennis players during many luncheons with his NIST colleagues. He enjoyed attending various tennis tournaments around Washington DC.

Alan was the beloved husband of 58 years of Anna Dekonschin Mighell. He met his wife when they both were at George Washington University. He proposed after dating two weeks. He was the

dear father of Dr. Mark Alan (Saskia) Mighell and Gregory Ronald Mighell; loving grandfather of Natasha, Chase, and Isabella Mighell; brother of Edwin Ronald Mighell and the late Ruth M. Weller. Alan is also survived by many more loving relatives and friends. (Some of the information of this article was obtained from his obituary published on the Web).

Personal memory by Winnie Wong-Ng

Alan was a good friend, an excellent scientist, and a gentleman. I first heard Alan's name when I was working for a database organization called JCPDS/ICDD in Swarthmore, Pennsylvania, in the early eighties. I was told that Alan was a world expert in crystallography, particularly in symmetry. Later when I attended my first Denver X-ray Conference somebody pointed him out to me. I had a poster exhibited there and I saw him standing in front of my poster for quite a long time. I became nervous and told myself, 'Oh, I hope I didn't make some big mistakes in symmetry determination'. Later on he told me he was indeed trying to make sure the symmetry of the crystals that I reported was correct. Thank God it was. I was quite relieved.

After I moved to NBS/NIST, we became good friends, and he taught me quite a bit about crystallography, particularly the importance of symmetry. He was such a hard-working and nice guy, always pleasant and glad to help. A group of us often had lunch together at the NIST cafeteria (or the neighborhood restaurants at the later dates) and we enjoyed each other's friendship very much. Those were the good old days!

I am very grateful that I have had the opportunity to know Alan for many years. I really miss him, and I will always remember him fondly.

Winnie Wong-Ng and Gasper Piermarini

References

[1] Santoro A, and Mighell AD. Determination of Reduced Cells. Acta Crystallogr. 1970;A26:124–127.

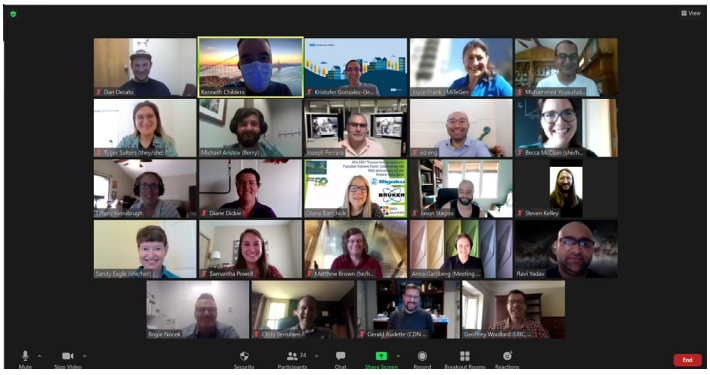
[2] Mighell AD, Karen (Himes) VL. Compound Identification and Characterization Using Lattice-Formula Matching Techniques. Acta Crystallogr. 1986;A42:101–105.

[3] Karen VL, Mighell AD. NIST*LATTICE—A Program to Analyze Lattice Relationships, Version of Spring 1991. 1991. (NIST Technical Note 1290). see also NBS Technical Note 1214 (1985).

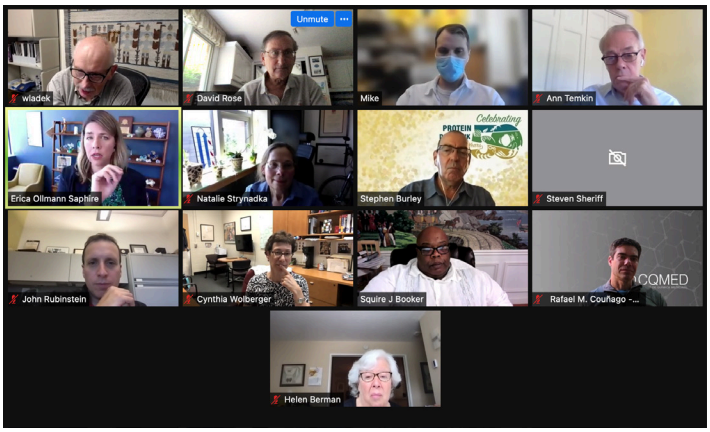
[4] Mighell AD, Hubbard CR, Stalick JK. Natl Bur Stand (US) 1981. NBS*AIDS80. A FORTRAN Program for Crystallographic Data Evaluation. (NBS Technical Note 1141).

[5] Mighell AD and Wong-Ng W, editor, Special Issue-Crystallography at NIST/NBS, J. NIST Research (2001).

YSIG Speed Mentoring Session



Transactions Sessions T1 and T2: Function Follows Form, Celebrating 50 Years of the Protein Data Bank.



Co-organizers: Stephen K. Burley, David Rose, Natalie Strynadka, and Rui Zhao

The ACA was honored to partner with the US-funded Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) to pay tribute to the PDB on the auspicious occasion of its Golden Anniversary.

Fifty years ago, when published three-dimensional (3D) structures of biological macromolecules numbered in the 10s, a visionary group of protein crystallographers meeting at Cold Spring Harbor realized the importance of sharing their data and storing it for reuse. Later that year in October 1971, the Protein Data Bank (PDB) was established as the first open-access digital data resource in all of biology. It not only revolutionized the concept of the "public repository" but emphasized the importance of open data to the advancement of science. Little could that group have known how critical the resource would become to generations of structural scientists and other researchers. More recent outreach and initiatives have broadened the impact of the PDB further into science education. And during the "Time of the Coronavirus", the PDB has played a central role in our response to the Covid-19 global pandemic by validating and biocurating SARS-CoV-2 protein structures before journal peer review and providing a central resource for rapid access to public domain data at no charge and with no limitations on usage. Today, the PDB provides a secure home for more than 180,000 experimentally-determined structures that impact scientific research and education broadly, literally from Agriculture to Zoology.

The 50th anniversary celebration began with a brief welcome from ACA President and Co-organizer, David Rose (University of Waterloo), then the current Director of the RCSB PDB and Co-organizer, Stephen K. Burley (Rutgers, The State University of New Jersey and University of California San Diego), introduced Day One of the Transactions Symposium and chaired the first sessions.

The T1 keynote speaker, Cynthia Wolberger (Johns Hopkins University School of Medicine) described how the post-translational modifications of ubiquitination and methylation complement each other in regulating histone plasticity in the nucleosome and, thereby, regulation of chromosomal access by the transcription machinery. This essential physiological activity is now understood in detail at the molecular level through studies using both X-ray crystallography and cryo-electron microscopy (cryo-EM). Cryo-EM has rapidly gained a prominent position in the arsenal of structural science, and in 2020 produced ~17% of publicly released PDB structures.

The second speaker of the first session, Michael Martynowycz (University of California Los Angeles/ Howard Hughes Medical Institute), focused on one of the newest applications of diffraction, micro-Electron Diffraction (ED). Relieved of the need for large individual crystals, ED techniques are being applied to structure determinations using crystals that are 100 to 1000 times smaller than traditional methods require. Rapid improvements to both sample preparation and to electron microscopes and electron detectors are contributing to the impact of this important new tool for both small-molecule and protein crystallography.

After a break, Co-organizer Natalie Strynadka (University of British Columbia) took the Chair and introduced John Rubinstein (Hospital for Sick Children, University of Toronto). John's talk focused on 'macromolecular machines.' The structures and dynamics of these protein complexes establish proton gradients across membranes, required for energy generation in the cell. V-ATPases are proton pump super-complexes and ATP synthases produce the energy storage medium, ATP. Those complexes specific to pathogenic bacteria are appealing targets for novel antibacterial compounds. Structures of these complex macromolecular assemblies can only be examined at atomic resolution by using single-particle reconstruction from Cryo-EM.

The next speaker, Squire Booker (Penn State) told an elegant story about deciphering, primarily using X-ray crystallography, the chemical details of the enzymatic reaction catalyzed by TsrM, a key enzyme in the biosynthesis of thiostrepton, a potent anti-Gram-positive-bacterial. The mechanism is distinct from related S-adenosymethionine enzymes in the nature of the chemical attack on the substrate and intermediate state.

Rafael Counago (UNICAMP, Campinas, Brazil) then described an effort, under the auspices of the Structural Genomics Consortium, to make use of many atomic structures made available by the PDB to develop targeted, cell-permeable anti-microbial compounds. Affinity and testing of these compounds can be carried out in live microbial cells using a bioluminescence resonance-energy transfer method developed in his laboratory. By focusing on essential enzymes in pathogenic species, his group hopes to generate novel inhibitors that could serve as staring points for drug discovery.

To complete Day One, Erica Ollman Saphire (La Jolla Institute for Immunology) described the enormous benefits of international collaboration through a consortium that was rapidly assembled to study COVID-19 immunotherapy approaches. By sharing data on large numbers of antibodies raised against the SARS-CoV-2 Spike protein, coming from both academia and industry, promising combinations of antibodies were identified and tested for efficacy. This approach, along with analysis of antibodies isolated from infected individuals, is forming the basis for a rapid response to SARS-CoV-2 Variants of Concern as they arise, including design of an engineered Spike protein as an antigen for eliciting broadly neutralizing antibodies.

Day Two of the Transactions Symposium began with the Nobel Lecture from Frances Arnold (California Institute of Technology) chaired by David Rose. Professor Arnold was awarded the 2018 Nobel Prize in Chemistry for her pioneering work in directed evolution of enzymes to perform specified reactions, central to the field of Synthetic Biology. Discovery of new protein catalysts with this strategy has yielded enzymes that can perform reactions not found in nature as applied to many societal and environmental problems, from medicine, to materials science, to bioremediation, to novel fuel sources. Currently serving as co-chair of President Biden's Council of Advisors on Science and Technology, Professor Arnold is providing a much-needed input of basic science and technology to policy making at the highest level.

Co-organizer Rui Zhao (University of Colorado Health Sciences Center) opened the next session. The T2 keynote speaker, Wayne A. Hendrickson (Columbia University), reflected on resolution and revolution in structural biology. Hendrickson was responsible for important technical advances in macromolecular crystallography that have benefited all structure depositors and PDB data consumers. Among all the Transactions Symposium speakers, he holds the distinction of being the sole founding PDB depositor, contributing the structure of lamprey hemoglobin (PDB ID 1lhb) in early 1973. Like many established protein crystallographers, Hendrickson concluded by describing how he is in the process of reinventing

himself as a cryo-electron microscopist to tackle even larger and more complex macromolecular machines.

The second speaker of the session, Wladek Minor (University of Virginia), brought attention to the current global health crisis caused by SARS-CoV-2, and how we have a unique chance to try and address societal and scientific issues that are often ignored. Minor then switched his focus to structural biology and how COVID-19 has helped to make it crystal clear how much the 3D biostructure data is impacting our lives. He concluded by recounting the rapid pace at which SARS-CoV-2 structures have been determined, deposited, validated, biocurated, and immediately released, highlighting the need for scrutiny of structures intended for use in structure-guided drug discovery campaigns.

After a break, Helen Berman (RCSB PDB Director Emerita, Rutgers, The State University of New Jersey) took the Chair for the final session and introduced Chris Sander (Harvard Medical School), who described his contributions to the decades-old quest of 3D fold prediction. His account came in two parts, the first focused on natural evolution and the second focused on experimental evolution. Information extracted from multiple sequence alignments of proteins undergoing selection in the wild or in the laboratory can be used to identify pairs of amino acid residues undergoing evolutionary co-variation that are useful for predicting 3D protein structures with accuracy rivaling experiment. He closed by discussing the recent outcomes reported from AlphaFold2 and RoseTTAFold and then provided several scenarios in which prediction would not be able to supplant experimental approaches.

The second speaker in this session, Eva Nogales (University of California Berkeley/Howard Hughes Medical Institute), presented the results of cryo-EM studies of two macromolecular machines involved in transcriptional regulation in eukaryotes (Transcription Factor IID, or TFIID, and the SAGA complex). Nogales' talk exemplified the power of the cryo-EM "resolution revolution." Elucidation of the mechanism of action of TFIID relied on determination of multiple structures at progressively higher resolution limits revealing a dynamic macromolecular complex that changes shape to interact with cofactors and bind the TATA box located immediately upstream of the transcription start sites of many messenger RNA-encoding genes.

The final speaker of the Transactions Symposium, Andrej Sali (University of California San Francisco), gave a forward looking talk focused on harnessing integrative, or hybrid methods, modeling approaches to mapping of biomolecular networks and spatiotemporal modeling of an entire cell. Sali introduced PDB-Dev, a Worldwide Protein Data Bank prototype repository currently available for archiving, validating, and analyzing integrative structures. He went on to describe the concept of Bayesian metamodeling (under development) that combines different types of heterogenous input models. This approach is currently being used to model in four dimensions (x,y,z, t) the workings of the pancreatic cell, which secretes insulin in response to elevated blood glucose levels.

Both days concluded with lively speaker panel discussions, which reiterated the enormous impact of the PDB and touched on various exciting new topics of interest to the audience.

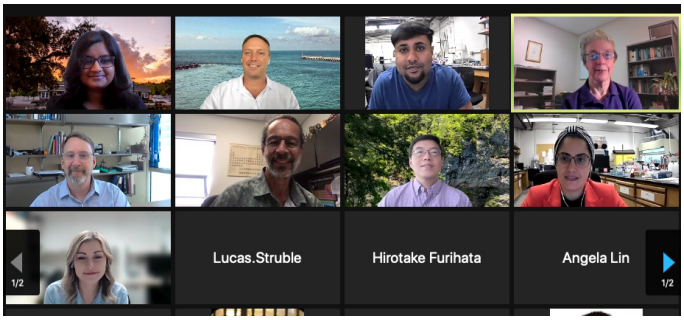
In closing, the ACA and the RCSB PDB thank the more than 50,000 depositors of PDB structure data. Contributions from our community of structural biologists over the past 50 years have built the PDB, establishing a global open-access data resource that is central to fundamental biology, biomedicine, bioenergy, and biotechnology/ bioengineering.

The ACA and the RCSB PDB also thank the following organizations for making financial contributions to the Worldwide Protein Data Bank (wwPDB) Foundation in support of PDB

50th anniversary celebrations around the world: Platinum-Novartis, ThermoFisher Scientific; Silver-Astex Pharmaceuticals, Bristol Myers Squibb, Bruker, Cambridge Isotope Laboratories, Dectris, Discngine, Genentech, Gilead Sciences, National Biomedical Research Foundation, OpenEye, Silicon Therapeutics; Bronze-Anton Paar, Cell Press, Rigaku. Corporate and Individual Donations can be made to the wwPDB Foundation in support of outreach activities that are crucial to the future of the PDB archive at foundation. wwpdb.org.

2021 ACA annual meeting session reports

1.1.1 General Interest



The session began with a talk by **Mono Joy** (Clarkson University) covering work aimed at determining the structural features responsible for the photochromic behavior of viologens-based metal-organic frameworks (MOFs). This was followed by a presentation by **Xioping Wang** (Oak Ridge National Laboratory) where he described the use of time filtering of event-based neutron TOF (time-of-flight) Laue diffraction in order to effectively expand the measured data beyond three dimensions. **Kraig Wheeler** (Whitworth University) then presented results from his work systematically expanding the topological differences between the components for quasiracemate crystallization. The final talk before the coffee break was given by **Carolyn Brock** (University of Kentucky). During her presentation she showed results demonstrating pervasive approximate symmetry from her extensive instigation of the packing in nearly 1500 organic, well-refined (R≤0.050), P1, Z>1 structures. Dr. Brock also discussed strategies for identifying approximate symmetry.

The first talk after the coffee break was presented by **Shefa Alomari** (Clarkson University). During the presentation Shefa presented data on how intramolecular radical formation induced chemical stability for several novel zwitterionic MOFs. Next, **Mrittika Roy** (University of California, Davis) showed how tertiary amine dications and radical monocations were synthesized and crystallized with high valent metal halides, producing X-Ray quality crystals. **Bryan Chakoumakos** (Oak Ridge National Laboratory) then provided a historical overview of how the Oak Ridge Research Reactor and the team of scientists who originally utilized it enabled chemical crystallography using neutrons as well as produced much of the basis for modern-day, computer-based crystallography. The final presentation of the session was presented jointly by **Dmitriy Soldatov** and **Mehdi Esmaeili** (both from the University of Guelph). During their talk they presented data from their work studying the solid state photoreactivity of cinnamic acid in order to investigate how the relative stability of different forms a molecular solid can affect the outcome of a solid state reaction.

1.1.1 General Interest II

The session opened with **Sara Soleimani** (Brigham Young University) presenting the development of a polymer forming crystallization chaperone, TESLAM, and its efficacy in producing well-diffracting crystals of Capillary Morphogenesis Gene 2. **Marcus Fisher** (St. Jude's Children's Research Hospital) presented on the individual water contributions of ligand binding, combining variable-temperature, high-resolution X-ray crystallography with calorimetry to understand how these energetics can be applied to drug design.

Next, **Jeffrey Lovelace** (University of Nebraska Medical Center) gave a presentation on how to decipher modulated superstructures that do not have significant changes in the chains composing the superstructure by comparing periodic atomic modulation functions in (3+1)D space.

Following the coffee break, **Angela Chang Sheng-Huei** (University of British Columbia) presented on the previously uncharacterized NFT2-domain in LD-carboxypeptidase Pgp2 which was identified by X-ray diffraction. Both the NFT2 domain and LD-carboxypeptidase domain of Pgp2 bind peptidoglycans and help induce the helical cell shape of Camplylobacter jejuni, a leading cause in food-borne gastroenteritis. **Prakash Nepal** (Northeastern University) talked about the use of X-ray microdiffraction in small angle X-ray scattering (SAXS) and wide angle x-ray scattering (WAXS) regimes in investigating polymorphisms in neurofibrillary tangle deposits from Alzheimer disease subjects. Next, **Yi Xue** (Tsinghua University) gave a presentation on the generation and use of realistic molecular dynamics (MD)-based diffraction photographs to solve the crystal structure of lysozyme. The talk expressed how this MD-based pipeline may improve computational tools in crystallography and aid in benchmarking MD force fields for biomolecules. **Jiangsheng Jiang** (National Institute of Allergy and Infectious Diseases) presented on the crystal structures of synthetic nanobodies complexed with the SARS-CoV-2 spike protein and its receptor-binding domain and discussed how structural analysis of the complexes can lend to development of new therapeutics. The final presentation was given by **Jahaun Azadmanesh** (University of Nebraska Medical Center), focusing on the neutron crystal structure of human mitochondrial manganese superoxidase dismutase (MnSOD) W161F mutant to explore the conditions leading to product inhibition and further investigate its concerted proton-electron transfer mechanism.

General Interest Chairs
Marc Giulianotti, Victoria Nicole Drago

1.1.4 Total Scattering: New Insights in Condensed Matter

Total scattering has enjoyed a renaissance over the last two decades owing to the increased availability of high-flux X-ray and neutron sources, improved detectors and associated electronics, and of course the dramatic changes in computing since the last millennium. This has enabled more detailed scrutiny of well-studied material classes, as well as opening previously inaccessible material states to observation.

In this year's session "Total Scattering: New Insights in Condensed Matter," speakers elaborated on: tunable vacancies in the classic Prussian Blue structure prototype; local structure perturbations in novel high-entropy alloys and oxides; novel battery materials (including multivalent charge storage); and the materials chemistry of tailored nanoparticles. Updates were delivered on the state of sophisticated in-situ capabilities, including grazing-incidence X-ray total scattering methods provisioned with interferometric sample position control enabling non-ambient investigations, and neutron total scattering environments for in-situ gas-flow studies and for in-situ battery cycling.

The breadth of total scattering studies discussed here, and the valuable insights provided, clearly reflect the importance of these techniques; total scattering extends the crystallographer's toolbox to the messy world of real, disordered materials. We are grateful to this year's speakers, and look forward to the growth of this important domain amongst the membership of the American Crystallographic Association.

Peter Metz & Matthew Tucker

2.1.1 Evolving Enzymes

Chairs: **Audrey Burnim, Kenny Childers, PhD** and **Ben Clifton, PhD**

On Monday August 2nd, the young scientist and small-angle scattering interests groups co-sponsored the Evolving Enzyme session at the ACA. This session was well attended with a peak of around 42 participants. The purpose of this session was to gather like-minded scientists from the rapidly growing and interdisciplinary field of structural molecular evolution. This subject of study combines bioinformatics and biochemical characterization to understand structure-function relationships in the context of evolution. This session was a great success and was able to bring together an international community of evolutionary enzymologists, spanning many different time zones.

The session began with an energetic talk by Professor **Michael Harms** (University of Oregon). His talk was titled "Ensemble epistasis: thermodynamic origins of non-additivity between mutations." His work in understanding the importance of epistasis on the energetic landscape of biomolecules was an excellent opener for the session as a prime example of the importance of the complicated rules underpinning the physiochemical basis of molecular evolution and described how common ensemble epistasis actually is in macromolecules. Next, we had a pre-recorded talk from Professor **Paola Laurino** (Okinawa Institute of Science and Technology) entitled "On the contribution of substrate flexibility to define Methionine adenosyltransferase specificity." This talk zeroed in on the importance of dynamics of an active site loop, which developed different specificities over the course of evolution, likely in response to varying intracellular concentration substrate.

After the coffee break, a prerecorded talk titled "Meet the Family: Structural and Kinetic Comparisons of Representative PEPCKs" was presented by PhD student **Sarah Barwell** (University of Waterloo), who was also present for a lively discussion of her work following the talk. Professor **Colin Jackson** (Australia National University), an established force in the field of molecular evolution then presented some of his group's newest work entitled "Structural and dynamic basis for evolutionary bifurcations in enzyme families."

PhD student **Franziska Sendker** presented an extremely unique system in her talk entitled "Discovery and investigation of a naturally evolved fractal-like protein complex." This system was a fascinating example of the molecular evolution of interfaces to influence higher order oligomeric structure. In the final talk of the session, Professor **Emily Parker** (Victoria University of Wellington) presented "Evolved and evolving allosteric regulation in the biosynthesis of aromatic amino acids" describing in-depth a long-standing research program in her lab. The molecular underpinnings of allosteric activation and the evolution of the mechanisms of aromatic amino acid biosynthesis was discussed.

The session was a great opportunity for young scientists interested in molecular evolution to interact with established researchers in the field and communicate research to evolve the field further.

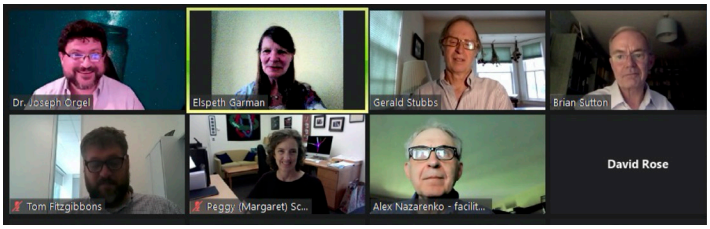
2.1.4 Magnetic Structure Determination: Advances and Applications

The magnetic structure determination session at the virtual 2021 ACA meeting attracted over 30 attendees from the Universities and National Laboratories. The session had 5 invited and 5 contributed talks on the application of advanced neutron/X-ray scattering techniques and data modeling on quantum and topological material research. **Dr. Alan Tennant** from the Oak Ridge National Laboratory (ORNL) introduced a way to apply advanced computation technologies, such as machine-learning, on handling the large numbers of simulations and volume of data for understanding fundamental physics. Then **Dr. Zachary Morgan** from ORNL showed a data modeling tool "rmc-discord" for performing the Reverse Monte Carlo (RMC) refinement of single crystal diffuse neutron scattering and correlated magnetic disorder. An experimental discovery of magnetic vortices in a square lattice was presented by **Dr. Erxi Feng** from ORNL. The work used machine-learning assisted Hamiltonian optimization and local magnetic susceptibility methods with half-polarized neutron diffraction to model diffuse scattering patterns and revealed magnetic ground states. Another experimental study on frustrated triangular and kagome lattice antiferromagnets was presented by **Dr. Zhiling Dun** from Georgia Institute of Technology. Professor **Ni Ni** from University of California, Los Angeles, gave the last invited talk in this session on how to integrate magnetism into topological insulators, where neutron diffraction technique is one of important techniques for characterizing structural stacking, disorder, and magnetism, and further guiding the design of magnetic topological materials.

Five contributed talks in this session were from **Dr. Xiaojian Bai** (ORNL), **Dr. Qiang Zhang** (ORNL), **Stephanie Gnewuch** (University of Maryland), **Madalynn Marshall** (Rutgers University), and **Dr. Xin Gui** (Princeton University). They talked about how to use polarized neutron diffraction on powder sample to determine anisotropic g-tensors of rare-earth magnets, "structural, magnetic ordering process and magnetic excitations in spinel $FeMn_2O_4$", toroidal orders in magnetoelectric materials, magnetic topological materials, and a ferromagnetic half-Heusler-type compound Cr_4PtGa_{17} with a breathing pyrochlore lattice, respectively.

Chairs: Huibo Cao & William Ratcliff

2.1.5 Rosalind Franklin: 101st Anniversary



It is 101 years since the birth of Rosalind Franklin (RF), famous for her part in the unravelling of the structure of DNA. However this great achievement constituted only a small part of her scientific output in a career which was sadly cut short due to her untimely death at the age of 37.

In this session, her enormous contributions to our understanding of the chemistry of coal, of the structure of DNA and of the three-dimensional arrangements of viruses were explored in depth,

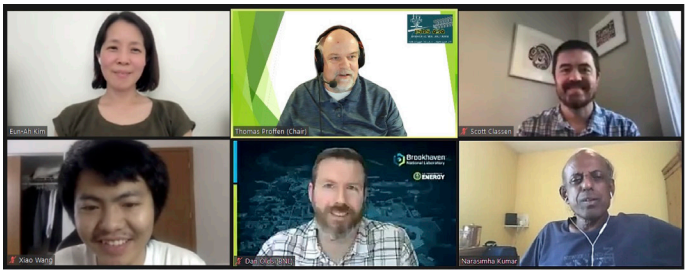
with talks on all three aspects of her work. To introduce RF, a general biographical overview of her family and career was given by **Elspeth Garman** (Oxford University, UK). This was followed by a detailed description by **Alexander Nazarenko** (SUNY Buffalo State College, USA) of the first observation of aromatic bond electron density made by RF. She published her results in Nature in 1950 and showed that it is necessary to consider electrons as being located between two carbon atoms, since the independent atom model fails. Her paper has been largely overlooked and the speaker concluded that appropriate recognition of RF's impact on charge density research is long overdue. The next speaker, **Margaret Schott** (Northwestern University, USA) explained RF's significant, fundamental and long-lasting contributions to our understanding of the molecular structure of sp2-based carbon materials. In particular, RF investigated the process of graphitisation using X-ray diffraction techniques and developed a structural model illustrating the potential of crystallites to fuse into well-ordered graphite. As highlighted by the following contributor, **Thomas Fitzgibbons** (The DOW Chemical Company, USA), RF's model is still of relevance, guiding research and development of new carbon materials today.

RF is best known for her work on DNA (1951-1953), and in particular, for the famous 'Photograph 51' of B form (92% humidity) DNA, seen without RF's knowledge by James Watson in early 1953. **Brian Sutton** (Kings College, London, UK) addressed the fascinating question of how close RF herself was to uncovering the structure of DNA. Tragically she died never knowing that her data had played such a key role in establishing DNA's structure, but today her contribution is fully appreciated and she rightly receives the recognition due to such an extraordinarily gifted scientist.

The final talk in the session was given by **Gerald Stubbs** (Vanderbilt University, USA) with backup from Joseph Orgel, and described RF's tobacco mosaic virus (TMV) work, carried out with Aaron Klug, Kenneth Holmes, and John Finch at Birkbeck College. The speaker had worked as a postdoc with Ken Holmes, and then continued to investigate TMV in his own lab. He described how the detailed structure published in 1989, 31 years after Rosalind Franklin's death, confirmed numerous results from her work, and reminds us of both her genius and her vision.
The session was attended by over 85 people, several of whom contacted the organisers afterwards to say how much they had enjoyed learning more about aspects of Rosalind Franklin's work.

Elspeth F Garman and Joseph Orgel

2.2.1 AI, Machine Learning, and Other Data Science Techniques Applied to Structure Determination



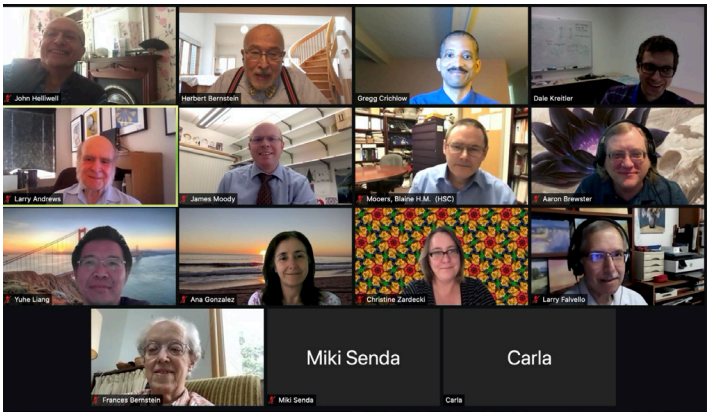
Advances in machine learning (ML) and artificial intelligence (AI) are already having a revolutionizing impact in many areas such as image, speech recognition or advancing self-driving cars. These techniques are starting to have an impact in materials science and beyond. The talks in session 2.2.1 provided an overview of the impact of AI, ML and related methods are having on the field of crystallography. The session was attended by 133 participants.

The first invited talk was given by **Dr. Eun-An Kim** from Cornell University. She presented how one can use machine learning and voluminous scattering data to discover order parameters and its fluctuations in X-ray diffraction data. Looking at a completely different application of machine

learning and computer vision, **Dr. Scott Classen** from the Advanced Light Source Berkely showed how these techniques can be used for sample centering. He also gave the audience a 'behind the scenes' look of the software and services used for the project. After the break, the second invited speaker was **Dr. Dan Olds** from Brookhaven National Laboratory. He presented an in-depth overview of the many areas machine learning and AI will have an impact at user facilities allowing to accelerate science discovery and making using a beamline more streamlined. He introduced a novel approach to use so-called reinforcement learning to have the system 'learn' what a good experiment looks like. The final two talks in the session touched on the use of machine learning and Cryo-EM. **Dr. Narashima Kumar** from Health Technology Innovations presented work aimed at automating 2D class selection in Cryo-EM. The final talk was given by **Dr. Xiao Wang** presenting the software Emap2sec+ used to assign structural labels with associated probabilities at each voxel in a cryo-EM map.

Thomas Proffen

2.2.2 Computing and Data Management



Session 2.2.2 was a half-day session on Computing and Data Management (CDM) with talks relating to useful methods in computing and data management (not just nice results) as a companion to another half-day session on Meeting the Challenges of Raw Data Management (MCRD). The session focused on methods now coming to the fore in solving crystallographic structures, including advances in improving and speeding up crystallographic pipelines, advances in using models and AI in starting and managing the solution process, advances in disaggregating data from multiple conformations and states, advances in integrating results from multimodal experiments across multiple scales, etc.

The session began with a talk for **Dale Kreitler** on "Discrete conformations of an enzyme are discernible via hierarchical clustering of X-ray diffraction intensities derived from multiple crystals." **Larry Andrews** spoke on "Discrete conformations of an enzyme are discernible via hierarchical clustering of X-ray diffraction intensities derived from multiple crystals. **Aaron Brewster** spoke on "Scaling up: processing XFEL data at kilohertz speeds using cctbx.xfel". **Blaine Mooers** spoke on "Literate programming with CCTBX and PyMOL in Jupyter notebooks." Finally **Gregg Crichlow** spoke on "The Life and Times of the PDB Format - Looking Towards the Future with mmCIF." The session concluded with a half hour of discussion.

Dale Kreitler's talk focused on the changes in best practices for MX data collection in which "Hierarchical clustering of X-ray diffraction intensities has recently been applied to multi-crystal datasets to determine the optimal combination of reflections for merging into final composite datasets. These methods have seen good success in macromolecular crystallography (MX), typically when target molecules that are recalcitrant to crystallization yield microcrystals which give rise to incomplete, partial datasets that represent small wedges in reciprocal space. In the present work we hypothesized that small deviations in atomic coordinates due to substrate binding in an enzyme protein crystal (relative to apo enzyme coordinates) would manifest as small differences in reflection intensities that would be discernible with agglomerative clustering techniques." He discussed a study of "apo enzyme crystals of a type C NRPS independent siderophore (NIS)

synthetase, DesD, in which apo enzyme crystals were soaked with an ATP substrate for varying time intervals. …"

Larry Andrews discussed approximate lattice similarity in which the definition of similarity is based on cells related by a scale factor. "A common problem is the accumulation of a list of unit cells in differing presentations. For instance, some may be primitive, some centered, or some not reduced, even though they are all measured from the same crystal form. … " A clearer appreciation of the similarities of lattices from multiple diffraction images can assist in clustering those images for appropriate merging in modern MX studies.

After the coffee break, **Aaron Brewster** focused on the challenges of processing XFEL data at very high data rates. "New XFELs are collecting 16 megapixel protein crystallographic images at kilohertz speeds. Experiments typically involve collecting multiple time points in a series or varying sample conditions through a range of physiological conditions, but in the true spirit of experimentation, biological results such as transition points, ligand interactions, and domain rearrangements are unable to be predicted ahead of time. Scientists need fast feedback from fully processed data to examine electron density maps directly so they can guide experimental procedures: collecting more data at certain settings or changing to new parameters entirely. To this end, we have built a processing pipeline that can run at kilohertz speeds. …"

Blaine Mooers discussed improved support for "literate programming" by use of Jupyter notebooks. "Computational notebooks like Jupyter notebooks facilitate the practice of literate programming. Literature programming involves writing prose with inserts of executable code. The output from the code is woven in amongst the prose in the document. The reader can interact with the code and explore the effects on the output of changing the values of parameters. The reader can import new sets of real or simulated data for analysis with the same code. The code can also be exported from the notebook into a script file for independent execution. Here, we provide support for literate programming by structural biologists in Jupyter Notebooks being run in JupyterLab via PyMOL code written in Python for passing commands from the Jupyter Notebook to PyMOL by means of the PyMOL's application programming interface (API) for Python. … "

In the last talk of the session, **Greg Crichlow** discussed to upcoming completion of the transition from the legacy Protein Data Bank punch card format to mmCIF format that has room for the wider range of fields needed in modern macromolecular studies. "The PDB file format was created when the Protein Data Bank was established In 1971. Originally designed to use 70 columns on punched cards, the format specified fixed column positions and column widths for all data items. As the science and technology evolved, this legacy PDB format can no longer support data representation for large complex structures. This includes large entries that do not fit the PDB file format (those containing >62 chains and/or >99999 ATOM records). … Since the late 1990s, PDB files are also available in mmCIF, an extensible machine readable format that is not limited by fixed column positions, and is extensible to support new data content. The legacy PDB format has not been modified or extended to support new content since 2012. Since 2014, legacy PDB formatted files have not been produced for entries containing multi-character chain ids or atom serial numbers with greater than five digits. …"

Session 2.2.2 and subsequent discussion reflected that we live in exciting and challenging times in which experiments and models are revealing more and more details especially about complex, dynamic systems and that the necessary data management and computational tools are rising to meet those challenges.

Herbert J. Bernstein and Dale Kreitler

2.3.1 Open Exchanges in Crystallographic Education

The speakers in our half-day session offered a variety of perspectives and techniques for promoting crystallographic education. The talks featured a mixture of topics, including novel classroom modules, virtual resources, and innovative active-learning exercises. **George Phillips** (Rice U) gave an account of recent developments with his X-ray View software that allows detailed simulations of X-ray diffraction experiments. **Aluwatoyin Asojo** (Hampton U) recounted her experiences with recruiting and retaining underrepresented students using protein X-ray crystallography. Additional examples of engaging undergraduate students with crystallographic methods by **Joe Tanski** (Vassar College) showed how to effectively integrate crystallography into advanced undergraduate labs as part of a discovery-based exercise. **Allen Oliver** (U Notre Dame) unfolded how the ACA's new crystallography literacy project plans to develop and archive educational resources that will be readily accessible via the web. **Charlotte Stern** (Northwestern U) gave an inspiring talk about crystallographic education and other resources at Northwestern U, with the highlight being a description of an inquiry-based upper-level undergraduate course dedicated to the synthesis and characterization of MOFS. After the break, **Yinka Olatunji-Ojo** (Cambridge Crystallographic Data Centre) gave an insightful perspective on their approach to global virtual instruction and how the CCDC has used interactive and engaging ways to transition materials despite the limitations of remote learning. Peter Horton (U Southampton) demonstrated the practical uses of a well-equipped diffraction laboratory and the effective use of these resources with online learning during the pandemic. **Krystle McLaughlin** (Vassar College) discussed the barriers and opportunities of making protein crystallography more accessible at PUIs. **Alain Beauparlant** (East Tennessee State U) showed how a well-placed video demonstration of the single-crystal X-ray determination of sugar could guide learners through the crystallographic process. To complete the session, **Michael Aristov** (UW Madison) offered perspectives of using a new online 3D resource for teaching symmetry and added several examples of modules that guide users through symmetry operations and other features of crystal structure.

Andy Torelli** and **Kraig Wheeler

3.1.1 Advances in Detector Technology

The detection of X-rays, neutrons, and electrons for diffraction and imaging techniques has changed dramatically over the last 20 years. This half-day session explored the most recent advances in detector technology as they apply to imaging and diffraction techniques.

The first speaker of the session was **Marcus Mueller** of Dectris. Marcus explained the advances in count rates, dual-energy discrimination, simultaneous read/write, and kilohertz frame rates of the EIGER2 detectors. Marcus also described the new features of Dectris' line of the direct-electron detectors. The second speaker of the session was **Roger Durst** of Bruker AXS. Roger reviewed state-of-the-art detector technology for XFELs and serial crystallography and ended with

a discussion of the technology in the Photon III series of detectors.

The third speaker, **Yasukazu Nakaye** of Rigaku, was unable to connect to the session due to internet issues. **Joe Ferrara** presented Yasukazu's slides at the end of the session. Joe reviewed the need for speed and described the advances in Rigaku's XSPA detector since 2019: larger aperture while maintaining a 56 kfps rate and introduction of GaAs as a sensor material.

In the second half of the session, **Kate Shanks** of CHESS, described the development of a variety of charge-integrating detectors for both X-rays and electrons. Kate also explored the tools needed to characterize these detectors for use with high-Z sensors. **Richard Riedel**, of ORNL, talked about two neutron detectors that were recently developed at ORNL, the Anger camera in use at HFIR and a TOF detector based on the Timepx3 sensor.

Anahita Pakzad of Gatan next described how Stela, a hybrid electron detector, integrates into the Gatan workflow for electron microscopy and diffraction. The last speaker of the session, **Jeff Lengyel** of Thermo gave an enlightening lecture on how DQE fails in the electron imaging experiment and proposed a new set of parameters called Critical to Quality (CTQ) metrics.

Christopher Russo & Joseph D. Ferrara

3.1.5 What I Learned from My First Structures

"What I Learned from My First Structures" was conceived as a platform to chronicle the development of technology and technique as embodied in what crystallographers of different generations had to learn in order to carry out their first structure analyses. In the actual event, the techniques described by the senior and junior speakers covered a time frame from the 1960's to the present.

The session was generously supported by Stoe.

Those speakers who conducted their first analyses in the 1960's and -70's -- **Bruce Foxman**, **Frank Fronczek**, **Bill Clegg** and **Larry Falvello** -- had used film methods, mostly Weissenberg photography, for geometric data collection and in some cases for intensity data measurements. **Frank** compressed the timeline by comparing the time it might have taken back then to conduct an analysis from start to finish -- he estimates a month -- to the time it took him to do an analysis on the day before the session -- less than a day from crystal selection to data base deposit, working in his spare time.

Larry discussed the importance of manipulating the direct-methods starting set of reflections in the analysis in the 1970's of cannabidiol, a natural product structure with Z' = 2.

Bill Clegg described photographic data collection as having taken about seven weeks, with the data measured by eye and hand-punched on paper tape. Bill also had to write a data reduction program for a new two-circle diffractometer that arrived while he was a student. He also commented that the more automation you get, the less sleep you get, an observation accredited by a lifetime of very productive work.

Bruce Foxman described the lasting impact of a few selected first structures on his path in science. The structure solution of ReI3 not only involved the laborious use of Weissenberg photography, but in order to reach an acceptable solution Bruce had to locate and correct an error in an established program that he was using for the refinement.

Carla Slebodnick did her early structures in the pivotal period in which structure determination was experiencing a metamorphosis as the widespread use of point-detector-based diffractometers yielded to the age of area detectors. Carla described the all-important procedure of defining the unique part

of the reciprocal lattice for data collection, usually according to the Laue class of the crystal. That was a key skill in the point-detector era but has been taken over now by software automation and the use of multiple data.

Leopoldo Suescun described a long professional path through crystallographic techniques, accompanied by photos of instruments that had played an important part in his work. Early work with single crystals was followed by a change to powder diffraction (Seifert Scintag PAD II). The purchase of a single-crystal diffractometer (Rigaku AFC7S) led to increased productivity and publication in well-regarded journals.

The youngest crystallographers in the program, **Norman Tran** and **Raúl Castañeda**, gave excellent presentations. **Norman** described the effects of non-crystallographic translational symmetry and how it undermines the assumptions of molecular replacement, with reference to his structure analysis of a putative protease from Gemella haemolyans. The lack of an adequate molecular replacement search model was a further problem. He used Phenix.mr_rosetta to solve the structure and emphasized the impact of improvements in crystallographic software.

Raúl caught everyone's attention with his detailed description of the advantages of using cactus needles for mounting crystals. This talk generated discussion and questions, with several attendees indicating that they would like to follow up on this topic.

The presentations in "What I Learned from My First Structures" seemed to exude the enthusiasm with which the speakers had approached their first experiences in structure determination. The question periods also reflected a high level of interest on the part of the audience.

Silvana Urcia-Romero and Larry Falvello

3.2.4 Getting the First Crystal

This session, consisted of 7 lectures, all focused on different aspects of macromolecular crystallisation. The first presentation, by **Eddie Snell** of the HWI discussed different facets of crystallography – from X-FELS based serial crystallography to neutron diffraction and the different crystal requirements for these. Next we had **Deborah Harrus** who discussed the potential future of data collection for crystallisation within the PDB. **Gabi Abrahams** presented how the PDB data can be used to create new crystallisation screens, and some of the factors that might be considered when doing so. **Chip Lesburg** described his interface for displaying and organising crystallisation images using disparate data sources including sample information, chemical information and image classifications from MARCO. The next two presentations discussed different approaches to getting diffracting crystals – **James Moody** showed how using the TELSAM protein self-association could be used to build diffracting crystals of target proteins, and **Miki Senda** presented the workflow that her group uses to produce not just a single well diffracting crystal but a system for obtaining enough crystals for a whole small molecule discovery campaign, and finally we finished with **Deepshika Gilbile** talking about her chip design for RT fixed target serial crystallography, which combines ease of setup with ease of data collection. The session wrapped up with opening the 'zoom floor' for discussion, which generated a lively discussion about AI, the impact of AlphaFold2, and the future of structural biology between the speakers and the audience.

All in all, the session showed the complexities of crystallogenesis, from deciding what crystals are required, to technologies for improving approaches through data visualisation and

mining, along with both biochemical, chemical and physical approaches to alleviating the crystallisation bottleneck. Perhaps most important was the recognition that capturing the details of how crystals are produced is critical, and yet so very non-trivial.

Sarah Bowman and Janet Newman

4.1.1: BioWAXS: Experiment and Interpretation

The session focused on emerging applications of wide-angle scattering (WAXS) from biomolecular samples, including time-resolved solution scattering experiments and imaging. WAXS data are rich in information, but they can be a challenge to interpret. The session highlighted the multiple ways this challenge is being addressed, including by novel experimental design, molecular dynamics (MD) simulation, and machine learning.

Jong Goo Kim, (presenting on behalf of Hyotcherl Ihee) at Inst for Basic Science KAIST, first provided an introduction into structural dynamics of proteins revealed by time-resolved x-ray diffraction in solution, denoted “x-ray liquidography”. The method was used to track ultra-fast dynamics of a homodimeric hemoglobin. Strikingly, the experiments revealed coherent (underdamped) oscillations of the protein upon photodissociation of carbon monoxide, in contrast to the commonly assumed overdamped protein dynamics in solution.

Giorgio Schirò, Institute for Structural Biology, CNRS, presented recent light-induced time-resolved WAXS experiments. Structural changes following photolysis of carbonmonoxy myoglobin (MbCO) were probed on the ps timescale using an X-ray free electron laser (X-FEL). The experiments revealed ultrafast oscillations of the radius of gyration (“protein quake”) which may represent the primary structural response, i.e. signal propagation from the binding pocket to the protein surface. Next, experiments were presented on photosensory proteins, phytochrome and the B12 photoreceptor CarH. These experiments followed transduction of light perturbation from sensing domains to the biological output (regulatory domain of phytochrome, and oligomeric state for CarH). In both cases, the structural changes involved in sensing and output occurred on very different time scales, suggesting a modular design with applications in optogenetics.

Lin Yang, Brookhaven National Laboratory, presented a new instrumentation installed at the Life Science X-ray Scattering (LiX) beamline at NSLS2. The new instrument is capable of collecting X-ray scattering intensities from ultra-small (0.006 Å-1) up to wide angles (3.2 Å-1). The power of the beamline was demonstrated by applications of the wide-angle data, covering both solution scattering and scattering at biological tissues.

Abdullah Al Bashit, Northeastern University, emphasized that WAXS data contains rich information, however the interpretation of the data in terms of real-space conformation remains a major challenge. Al Bashit argued that machine learning models can be trained to map the noisy reciprocal-space features in the data onto specific conformations of a 12-base pair RNA duplexes. The presentation further showed that ensemble modeling was needed to fit experiential data of the RNA duplexes at various salt conditions.

Yen-Lin Chen, Cornell University, presented scattering data from short RNA duplexes. The WAXS region contains oscillatory features, or a “fingerprint”, that differs from the canonical A-form pattern in potassium or magnesium salts. By using MD simulations to train a machine learning (ML)

algorithm for feature extraction, Yen Lin showed that the WAXS data encodes the helical parameters, such as radius and twist, and that the trained ML model can robustly extract these parameters from experimental data. Interestingly, an analysis of the ML model revealed which features in the WAXS were most important for classification.

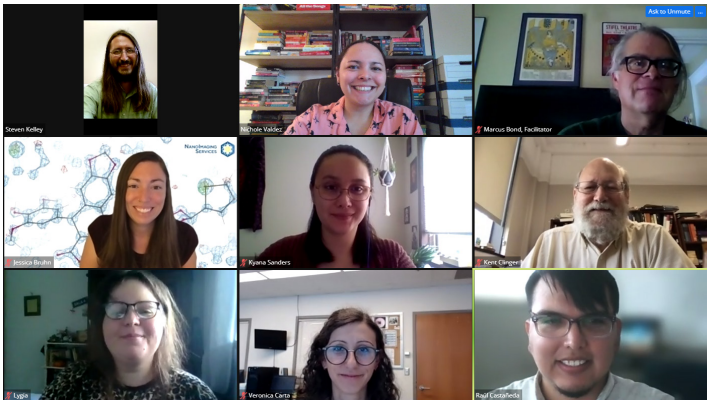
Weiwei He, New York University Abu Dhabi, presented structures of DNA/RNA helix conformations obtained by MD simulations that were validated and refined against small- and wide-angle X-ray scattering (SWAXS) data. The presentation highlighted the complementarity of atomistic simulations and X-ray solution scattering. Using machine learning approaches, Weiwei He was able to correlate features of the one-dimensional SWAXS curve with real-space features of the helix.

Philip Anfinrud, National Institutes of Health, presented the new BioCARS beamline at the APS, which is capable of measuring high-precision X-ray solutions scattering data simultaneously at both small and wide scattering angles. A new sample cell design whose temperature can be controlled over a wide range allows for both time-resolved temperature jump experiments (T-jump) and equilibrium measurements (T-ramp). The speaker presented new data that precisely resolved the modulation of the radius of gyration of a protein as a function of temperature, likely providing a direct probe of the modulations of the hydration layer with temperature. Additionally, new data on nucleic acid unfolding with temperature demonstrated the potential for combining T-jump and T-ramp experiments to discover folding intermediates, extract thermodynamic parameters, and ultimately to reveal unfolding mechanisms.

A lively hour-long discussion followed the formal talks. We are grateful to Dectris, Xenocs, Bruker, Anton Paar, MiTeGen, and Rigaku for sponsoring the session.

Jochen Hub and Steve Meisburger

4.1.2 Cool Structures



Cool Structures was conducted as a single session on Day 5 of the 2021 ACA meeting and chaired by **Dr. Steven Kelley** and **Dr. Nichole Valdez**. The session is one that has reoccurred perennially at ACA meetings and focuses on fundamental science learned from small molecule crystal structures and prominently features student speakers. This year's session included seven talks covering a broad range of small molecule structural science, and was well-attended with an average of 40 viewers per talk.

The session was opened by **Kyana Sanders** (University of Wisconsin), named as this year's Margaret C. Etter Student Award winner. Kyana presented on chemical pressure-driven epitaxy in intermetallic systems and how these lead to eptiaxial vs. intergrowth of separate phases. The talk explored how the understanding of chemical pressure-driven crystal growth had led to increasingly sophisticated design of new intermetallic phases based on different parent structures.

The second talk was presented by **Dr. Veronica Carta** (Indiana University), who presented the crystal structures of an isomeric and polymorphic family of palladium(II) complexes with perfluorinated ligands. Noncovalent F···F interactions, which are particularly subtle among halogen-halogen interactions, were shown to play roles in polymorph formation of both isomers of

the metal complex.

The first half was closed by **Dr. Jessica Bruhn** (Nanoimaging Services, Inc.) who discussed a micro-ED pipeline developed in her organization specifically for high throughput structure determination of small molecules. All aspects from data collection through structure refinement were covered along with discussions on how these steps are optimized. This cutting edge topic prompted an especially energetic discussion with the audience during the break.

The second half of the session was opened with a talk from **Prof. Kent Clinger** (Lipscomb University) who presented on the crystal structure determination of tetrahalogenated tricyclo[7.1.0.04,6]decanes. After taking us through the experimental challenges associated with isolating and refining such a conformationally-diverse multicyclic system, the talk was closed with an interesting historical perspective on some of the pioneers in structural science and their continuing influence and connections with the speaker's own research.

The next talk was presented by **Prof. Marcus Bond** (Southeast Missouri State University), who presented on the crystallization and structure determination of a family of aminopyridinium bromcuprate complexes. Prof Bond's research revisited a known system from the literature and found a wealth of undiscovered structural diversity owing to varying coordination modes of the pyridine moiety and participation of the solvent.

This talk was followed by a presentation from **Dr. Lygia Silva de Moraes** (Free University of Brussels) on polymorphism in 2-benzoyl-N,N-diethylbenzamide, an important pharmaceutical molecule. The long-standing ambiguities on the thermal properties of polymorphs in this system were presented, along with the contributions of Dr. de Moraes and her colleagues in resolving these with combinations of thermal studies and variable temperature diffraction experiments.

The interface between small molecule science and medicine was continued in the final talk of the session by **Dr. Raúl Castañeda** (New Mexico Highlands University), who presented on the use picolinamidine ligands to stabilize water-soluble paramagnetic metal complexes for use as MRI contrast agents. The potential of this ligand system was demonstrated through a large family of metal complexes varying in both the metal and the counter ion.

Thanks, and please give the majority of the write-up credit to Steven (:

Nichole Valdez, Ph.D.
R&D Laboratory Support Technologist
Office: 897/2497
Sandia Cell: 505-934-0003
Email: nrvalde@sandia.gov

4.1.4 Large-scale Facility Upgrades

Chairs: Ana Gonzalez and Bryan Chakoumakos

Upgrades are part of the life cycle of successful large-scale user facilities, they are necessary to provide new technical capabilities that facilitate state-of-the-art performance and enable new challenging experiments. The purpose of the Large-Scale facilities upgrade session was to highlight recent developments and plans in several user facilities; including LCLS II - which can provide a four order of magnitude improvement in number of pulses and average brightness compared to the LCLS; the Spallation Neutron Source (SNS) second target station, that will deliver a 25 times increase in brightness and 4 times the neutron energy range; CHESS, recently converted to a third generation dedicated storage ring; ESRF, which has recently completed an upgrade to a 4th generation storage ring based on a MBA lattice, and APS, that will undergo a similar upgrade in 2023. The focus of the session was to describe the impact of these upgrades for different techniques and research areas.

Andy Aquila opened the session with a description of the high energy high rep-rate upgrade to the Linac Coherent Light Source (LCLS-II HE) hard X-ray Free Electron Lasers. The combination of new accelerator and detectors can read out at up to 25 kHz allowing a better time resolution for studies of motions in biomolecules during stochastic or triggered motions, with an improvement of 10-20 times over the current capabilities of the LCLS.

The following two talks focused on plans for the Second Target Station (STS) at the Spallation Neutron Source (SNS). **Yaohua Liu** introduced new diffractometer concepts proposed for the STS, complementing those of the SNS First Target Station (FTS) and the High Flux Isotope Reactor (HFIR) at the ORNL; he presented examples of how the higher peak brightness and the broader spectrum can achieve measurements that are not feasible at existing neutron diffractometers in the USA or abroad. **Qian Shuo** spoke about Centaur, an instrument designed for small- and wide-angle neutron scattering (SANS and WANS) at the STS, covering the resolution range between tenths and hundreds of nanometers. The design can also be used as a direct geometry spectrometer for probing the dynamics of relatively large length-scale structures and will enable time-resolution studies of a variety of materials in the second scale.

The second part of the session was dedicated to synchrotron source upgrades. **Uta Ruett** opened with an overview of the plans for the APS upgrade, to be completed in 2024. The new source will operate at 6 GeV and will produce highly coherent radiation even at high energy. Of the new beamlines built to take full advantage of the new source, she focused on 11-ID-D, optimized for total scattering, focused into the submicrometer range, and dedicated to the study of new materials from in-situ synthesis and manufacturing to functionality studies. **Yu-Seng Chen** spoke about upgrades to the ChemMatCARS, funded by the National Science Foundation. ChemMatCARS will build a new beamline on a canted undulator, which will allow the Advanced Crystallography Program to become 100% dedicated as a small molecule beamline. He also discussed new experiments that could be carried out after the upgrade.

On the subject of benefits of synchrotron upgrades for structural biology applications, **Daniele de Sanctis** provided a report of a new flagship facility at the ESRF that fully exploits the characteristics of the recently upgraded storage ring. The project EBSL8 aims to the construction of a new beamline built on the ID29 section entirely dedicated to room temperature serial crystallography. This beamline incorporates many optics and instrumentation at the forefront of development. Time-resolved experiments will be enabled by the extremely high flux, a submicron focus and microsecond pulsed X-ray beam. **Bi-Cheng Wang** followed with a historical introduction to the properties of different generations of synchrotron sources and a description of the plans for the SouthEast Regional Collaborative Access Team (SER-CAT) to continue their user program during the APS upgrade. **Marian Szebenyi** closed the session with an update of the new facilities at MacCHESS for structural biology (MX and BioSAXS), both for conventional experiments and for special and new techniques, like applying serial crystallography techniques for MX at room temperature and measurements at high pressure.

4.1.5 Structural Biology of Infectious Diseases

On Wednesday, August 3, a session on Structural Biology of Infectious Diseases was held that was sponsored by the BioMac, Cryo-EM, and Industrial SIGS. The Session was also graciously supported with funding by MiTeGen, Douglas Instruments, SPTLabTech, and ThermoFisher Scientific. Featuring a series of talks from graduate students, postdoctoral fellows, faculty, and industry scientists, the main theme of the session was to highlight how structural science has contributed to advancing the understanding of the molecular

basis of infectious diseases and applying this knowledge base to develop therapeutic strategies to combat various pathogens including SARS-CoV-2.

Iga Kucharska (Hospital for Sick Children, Toronto) opened the session by presenting the structures of a series of potent monoclonal antibodies bound to the Plasmodium spp. circumsporozoite protein (CSP) which contains an unusual central region of multiple amino acid repeats. Antibodies targeting these repeats have the ability to inhibit sporozoite infectivity, and antibody clustering around CSP provides a general immune mechanism. **Lyndsey Backman** (Massachusetts Institute of Technology) presented the crystal structure of hydroxyproline dehydratase (HypD) which is the second most prominent glycyl radical enzyme in the human gut microbiome. HypD is involved in the reversal of trans-4-hydroxy-L-proline (4-Hyp) to 1-pyrroline-5-carboxylic acid. Combining both structural and biochemical investigations has led to the identification of catalytic residues involved in the mechanism of 4-Hyp dehydration. **Baldeep Khare** (Purdue) presented the impressive cryo-EM reconstruction of the Usutu SAAR-1776 virus at 2.4 Å resolution. This is the highest resolution structure of a flavivirus determined to date and has revealed many structural insights which may have implications for the wider field of flavivirus biology.

After the coffee break, **Celia Schiffer** (University of Massachusetts Medical School) described her laboratory's approach to avoiding small-molecule drug resistance by rationally designing inhibitors that fit within the natural substrate envelope. As evidence of the power of this approach, which now includes machine learning, she described its application to the development of potent inhibitors for hepatitis C virus NS3/4A protease, HIV-1 protease, and SARS-CoV-2 Mpro. Next **Debanu Das** (Accelero Biostructures) described his approach to fragment-based drug design centered on ultra high-throughput crystallography screening, which simultaneously provides hit identification and binding location. This technology is now being applied to numerous drug discovery programs, including those targeting the spike protein of SARS-CoV-2, the causative agent of COVID19. **Daniel Kneller** (Oak Ridge National Laboratory) presented research from his postdoctoral studies investigating the mechanism of the SARS-CoV-2 Mpro. He was able to determine the first room temperature X-ray structure and the first neutron diffraction structure of this important drug target. The neutron diffraction studies revealed that the non-canonical catalytic dyad is zwitterionic, and that covalent inhibitor binding modulates protonation states, providing new insights for drug development. The last speaker of the session, **Gordon Joyce** (Walter Reed Army Institute of Research), described his laboratory's use of structural information to design novel vaccine candidates for SARS-CoV-2. These include a self-assembling ferritin-based nanoparticle that displays multiple copies of the SARS-CoV-2 spike protein on its surface. The vaccine candidate elicits high titers of neutralizing antibodies in mice and macaques, and recently entered human clinical trials.

George Lountos & Jason McLellan

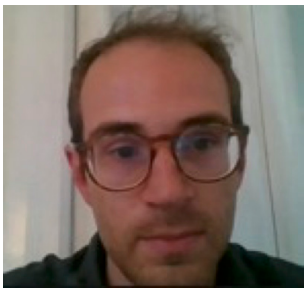
4.2.2 Meeting the Challenges of Raw Data Deposition

The ability to reproduce experimental results (the basis of a publication or other scholarly work) strongly relies on the availability of primary experimental data. The Structural Biology community recognizes this and has encouraged the sharing of research data since its birth.

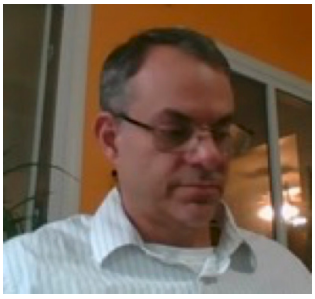
Today, the importance of archiving the raw data (the images and their associated metadata) leading to a structure has come to the forefront as reflected by the work of the IUCr and the ACA in this area. In addition, funding agencies are particularly interested in the reproducibility of the work they fund.

Session 4.2.2 consisted of four talks related to data archiving and the use of data archives to advance science.

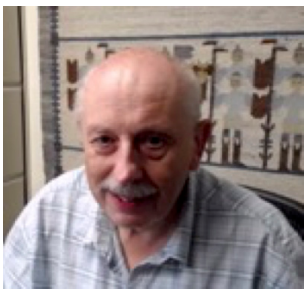
The first talk was presented by **Dr. Marek Grabowski** University of Virginia Charlottesville, VA who provided an introduction for the need to archive raw diffraction images using FAIR principles. He then went on to provide an overview of the Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC) established in 2016 at the University of Virginia and gave a five-year progress report. The Resource currently contains 9402 data sets (5776 structural projects, ~350 data sets added per year) that have been used for studies ranging from automated image processing and structure determination to the modeling of diffraction artifacts (ice rings), classifying dynamic protein polymorphs, and validating & improving structural models including a recent study related to SARS-CoV-2 drug design. More information about how to access the Resource can be found at proteindiffraction.org.



Dr. David Moreau Cornell University Ithaca NY, then presented a talk on ice in biomolecular crystallography. His studies extend the work of Andrea Thorne which revealed that 20% of PDB entries display ice contamination by determining the prevalence of different ice forms in the crystal and how these ice forms affect integrated intensities. To do this he used images from the IRRMC and structure factors from the PDB. Initial analysis showed hexagonal, cubic, and stacking disordered ice contamination. Several software tools were presented to analyze ice forms and their prevalence from diffraction images. In addition, since ice diffraction is not accounted for during image integration, tools for identifying ice diffraction biases in the resulting structure factors were also developed. The software can distinguish between hexagonal, cubic, and stacking disordered ice and ice related artifacts can be detected to high accuracy. The analysis also showed that hexagonal ice is becoming more prevalent in PDB entries which is indicative of very poor cryocooling and should be a concern of the community.



After the coffee break **Dr. Alexei Soares** Brookhaven National Laboratory Shirley, NY presented his work on classifying diffraction data from dynamic proteins according to the individual polymorphs present in the crystal. The microbeams at NSLS II offer the ability of identifying polymorphous crystals or polymorphous domains in larger crystals. A set of software tools has been developed based on the Spring8 KOMA tools. The tools include automated data clustering based on the similarity of unit cell parameters and reflection intensities - to identify possible biological polystates, polynomial-based amplitude modeling as a function of pH - to identify possible polymorph transitions, Ca-based distance analysis of mainchain contacts – to identify residues of interest and cluster-based positional (x, y, z) ellipsoid analysis - to quickly detect interesting features. Several proof-of-concept examples of the tools were presented including the analysis of mixed-state data from chymotrypsin crystals that showed that the data populate an arc of the reaction trajectory as chymotrypsin is converted into chymotrypsin. A paper describing this work is in preparation.

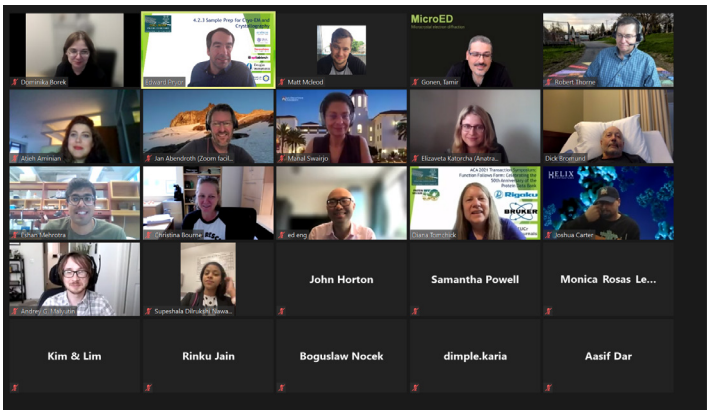


The last but not least talk was presented by **Dr. Wladek Minor** University of Virginia Charlottesville, VA, who provided an overview of the rapid response by the scientific community to biomedical challenges and threats. He argued that threats like COVID-19 require analyzing medical data in the context of other in-vitro and in-vivo experimental results. Recent advancements in biochemical, spectroscopical, and bioinformatics methods may revolutionize drug discovery, albeit only when these data are combined and analyzed with an effective data management framework like an Advanced Information System proposed in 2017. The progress on AIS is too slow, but creating such a system is a Grand Challenge for biomedical sciences. By definition, a Grand Challenge is an ambitious, complicated, and extremely difficult long-term project, and people looking for immediate returns will not always appreciate the efforts that lay a foundation for subsequent works.

*It is with great sadness and a heavy heart, we would like to inform you that **Dr. Marek Grabowski** passed away on August 11th. He had a sudden and unexpected medical emergency while jogging. Marek was a brilliant scientist, a great friend, and a magnificent, always smiling person. He published many papers that attracted a significant number of citations. He was a frequent presenter on ACA and IUCr Congress meetings. He will be missed very deeply.*

John P. Rose & Wladek Minor

4.2.3 Sample Prep for Cryo-EM and Crystallography



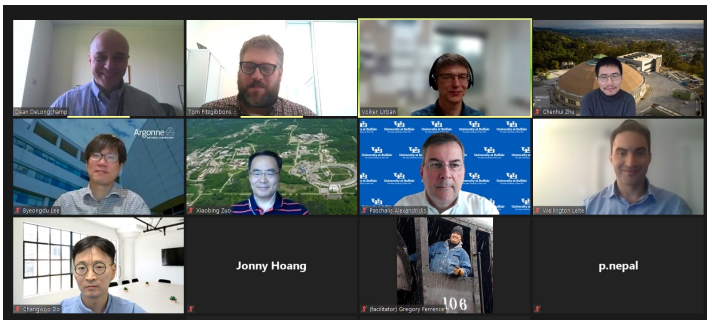
The "Sample Prep for Cryo-EM and Crystallography" session (4.2.3) took place on day three of the 2021 ACA meeting and was attended by over 115 participants. This session was chaired by **Eddie Pryor** from Thermo Fisher Scientific and sponsored by the Cryo-EM and Best Practices Special Interest Groups. The session was kicked off by **Rosemary Cater** from Columbia University who gave an exciting overview of utilizing Fab antibody fragments to aid in the structure determination of small membrane proteins by Cryo-EM. This was followed by **Tamir Gonen** from UCLA and HHMI who presented an overview of both protein and small molecule MicroED, with an emphasis on the sample preparation steps. After the coffee break, **Robert Thorne** from Mitegen resumed the session by introducing Mitegen's SSX system, a new device for serial synchrotron crystallography, as well as some exciting data of Cryo-EM grid vitrification using their Nanuq system. **Atieh Aminian** from Thermo Fisher Scientific presented novel solutions to accelerate Cryo-EM sample screening, including results integrating mass spectrometry data to evaluate samples for the Cryo-EM workflow. In the penultimate talk, **Supeshala Sarath Nawarathnage** from Brigham Young University showed exciting results using TELSAM as a crystallization chaperone for protein targets, including the human TNK1 UBA domain. Wrapping up the session, **Dominika Borek** from UT Southwestern Medical Center presented multiple strategies to improve the vitrification and

data collection of proteins for Cryo-EM which were tested on a handful of benchmark proteins including ApoF, HemQ, and GroEL.

Eddie would like to extend a special thank you to the session facilitators, and to the corporate sponsors of this session: Anatrace, Molecular Dimensions, Thermo Fisher, SPT Labtech, Douglas Instruments, and NanoImaging Services for their generosity.

Eddie Pryor

4.2.4 Self Assembly in Soft Matter Systems

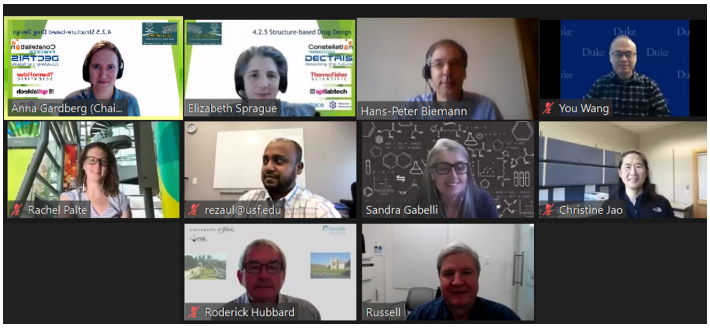


The "Self-Assembly in Soft Matter Systems" session took place on Wednesday August 4th and was attended by over 35 participants. The session was chaired by **Tom Fitzgibbons**, Dow Chemical, and **Volker Urban**, Oak Ridge National Laboratory and focused on the development of new methods and structures that have been applied to study the self-assembly of polymeric based systems. Distinguished professor of chemical engineering at the University at Buffalo, **Paschalis Alexandridis**, kicked things off with an invited talk about using molecular dynamic simulations with small angle scattering to look at the effect of small molecule additives to the self assembled structures present in block copolymer solutions. Professor Alexandridis showed how through the combination of small angle scattering and molecular dynamics simulations small molecule additives could be located within self-assembled micelles. Following

professor Alexandridis' talk, **Dr. Changwoo Do** from Oak Ridge National Laboratory presented the use of contrast matching and differences in contrast observed with SANS and SAXS measurements to elucidate the structure of block copolymer systems. **Xiaobing Zuo** from Argonne National Lab continued the discussion of using SAXS to characterize soft matter self-assembly at the Advanced Photon Source. **Chenhui Zhu** from the Advanced Light Source of Lawrence Berkely National Laboratory gave a talk that focused on using resonant soft X-ray approaches to study complex self assembled structures that form a double gyroid pacing geometry. By taking advantage of the unique contrast afforded soft X-rays, the complex packing structure could accurately be described. Following the short coffee break **Wellington Leite**, a postdoctoral fellow at Oak Ridge National Laboratory, provided insights into the self-assembly of bicelles for biological systems. **Byeongdu Lee** from Argonne National Laboratory then gave a talk that focuses on how SAXS has been used to look at grafting onto nanoparticles. In this case, Dr. Lee was showing results on DNA grafted nanoparticles and the power that SAXS with its associated modeling can provide to the analysis. The session ended with a second invited talk by **Dr. Dean DeLongchamp** from the National Institute of Standards and Technology. In his talk he focused on the new technique of polarized resonant soft X-ray scattering. In this new method the polarization of the beam can be used to deduce orientation differences between samples with unique chemical specificity provided by resonant soft X-ray scattering. Through a combination of this method and the newly developed forward scattering simulations developed by his team and collaborators Dr. DeLongchamp was able to show the relative orientation of polystyrene chains grafted to a nanoparticle. Overall, the session was very well received by the attendees and speakers. The representation from our national labs and academia made for very fruitful discussion around the new technologies and advances made in the field of studying self-assembly in soft matter systems. We look forward to have future sessions like this at upcoming ACA meetings.

Tom Fitzgibbons and Volker Urban

4.2.5 SBDD Session Summary



In session 4.2.5 we explored applications of structural biology methods to drug discovery, including structure/function studies, hit validation, lead optimization challenges and fragments with a particular interest in examples involving a variety of techniques. We featured a mix of speakers representing both academic and industrial

institutions who presented their work involving small molecule and antibody therapeutics. With over 70 participants, we had an engaging session that encapsulated the diverse role of structural biology and complementary biophysical techniques in drug discovery.

We opened our session with a crystallography-based talk from **You Wang** (Duke University) who described the X-ray crystal structure-guided optimization of a small-molecule fungal FTPase inhibitor. The second speaker, **Md Rezaul Karim** (Moffitt Cancer Center), presented some intriguing complementary crystallographic and SAXS studies to elucidate ligand-induced global conformational changes in TAF1 tandem bromodomains in the quest to find a dual TAF1-ATR inhibitor as a potential cancer therapeutic. **Rachel Palte** (Merck & Co) then moved us toward the macromolecular therapeutic realm with a mesmerizing talk about the analysis of paratopes and epitopes of 5 anti-hArg antibodies via cryo-EM structural studies of complexes consisting of antibodies bridging trimers of hArg1. Her team obtained local resolutions of 3.5 Å for these complexes, consisting of multiple hArg and mAb molecules, which are greater than 650 kDa in size.

After the coffee break we continued with more cryo-EM from **Christine Jao** (Genentech) who captivated us with how she utilized protein engineering and chimeras to advance drug discovery efforts for the Nav 1.7, a pain-sensing voltage-gated sodium channel. Next up and moving beyond small molecule therapies, **Sandra Gabelli** (Johns Hopkins School of Medicine) highlighted her group's recent work towards developing bispecific antibodies and CAR-T cells that target intracellular cancer mutations via MHC-neoantigen complexes presented on the cell surface. Through the application of crystallography combined with cellular assays, biophysics and computation, it was a fascinating tale of how antibodies can distinguish between proteins differing by a single amino acid. Finally, the last two speakers in the session presented their work focusing on fragment-based drug discovery. **Russell Judge** (Abbvie) described his team's path starting with a fragment hit for Bcl-XL and overcoming many challenges beyond potency to develop a first-in-class orally active inhibitor. **Rod Hubbard** (Vernalis and York University) wrapped up the presentations by spotlighting examples where NMR, SPR and high throughput crystallography were critical to advancing fragment-based lead discovery for several disease targets. We concluded the session with an interactive discussion covering the presentations as well as our experiences in structure-based drug discovery.

A huge thank you to our facilitators for their technical assistance: Emilia Arturo and James Moody; and to our sponsors for their generous support of the session: Constellation Pharmaceuticals, Dectris, Thermo Fisher Scientific, SPTLabtech, Anatrace/ Molecular Dimensions.

Elizabeth Sprague, Anna Gardberg and Hans-Peter Biemann

WK1: Small Angle Scattering for the Study of Soft Mater Systems

Organizing and carrying out a workshop for virtual participants is not ideal, but the members of the small angle scattering special interest group along with instructors from beyond the traditional ACA membership made do with what was provided and were able to assemble a strong 3 day workshop for people interested in applying scattering methods to soft matter systems. The workshop allowed participants to learn from lecture based approaches as well as gain hands on training on the use tools that have been developed for studying polymer and colloidal based systems. The workshop was successful in reaching 15 registered participants and was taught by 5 co-instructors across academia, industry, and our US national lab synchrotron sources.

The workshop was spread over 3, four hour, sessions from Monday August 9 – Wednesday August 11th. During the first day the participants were provided insight into the SAS measurement and the various hardware approaches to collecting the data. Industrial sponsors Rigaku and Anton-Paar were also present to give insight into how the approaches shown in the session, which focused on synchrotron and neutron sources, could be scaled down to laboratory based systems. The bulk of the 1st day was given to **Tyler Martin** who walked participants through the pyPRISM workflow using Google Colab. PRISM modeling of polymer systems is a powerful tool to understand many thermodynamic properties of polymer solutions. From the pyPRISM toolbox the users learned how to calculate many of the parameters associated with polymer solutions while also model the SAS behavior of the systems.

The second day of the workshop was headed by **Jan Ilavsky** of the Advanced Photon Source and professor **Greg Beaucage** of the University of Cincinnati. Professor Beaucage explained in detail the unified fit model to describe the structure of complex hierarchical materials that are often found in polymer science. Professor Beaucage showed how the model could be used to understand unimolecular systems such as branched polymer chains as well as self assembled macrostructures like wormlike micelles and colloidal aggregates. Jan Ilavsy then led the participants through a hands on demonstration of the IRENA package within IgorPro. This software package developed by Dr. Ilavsky has integrated the Unified fit model developed by professor Beaucage into a easy to use graphical user interface. New functions associated with the tool were also demonstrated such as bead modeling of hierarchical structures based on the solution of the unified fit model.

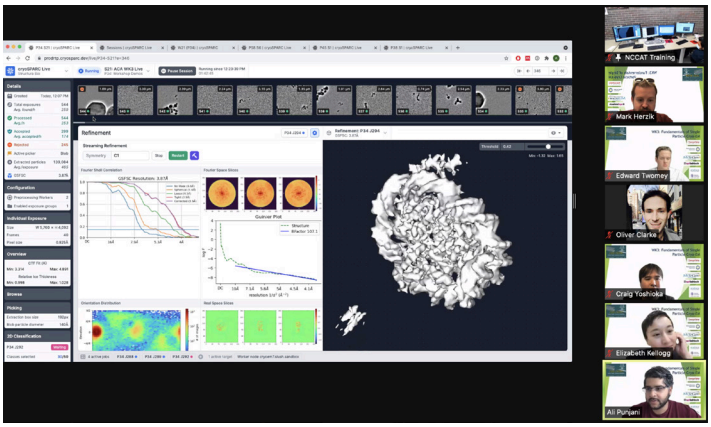
During day 3, professor **Lucia Fernandez-Ballester** from the University of Nebraska and **Tom Fitzgibbons**, a research scientist from Dow Chemical, led a lecture describing the in situ analysis of polymer systems using a combination of WAXS and SAXS. Professor Fernandez-Ballester provided a lot of first hand knowledge to the participants on how to design and carry out detailed crystallization studies at various beamlines as well as the difficulties present in scaling down industrial processes to lab based fixtures that can fit within a beamline hutch. She then stepped the class through the fundamentals of WAXS analysis and polymer crystallization using examples from her extensive flow-induced crystallization work. Between the two main speakers, Anton-Paar and Rigaku provided the participants information on their new in situ stages that can be used in either their in house PXRD systems or at various beamlines for in situ polymer analysis. Dr. Fitzgibbons then provided several real world examples of using in situ WAXS and SAXS experiments to understand the role of additives to polymer and paraffin crystallization and deformation.

Overall the workshop was able to provide participants insight into the methods and analysis that materials science practitioners experience using SAXS and WAXS to study polymer systems. We as instructors and organizers hope to see

more materials science based programing in the future at ACA meetings.

Tom Fitzgibbons

WK3: Fundamentals of Single Particle Cryo-EM



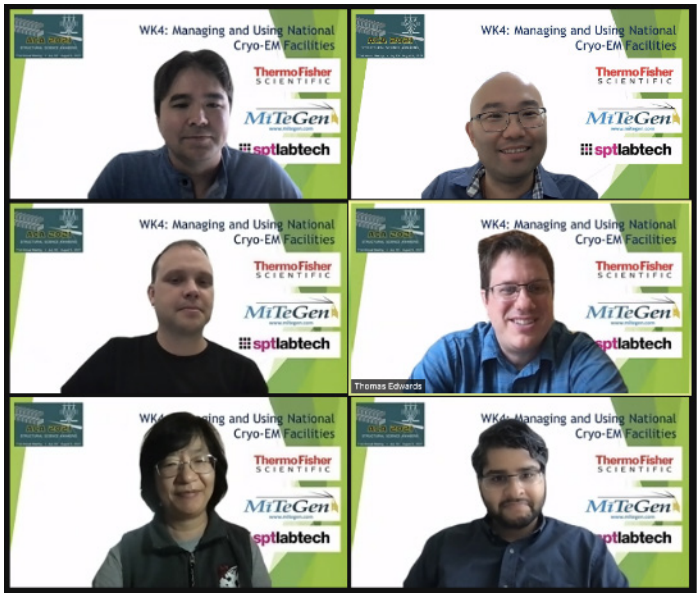
Ali Punjani (Structure Bio) leads a live cryoSPARC Live demonstration using data streaming in real-time from data being collected at NCCAT (Ed Eng).

Mark Herzik (UC San Diego), Elizabeth Kellogg (Cornell), and Edward Twomey (Johns Hopkins) organized this year's Fundamentals of Single-Particle CryoEM Workshop. This virtual workshop was designed to accommodate registrants of disparate educational backgrounds to provide an opportunity to obtain a critical understanding of current best single-particle cryoEM practices, latest advances in sample preparation technologies and data processing strategies, as well as provide insights into where the field is moving. Instructors included Eva Nogales (UC Berkeley), Chris Russo (MRC-LMB), Michael Cianfrocco (U Michigan), Chi-Min (Mimi) Ho (Columbia), and Oli Clarke (Columbia). In addition, registrants were introduced to the NIH-funded National CryoEM Centers (Ed End; NCCAT, Craig Yoshioka; PNCC), how to apply for time at these centers, what to expect when samples are sent to these centers, and expectations during and after data collection. Importantly, at this workshop the very first live cryoEM data collection at NCCAT (Ed Eng) was broadcast in real-time during the workshop and one of the instructors, Ali Punjani (Structura Bio) led the first live cryoSPARC Live demonstration using data that was being collected in real-time at NCCAT. Such a feat had never been accomplished before and represents the latest advances in cryoEM data processing software and microscope capabilities, whereby, during the workshop, a ~3.4 Å cryoEM reconstruction of a nucleosome was obtained.

This workshop was made possible by generous contributions from our sponsors, including: MiTeGen, Thermofisher Scientific, Nanoimaging services, Anatrace, Molecular Dimensions, and SPT Labtech.

Mark Herzik, Elizabeth Kellogg, and Edward Twomey

WK4: Managing and Using National Cryo-EM Facilities



The one-day workshop "Managing and Using National Cryo-EM Facilities" was held via Zoom as part of the ACA annual meeting on Monday, August

16, 2021, in conjunction with the ”Fundamentals of Single Particle Cryo-EM” workshop held the following two days. The workshop was organized by **Ed Eng** (NYSBC/NCCAT) & **Craig Yoshioka** (OHSU/PNCC) and included **Thomas Edwards** (FNLCR/NCEF), **Anchi Cheng** (NYSBC/SEMC), **Ali Punjani** (Structura Biotechnology Inc.) and **Corey Hecksel** (Stanford-SLAC/S2C2) as instructors.

Close to 50 attendees learned how recent advances in cryo-EM methods and technology have greatly extended its resolution and the amount of information it can provide about viruses, proteins, and other important biomolecules. The goals of the workshop were not only to discuss the infrastructure and operations needed to run a cryo-EM facility but how to interface with the national service centers. Over the course of the day, a variety of topics were covered including 1) cryo-EM operations, 2) IT Infrastructure and 3) User Training.

Cryo-EM instrumentation is being installed at many universities, and is also available at large multiuser facilities both in the U.S. and worldwide. The NIH CommonFund has sponsored the Transformative High-Resolution Cryo-electron Microscopy Program to broaden access to high-resolution cryo-EM for biomedical researchers has created national service centers, and enabled the cultivation of a skilled workforce through the development and implementation of cryo-EM training material. The three National cryo-EM Service Centers offer usage of state-of-the-art equipment, technical support, and cross-training for the production and analysis of high-resolution data. The shared landing site for the resources at the national centers may be found at https://www.cryoemcenters.org/. These offerings are available at no charge for non-profit use, eliminating the high-cost barrier usually associated with cryo-EM.

Ed Eng** & **Craig Yoshioka

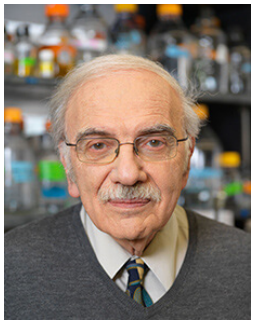
ACA HISTORY

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

History Project Update

Virginia Pett

Oral Interviews



Mario Amzel

Mario Amzel (1942 - 2021) grew up in Buenos Aires and studied science at university, where he became interested in relating thermodynamics to structure. Throughout his career he was trying to answer the question, "Can you go from coordinates to thermodynamics?" After a military coup in Argentine, he and a group of others went to Universidad Central de Venezuela, where he received his Ph.D. He then came to Johns Hopkins to the lab of Roberto Poljak where they determined the first structure of a Fab fragment: "It was the first structure that allowed people to know how antibody recognize antigens." During his career he has been particularly interested in how mutations affect function, in enzymes and in sodium channels. For the future of structure determination he predicts, "Eventually, my impression is that many of the structures will have to be determined crystallographically and will have to be combined, combined with EM structures, and that will be where we are going to look for the answers." Finally, he gives his philosophy of research: "I'm not here to make a medication. I'm here for people to understand how things work." Click here to read his 2020 interview with David Zierler.

Jenny Glusker

Jenny P. Glusker describes her life and scientific career in this oral interview with David Zierler of the American Institute of Physics. Jenny Pickworth worked with Dorothy Hodgkin at Oxford on the structure of vitamin B12. She came to the USA, married Don Glusker, and did postdoctoral research at Caltech with Linus Pauling, Robert Corey, and Dick Marsh. She joined Lindo Patterson at the Institute for Cancer Research in Philadelphia, where she had an illustrious career researching small molecule structures and their interactions with DNA and proteins. She became expert at the interactions between metals and proteins. She and Kenneth Trueblood wrote a primer, Crystal Structure Analysis, which presents a clearly written description of the process, including the mathematics.

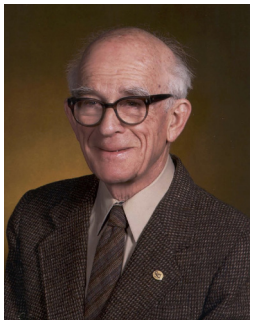
Robert Rosenstein Bequest

Robert Rosenstein

At the 2021 Business Meeting of the ACA, Treasurer Ilia Guzei reported a $250,000 bequest from Robert D. Rosenstein (1922 – 2017). The funds will be used for education and training of structural scientists. Art Olson characterized Rosenstein's career as follows: "Bob was a crystallographer's crystallographer, teaching the science and art of the subject for

many years in the Crystallography Department at the University of Pittsburgh." Ned Seeman, who had been a graduate student in that department, commented, "Bob was arguably the best teacher I ever encountered." You can read more about his life in comments by Art Olson, Helen Berman, and Ned Seeman at ACA History online.

Sidney C. Abrahams (1924 - 2021)



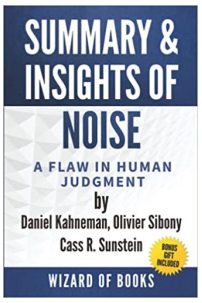
Sidney Abrahams

Sidney wrote his "Living History" for ACA RefleXions magazine in 2011; his memoir was one of the first to be published online at ACA History. Abrahams had a distinguished career at Bell Labs, as president of the ACA (1978), as editor of Acta Crystallographica (1978-87), and extensive participation in commissions of the IUCr. Several obituaries were recently added here.

2020 Transactions now online

I thought readers would want to know where to find the Transactions from the 70th Annual Meeting of the American Crystallographic Association, "Structural Science—New Ways to Teach the Next Generation." This excellent collection of papers on teaching crystallography is published in an open-access issue [Structural Dynamics 8, 040401 (2021)]. Of course, this Transactions is not history – it is a forward-looking compilation of methods for educating future structural scientists.

Virginia Pett



Book Review: Noise: A Flaw in Human Judgment

ISBN: 978-031645140
By Daniel Kahneman, Olivier Sibony and Cass R Sunstein

Jeanette has been swamped with work and so you'll have to suffer through one of my reviews. I picked this book up because the title caught my attention and I really enjoyed Thinking, Fast and Slow by the first author. When I think of noise I think of the noise in linear systems, specifically X-ray instrumentation, the leaf blowers on Zoom calls, or pops and clicks on vinyl albums. I never thought of human judgment as being noisy. Biased, yes, but not noisy. In this book you will learn we are very noisy, indeed.

The authors start with a basic description of the error model for human decision making using bias and noise, then describe a number of every day phenomena that are noisy: insurance premiums, medicine, child custody, forecasts, asylum decision, personnel decisions, bail decisions, forensic science and patents. The authors use studies of the various phenomena to illustrate their points throughout the book.

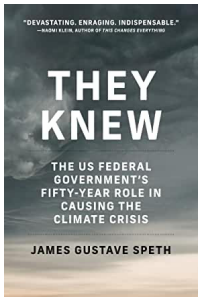
The first part of the book is devoted to understanding the difference between bias and noise, and introduce the concept of a noise audit (how to properly execute one is described in detail in Appendix A). In part to the authors analyze human judgment and separate noise in decision making, pattern noise, into to two parts, level noise and occasion noise. The former is the noise in decisions between individuals and the latter the noise in decisions for a given individual at different times. Part 3 delves into ways to standardize decision making to minimize noise. Part 4 considers human psychology, the sources of noise in decisions and why humans filter noise so well. Part 5 looks at improving judgment and reducing error through a concept dubbed decision

hygiene. Part 6 addresses the issue dealing with noise when you can't eliminate it.

Appendix B provides a checklist to reduce bias in decision making and another Appendix addresses predictions and reminds me of Bayesian analysis without the math.

I enjoyed this book so much that I thought I would throw an idea: start a book club where we could get together on Zoom and discuss this book. If you are interested email me at joseph.ferrara@rigaku.com.

Joseph Ferrara



Book Review: They Knew: The US Federal Government's Fifty-Year Role in Causing the Climate Crisis

ISBN: 9780262542982
By James Gustave Speth

They Knew is not like most books about the climate crisis. Despite the presentation of its publication as a book, it is in fact a copy of the author, James Gustave "Gus" Speth's expert testimony in the case Juliana vs. the United States. In 2015, 21 youth plaintiffs filed a lawsuit against the United States claiming that government officials had violated their unalienable rights to life and liberty by pursuing a national agenda in support of fossil fuel consumption despite having extensive knowledge regarding the negative and inevitable impact of such behaviors on the (near) future climate of the planet.

The case is still ongoing--as of the writing of this review, the plaintiffs are in the middle of settlement negotiations. However, despite the frequent legalese in the introduction, which was written by the two adult litigators leading the plaintiffs case, Julia Olsen and Philip Gregory, the rest of the book is much more rooted in history and the science of those historical times. You do not need to be a lawyer to parse the majority of the book, though the introduction definitely tests the reader's basic knowledge of legal terminology.

Speth's book is divided into 9 chapters, prefaced by an introduction in which he explains his pro bono role as an expert providing testimony on behalf of the plaintiffs in Juliana. He also clarifies that though this testimony was originally written and presented in 2018, he reviewed, revised, and updated it in 2020 to include the full impact of the most recent administration.

In the first chapter, he lays the groundwork for what the United States government knew about climate change at the beginning of the Carter administration. The following 7 chapters are broken out by presidential administration, from Carter through to Trump. In each chapter, Speth outlines both the advances in understanding of climate science during that president's term, as well as how the policies they enacted and supported impacted the well-being of the environment at that time. No administration comes out of Speth's testimony entirely spotless, though perhaps the worst offender is the most recent one, from 2017-2020. Under Trump's presidency, almost all previously enacted climate protections were undone, and any progress made during previous administrations was entirely lost. The full list, provided in bullet form for ease of reading, is indeed still difficult to digest.

The final chapter contains Speth's damning conclusion--as the title of the book suggests, "they knew" (the "they" in question being the United States government) how the actions and policies enacted by the various administrations of the past 40 plus years would negatively impact future generations. But Speth keeps his testimony very factual, leaning on evidence from verifiable sources such as recorded speeches and official

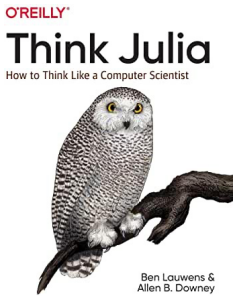
documentation. He doesn't try to posit why these decisions were made, only that they were in spite of the mounting scientific evidence that they would have dire consequences in the near future.

The book ends with an appendix written again by Olsen and Gregory, updating the reader as to the status of Juliana as of the time of the book's publication.

The last hundred or so pages contain all Speth's extensive references, as well as a note confirming his professional background as it qualifies him to provide testimony in Juliana.

They Knew is not a fun, light, or entertaining summer read, but it certainly casts a bright and educational light on a dark history of covering up climate change.

Jeanette S. Ferrara, MFA



Book Review: Think Julia: How to Think Like a Computer Scientist

ISBN-13: 978-1492045038
By Ben Lauwens and Allen B. Downey

I will be the first to admit I missed the boat on Python as a coding language. So when a colleague mentioned this new language from MIT called Julia that was very efficient and fast, I decided to look into it. I was pleasantly surprised at the compactness of the download and the wealth of information available online. You can see this in the useful links and videos listed above. I generally look to O'Reilly for books on computer science and related topics, so I picked up Think Julia.

The book first elucidates some fundamental programming concepts as well as installing and running Julia. The book progresses through more complex and abstract concepts: variables, expressions and statements, functions, conditionals and recursion, iteration, strings and arrays, dictionaries, tuples, files, structures and objects, structures and functions, multiple dispatch, subtyping, and debugging. The authors also provide details on syntax and the utilities in the base Julia distribution. Interspersed throughout the text are case studies diving deep into particular problems. Each chapter ends with hints for debugging, a glossary, and a set of exercises.

I do have one minor complaint: the book was written with the Julia 1.0 base in mind, and some features of the package associated with the book did work with the current distribution, 1.6. Nevertheless. I found the book an easy and enlightening read, and Julia a lot of fun.

Joseph Ferrara

Puzzle Corner

For Fall, we have a symmetry puzzle about car wheels, a new Crystal Connections and a new DISORDERED puzzle. The solutions to the previous puzzles are also given, along with mention of those who provided them.

Crystal Connections #21:
Find the answers to these clues and what they have in common.

1. Painted on barns in Pennsylvania Dutch country.
2. Cars have four of them.
3. Typically found on doors of crystallography labs.
4. Posted on labs with BSL-2 rating or above.
5. Sand painting created by Buddhist monks in order to be ritualistically destroyed.
6. Circle Limit III, Path of Life, and Snakes, for instance.
7. Used to control a watercraft's rudder from its helm.
8. At the end of a rope, thrown to a drowning person.
9. In Gothic cathedrals, stained glass structures radiating outward like flower petals.
10. Ice I_h, photographed by Wilson Bentley and much later by Kenneth Libbrecht.

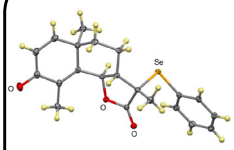
Solution to Crystal Connections #20:
All pertain to Baltimore, the originally planned site of ACA2021

1. Emily Dickinson wrote a poem about the song of Icterus galbula, for which this baseball team is named. **Baltimore Orioles (The Oriole's Secret)**
2. "And **The Raven**, never flitting, still is sitting, still is sitting…" This poem led to the name of a pro football team.
3. The author of that poem, who also wrote "The Gold-Bug," which involved cryptograms. **Edgar A. Poe** died and is buried in Baltimore.
4. The **Baltimore Classification System** groups viruses based on genome replication strategy.
5. The "Star-Spangled Banner" was written during its bombardment in 1814. **Ft. McHenry**
6. In Monopoly, the "B&O" railroad. **Baltimore and Ohio**
7. Considered the first research university in the United States. **Johns Hopkins**
8. The Preakness Stakes horse race is held here. **Pimlico Race Course**
9. The Susquehanna, Potomac, Rappahannock and James Rivers drain into **Chesapeake Bay**.
10. Randy Newman song which contains the line "beat up little seagull on a marble stair". **Baltimore**

DISORDERED

Correct these anomalous spellings to resolve the ambiguity

FHOTO	H O O F T
DEFILER	F R I E D E L
RICHLA	C H I R A L
TRAFCO	F A C T O R
KEPS	S P E K



x=0.986(8)

If you report the incorrect absolute structure, the referees will give you…

Answer:

A L O T O F F L A C K

DISORDERED

Fill the boxes correctly to arrive at the right place

IDLY	
PYRONET	
DERNHOGY	
NASTIGCK	
MACERATE	

The most interesting part of moving an X-ray lab

Answer:

Observational Symmetry Puzzles:

1. What is the most common order of rotational symmetry (idealized, neglecting manufacturer's logos, bolt holes, valve stems, etc.) for automobile wheels? How common are other orders? Take a guess, observe for a few days, and let me know what you find.
2. How common are wheels without mirrors in addition to the major rotation axis? Those that don't are, of course, chiral. Are the left-side wheels mirror images of the right-side wheels (i.e. are these cars meso or homochiral, wheel-wise)? Again, guess and then observe.

Solution to Crystoquote #11:

My attraction to crystallography initially was, frankly, totally aesthetic. It's a beautiful science. I think many of us who became crystallographers were attracted by that beauty.
- **Helen Berman**

Comments on the previous puzzles:

Frances Bernstein was the first to provide the solution to the Flack DISORDERED puzzle, and **Joel Harp** provided the solutions to Crystoquote #11 and Crystal Connections #20.

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

Frank Fronczek – ffroncz@lsu.edu

MiTeGen
www.mitegen.com

MiTeGen was proud to sponsor the 71st Annual Meeting of the American Crystallographic Association! We believe that such events are essential to supporting the ACA and our scientific community.

Our goal is to serve as a resource to fellow researchers and we want to be sure you know about technologies we highlighted at this year's ACA meeting:

- Increased drop protection while harvesting - Watershed™ Humidified Harvesting Instrument
-
- Cutting edge mounting system - Sample supports for Serial crystallography and more
-
- Leading sample storage and shipping
  Unipuck Starter Kits
  Cryogenic RFID Sample Tracking System

- Simplified crystal harvesting - Mounts and Loops for Better Diffraction

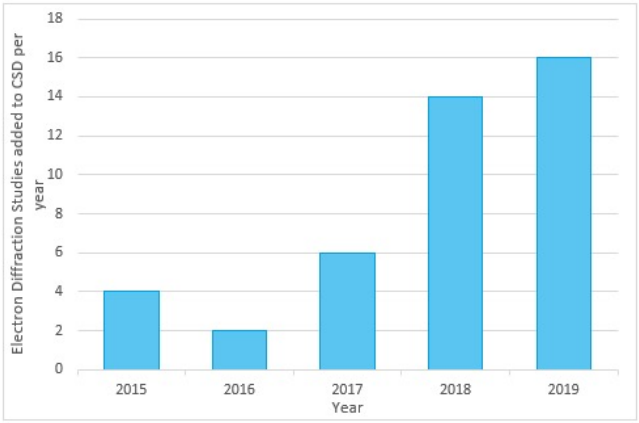
Remember to connect with researchers, discover events, and learn about our New Lab Program with a free subscription to our monthly newsletter or take a look at our new Jobs Board.

If I can be of any assistance, please reach out to me by email joyce@mitegen.com or schedule a call with me by phone or video.

CCDC

The Cambridge Crystallographic Data Centre (CCDC) is a world-leading expert in structural chemistry data, software, and knowledge for materials and life sciences research and development. We specialize in the collation, preservation, and application of scientific structural data for use in pharmaceutical discovery, materials development, and research and education.

Microcrystal electron diffraction supports a new drug development pipeline



The number of structures measured with electron diffraction added to the CSD 2015–2019.

To date, solving structures of potential therapeutics using X-ray diffraction (XRD) has been an assumed, pivotal step in the drug development process. But a recent paper by a team of researchers led by NanoImaging Services shows how microcrystal electron diffraction (MicroED) is growing to obtain the structures of potential pharmaceuticals.

"Growing large crystals is a huge bottleneck for those interested in determining crystal structures," said author Dr. Jessica Bruhn, Scientific Group Leader – MicroED at NanoImaging Services.

"MicroED can work with crystals of almost any size as it is generally fairly straightforward to break large crystals into a size suitable for MicroED."

Developments in automated data collection and data processing have led to increased interest in electron diffraction as an XRD alternative. Currently, there are over 100 unique datasets determined using electron diffraction in the CSD's June 2021 web and desktop offerings. Suzanna Ward is the Head of Database at the CCDC.

"Electron diffraction is truly one of the most exciting and rapidly evolving areas of structural science," Ward said. "Recent publications already show how it could help to speed up the development of new drugs, and we are eagerly anticipating how it might impact the volume and breadth of data we are able to share through the CSD. I think we have an interesting journey ahead of us, and it will be intriguing to see how 3D electron diffraction will be utilized in both industry and academia in the coming years."

For more information on how to access and deposit electron diffraction structures in the CSD, read this blog by CCDC Data Integrity Research Scientist, Natalie Johnson on Electron Diffraction Data in the CSD.

Read our full Q&A with Dr Jessica Bruhn, Scientific Group Leader – MicroED at NanoImaging Services.

Read the full CCDC and NanoImaging Services press release.

Upcoming CCDC events

CCDC has several exciting events coming up, and we'd love to see you there. View all our events on our webpage. Here are a few highlights.
November's virtual workshops

CCDC hosts recurring Virtual Workshops that provide hands on opportunities to improve your skills in various CCDC tools and applications. We're hosting three in November - and they're free to attend.

Virtual Workshop: deposit your crystallographic data in the CSD

- Which data and data files you can submit to the CSD.
- How you can enhance your deposited data.
- What happens to your data after deposition and how you can manage them.
- What the benefits of sharing your structural data with the community are.

Date: 2 November 2021
Time: 6:00 to 7:45 (ET) / 10:00 to 11:45 (GMT)

Register here

Virtual Workshop: learn the basics of protein-ligand docking using GOLD

- The basics of GOLD and our Hermes interface.
- How to run a standard protein-ligand dock.
- How to identify the correct binding modes reliably and with confidence.
- The basics of how GOLD can be used in virtual screening and lead optimization.

Date: 9 November 2021
Time: 11:00 to 12:45 (ET) / 15:00 to 16:45 (GMT)

Register here

Virtual Workshop: intermediate Mogul, assessing molecular geometries

- Interpreting usual and unusual results given context.
- Analyzing the impacts of specific groups.
- Assessing new drugs in the pharmaceutical industry using Mogul.

Date: 16 November 2021
Time: 08:30 to 10:15 (ET) / 12:30 to 14:15 (GMT)

Register here

Focus on MOFs talk and networking event

ELECTRON DIFFRACTION (MICROED/3DED) WORKSHOP

This workshop is for X-ray crystallographers interested in finding out more about electron diffraction and how to get started. Presentations are intended to introduce the technique and will be a mixture of practical and educational. We will include the basis for the technique, how it differs from X-ray crystallography, and a demonstration of how to operate the XtaLAB Synergy-ED electron diffractometer and how to handle data from it.

Oct 27, 2021 08:00 AM
Oct 28, 2021 08:00 AM

Time shows in Central Time (US and Canada)

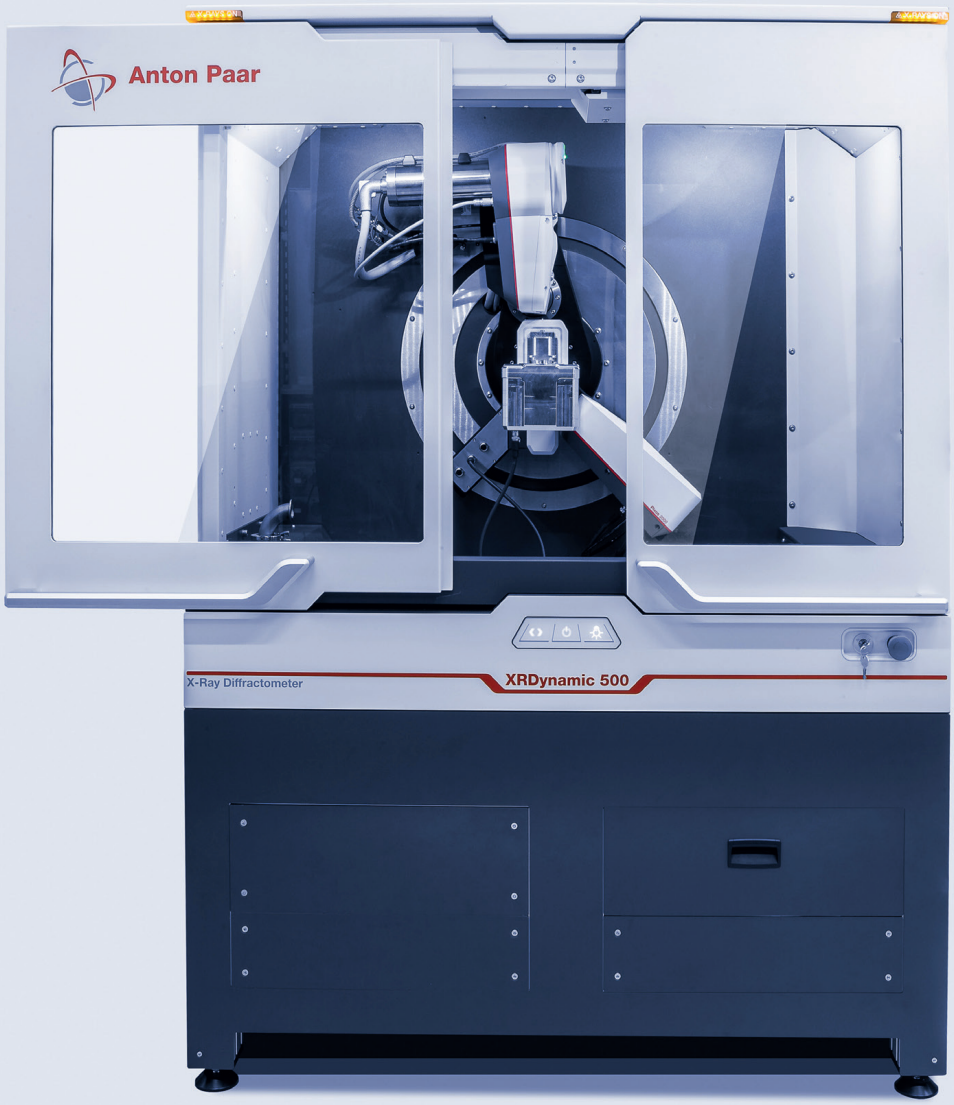
Register Now

2021 Corporate Sponsors

DIAMOND SPONSOR ($2,200/Year)	RUBY SPONSOR ($1,800/Year)	EMERALD SPONSOR ($900/Year)
MiTeGen	Anton Paar	charlessupper company
Rigaku	ThermoFisher SCIENTIFIC	Douglas Instruments
sptlabtech	DECTRIS detecting the future	rayonix
anatrace / Molecular Dimensions		ICDD
STOE SINCE 1887		CIA CRYO INDUSTRIES OF AMERICA, INC.
ARI Art Robbins Instruments		NanoImaging Services
BRUKER		PROTO MANUFACTURING
		CCDC advancing structural science
		ATPS, Inc.
		AIP American Institute of Physics

Thank you to all our Corporate Members for their continuing support!
We also welcome new members. If you are intereseted in becoming a Corporate Member, please follow the link below:
https://acas.memberclicks.net/corporate-membership

Anton Paar



DRIVING XRD:
XRDynamic 500

- Versatile powder diffractometer for all XRD applications
- Large goniometer radius, evacuated beam path: supreme data quality
- Maximum efficiency via automatic optics and alignment routines
- State-of-the-art components: from high-end pixel detectors to innovative X-ray optics

Get in touch: **www.anton-paar.com**