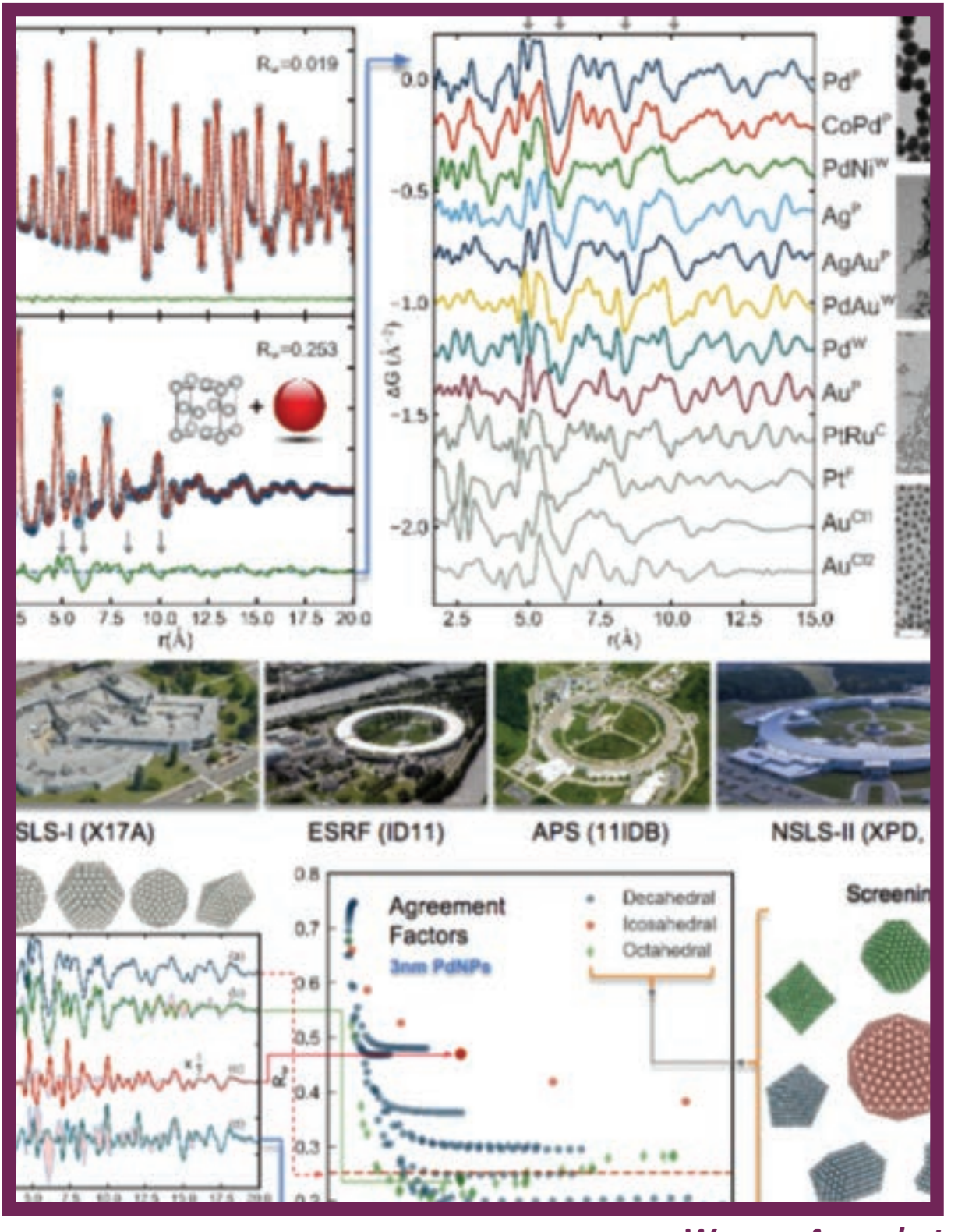
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 3

Fall 2018



Warren Award at Toronto ACA Meeting

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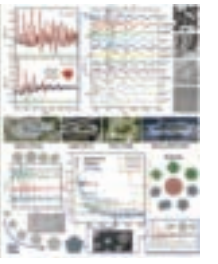
Lisa Keefe
2018 ACA President



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President's Column


Lisa Keefe

As many have noted, the science presentations at the 2018 annual meeting in Toronto highlighted impressive discoveries in groundbreaking research, the life-long achievements of Buerger awardee Frank Hawthorne (crystal chemistry of major mineral groups) and Warren awardee Simon Billinge (characterizing structures of nanomaterials), the remarkable scientific advances of Etter Early Career awardee Jason McLellan (structure-based approaches to treating viral infections), and the innovative approaches to structure-based drug design presented in the Transactions Symposium. Indeed, the impact of structural science reverberates across the many disciplines within the ACA, and has been felt for generations since the beginnings of crystallography. The efforts of our fellow structural scientists do not go unnoticed, evidenced by the prestigious awards bestowed upon our mentors and colleagues over the many years during which crystallographic techniques have developed and enabled the structure solution of molecular complexes that long eluded us. What are the elements that have nurtured these successes?

The scientific environment in which crystallography has flourished is one in which researchers respectfully embrace the differing perspectives and backgrounds of colleagues. The ACA has a long history of embracing and supporting all scientists studying structure—a practice that has strengthened the society and fostered fruitful collaborations—resulting in innovative scientific discoveries. While many researchers are of the opinion that the ACA has long promoted a healthy and inclusive environment that meets its members' needs, it is prudent to routinely re-assess policies and practices to determine how ACA can better align with the membership and what new strategies can be developed that will further promote scientists pursuing careers in the study of structure.

This year, ACA reaffirmed its commitment to diversity and inclusion. Now posted on the ACA website, the statement reads: "The American Crystallographic Association is committed to diversity and inclusiveness in our membership, as well as in all activities, events, and programs, and services. Scientific innovation requires bringing together both diverse ideas and people from varied backgrounds who may have different world views and ways of solving problems. The ACA seeks to include and engage members across age, gender identity and expression, race, nationality, ethnicity, physical ability, marital status, sexual orientation, socioeconomic status, military or veteran status, or any other facet of social diversity in our society and seeks to remove obstacles to their professional growth and advancement. Through our actions at the international, national, and local levels, we strive to promote inclusion in academic, industrial, and government institutions for both current and future members of our organization." ACA Council is committed to affecting changes to ensure diversity and inclusion for the benefit of all members of ACA. As a first step toward that goal, Council sought your input via the ACA Member Survey that was emailed to all members this past summer. Approximately half of the membership responded; your thoughtful responses are highly valued. Review and analysis of those responses are in progress in order to identify areas in need of improvement and to develop impactful strategies for strengthening diversity and inclusion. In the second step, Council will respond to the results of the survey and develop a comprehensive strategic plan to enhance the value of ACA membership.

ACA's commitment to enhancing value is broad reaching. This reach encompasses differing scientific perspectives, arenas of scientific inquiry, and the methodologies and techniques for studying structure. Whether it be conducting basic research, teaching, providing service, or developing new technologies, ACA aims to recognize members' achievements with either the distinction of ACA Fellow or a variety of awards. Candidates for these honors must be nominated; all members of ACA are eligible to submit a nomination. Details about the awards and ACA Fellows, including nomination forms, are posted on the ACA website. This is your call to action: nominate a mentor or colleague for ACA Fellow or for an ACA award.

ACA fully embraces the full spectrum of structural science communities. Whether it be small molecule or macromolecule, experiment or theory, single crystal X-ray diffraction or neutron diffraction or SAXS or NMR or cryoEM, the study of structure binds us. New elements of structural science diversity within ACA are warmly welcomed. To note, the excitement for new approaches to studying structure that were generated by the most recently formed SIG, the cryoEM SIG, illuminates how scientific diversity contributes to the potential for scientific breakthroughs. The SIGs drive the content for the sessions at the annual meeting and consequently set the overarching scientific focus for the annual meeting. The scientific diversity of the SIGs is what gives ACA its many appealing facets.

ACA supports crystallographers in all of North America and South America, and lends support to our sister organizations world-wide in Europe, Asia, and Africa. Our diversities structure the environment in which we collaborate and innovate. Our subscription to a culture of respect fosters borderless research and fruitful collaborations. Our shared passions drive discovery.

Lisa Keefe

Photo by Richard H. Bromund.

The ACA's **68th Annual Meeting** kicked off in Toronto on Friday, July 20, 2018 with four full-day **Workshops**: **Cryo-EM – A Guide to High-Resolution Structure Determination**; **Molecular Art & Animation in 3D**; **Applications of Small Angle Scattering to Structural Biology: An Introduction**; and **Rietveld Refinement and Pair Distribution Function Analysis of *In Situ* X-ray Scattering Within GSAS-II**. A **First Time Attendee and Student Meeting Orientation** was held Friday evening. This was followed by a **Special Plenary Lecture** by **John Polanyi**, 1986 Nobel Laureate in Chemistry. The **Opening Reception Exhibit Show**, generously hosted by the exhibitors, capped off the evening. Reports from the **Workshops** and from this year's **Travel Award Winners** will be featured in our Winter issue of *ACA RefleXions*.

The scientific sessions began on Sunday with the presentation of the 2018 **Warren Award** to **Simon Billinge**. Simon's Warren Award winning work is featured on our cover (see also ***What's on the Cover*** on p. 6). New this year was a **Three Minute Thesis** session during which select poster presenters were invited to give an oral presentation of the thesis and significance of their work. The Sunday sessions also included the **ACA Transactions Symposium**: **Shining a Light on Structure-Based Drug Discovery**, chaired by **Steve Soisson** and **Vincent Stoll** (pp. 20-23).

On Monday **Frank Hawthorne** received the 2018 **Buerger Award** (featured on the cover of the Spring 2018 issue of *ACA RefleXions*), and **Jason McLellan** received the **Margaret C. Etter Early Career Award**, on Tuesday. In addition to the award lectures and poster sessions, over 40 separate scientific sessions were held on a variety of topics related to the structure of matter (see pp. 20-52, ***Toronto ACA Meeting Scientific Sessions***).

The meeting wrapped up Tuesday evening with ACA's annual **Awards Banquet**. The evening's program was chaired by ACA President, **Lisa Keefe**, and included announcement of the **ACA Fellows – Class of 2018**: **Andrew Allen, James Britten, Majed Chergui, Wladek Minor, Thomas Proffen, Janet Smith** and **Robert Von Dreele** (see pp. 8-12). The ACA honored this year's 14 **Poster Award Winners** from among the exceptional array of posters presented at the meeting (see ***Poster Prizes in Toronto***, pp. 53-54). This year's awards banquet program featured a talk by **Natasha Myers**, Dept. of Anthropology, York University. To cap off the evening, guests were treated to musical entertainment by the **Stringhoppers**.

Gerald Audette and **Tiffany Kinnibrugh** were **Program Chairs** for the meeting; **Louise Dawe** and **David Rose** were **Posters Chairs**; **Richard Bromund** coordinated the **Session Photos** with assistance from ACA's **Kristina Vitale**; and **Richard Bromund** and **Virginia Pett**, ACA's **Videography Team**, recorded the award lectures and the Polanyi interview. AIP Publishing's **Robert Finnegan** did his usual great job with the **Exhibit Show**.

RefleXions from Canada

Tomislav Friščić

This was a particularly exciting summer for crystallographers in Canada, as the Annual ACA meeting took place in Toronto, Ontario, organized under the watchful eye of **Gerald Audette** from York University and **Tiffany Kinnibrugh** from Elmhurst College. As I expect that this edition of the ACA RefleXions is fully dedicated to the events and sessions that took place at this meeting, let me simply state that it was both a riveting and a dynamic event, which provided an excellent opportunity to bring together crystallographers not only from USA and Canada, but also from all corners of the world. I would also like to highlight that, besides the **2018 Annual ACA Meeting**, Canada has this Summer also been the home for a number of other meetings related to crystallography and solid-state sciences. Specifically, the **11th Canadian Powder Diffraction Workshop** was held in the period 25-29 July 2018 in Hamilton, Ontario, immediately after the Annual ACA meeting in Toronto. The workshop was organized by **Jim Britten** (McMaster University) and **Patrick Mercier** (National Research Council), and more information can be found on the webpage: **https://xtallography.ca/index.php/xtal/meetings/cpdw-11/**.

I am very happy to report that, together with **Louis A. Cuccia** from Concordia University and **James D. Wuest** from Universite de Montreal, we have organized the fifth edition of the **Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec** meeting (**CEMWOQ-5**) at the Department of Chemistry, McGill University. It is great to see this young tradition of solid-state chemists and crystal engineers in Canada develop. This year, as before, the meeting has hosted a number of Canadian and International speakers, with plenary lectures provided by Prof. **Joel Bernstein** from New York University and Prof. **James D. Wuest** from Universite de Montreal. Over 50% of speakers at the meeting were graduate, undegraduate students or post-doctoral researchers, with research topics ranging from designing organic magnetic materials and metal-organic frameworks (MOFs), to structure determination using NMR Crystallography. More on

Figure 1. (a) Attendees of the powder X-ray structure solution workshop that preceded the CEMWOQ-5 meeting at McGill University, Montreal; (b) Plenary Lecturer Prof. Joel Bernstein explaining details of polymorphism to the audience at CEMWOQ-5 and (c) one of the breathtaking sights from the Sagamore 2018 Conference held in Halifax, Nova Scotia.
Photo credit: (a) and (c) Krešimir Molčanov, Ruđer Bošković Institute.

this meeting can be found at the webpage: **http://friscic.research.mcgill.ca/CEMWOQ5.html** .

We are all looking forward to the sixth meeting in the series, which will apparently be organized just before the next year's **Canadian Society for Chemistry** (**CSC**) annual meeting, in May 2019 at Concordia University.

This year's **9th Canadian Chemical Crystallography Workshop** (**CCCW18**) was organized at Edmonton, Alberta, from 22-26 May 2018 as a satellite meeting of the **101st CSC Annual Meeting**. The speakers have included M. Ferguson, Bob McDonald, Arthur Mar, Anton Oliynyk (University of Alberta), Paul Boyle (Western University), Jim Britten (McMaster University), Charles Campana (Bruker AXS), Louise Dawe (Wilfried Laurier University), Brian Patrick (University of British Columbia) and Horst Puschmann (Durham University). I was told that the workshop addressed a wide range of topics, from foundations of crystallography to crystal growing and advanced structure solution techniques. More on this meeting can be found on the webpage: **https://xtallography.ca/index.php/xtal/meetings/cccw18/program-2/** .

This year, Canada was also the host for the **19th Sagamore 2018 Conference on Quantum Crystallography**, which was held from 8 to 13 July 2018 in Halifax, Nova Scotia. The Conference Chairs were **Chérif Matta** (Mount Saint Vincent University) and **Paul Ayers** (McMaster University) and I was told by one of the international participants (Krešimir Molčanov, Ruđer Bošković Institute) that it was an excellent match of super science and breathtaking views. More on this meeting can be found on the corresponding web address: **http://www.sagamore2018.ca/** .

Finally, Summer 2018 also saw the **8th Annual CLS Mx Data Collection School** held from 4 to 8 June 2018, at the Canadian Light Source in Saskatoon. It was an intense 5-day hands-on synchrotron data collection school, with lectures and experiments in macromolecular crystallography, featuring **Brian Mark** from the University of Manitoba as the Invited Speaker who guided participants through structure solution techniques. More information on this meeting can be found at: **https://cmcf.lightsource.ca/school/mxschool/** .

This highlight would not be complete without highlighting some of the activities of our **Canadian National Committee for Crystallography** (**CNCC**) which has awarded the first crop of **Larry Calvert Travel Awards**. These awards, first announced on 1st April 2018, have assisted the participation of Canadian students, postdoc and researchers at crystallography-related conferences, such as the Macromolecular Crystallography Workshop at CLS and the ACA Annual Meeting in Toronto. More information on the Larry Calvert fund, including eligibility and upcoming deadlines, can be found on the webpage: **https://xtallography.ca/index.php/student-funding/63-2/** .

More details on the mission and activities of the CNCC, as well as on recent or upcoming crystallography meetings in Canada can be found on the webpage organized and maintained by Louise Dawe of Wilfrid Laurier University: **https://xtallography.ca/** .

As is customary in this column, I would also like to highlight some of the top researchers in Canada, and this time it will be **Matthew J. Harrington**, who recently joined the Department of Chemistry at McGill University. Harrington is a rising star, working at the interface of structural chemistry, chemical biology and materials science. His growing research group at McGill University (Figure 2a) is using a plethora of advanced materials characterization techniques, including a range of methods based on X-ray diffraction, to tackle critical questions in biological materials science. He

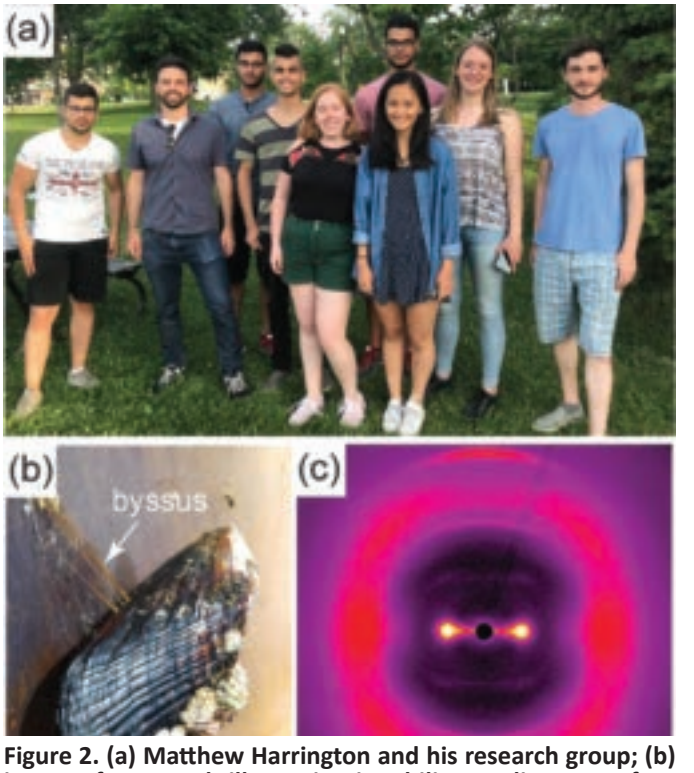


Figure 2. (a) Matthew Harrington and his research group; (b) image of a mussel, illustrating its ability to cling to surface using the byssus, a set of tough, self-healing fibers and (c) X-ray diffraction image of the mussel byssus thread.

obtained a Bachelor's degree in biological sciences at University of Delaware (2002) and, after a year in industry, he performed doctoral work with Prof. J. H. Waite at University of California Santa Barbara (2008), focusing on biochemical characterization of proteins comprising biopolymeric materials. This was followed by a prestigious Alexander von Humboldt postdoctoral fellowship at the Max Planck Institute of Colloids and Interfaces (MPIKG) – a highly renowned German institute at the forefront of research on biogenic and bio-inspired materials. Before beginning his current position as an Assistant Professor of Green Chemistry at McGill University in 2017, Harrington led his own

research group for seven years in the Biomaterials Department at the MPIKG, integrating his expertise in biology, chemistry and materials science into a focused research program aimed at elucidating structure-function relationships in protein-based biological materials. Here, I would like to highlight his two recent contributions, both published in the high-impact journal *Nature Communications*. Specifically, *Nature Commun.* **2017**, *8*, 974 investigates an exciting biological model system for circular materials processing: it elucidates a novel, unprecedented fiber assembly mechanism by which a fluid suspension of lipid-protein nanoglobules found in the velvet worm slime can be reversibly formed into highly stiff, polymeric fibers by simple mechanical drawing. While dissolving fibers in water leads to the re-formation of nanoglobules, the fibers can be re-drawn from this solution, presenting excellent potential to use such biological self-assembled systems in the design and development of new ways to make materials.

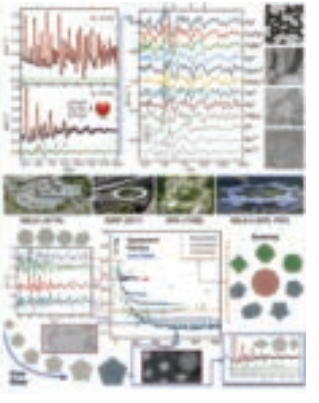
The second communication, *Nature Commun.* **2017**, *8*, 14539, presents a fascinating study of how marine mussels self-assemble tough and self-healing biopolymeric fibers with complex structural organization and function. The study is multi-faceted and interdisciplinary, relying on the use of a wide range of techniques, including a novel combination of traditional histological tissue staining and cutting-edge confocal Raman spectroscopic mapping. The focus of the study was the mussel byssus (Figure 2b,c), a collection of tough and self-healing fibers that glue mussels to rocky surfaces in seashore habitats. As Matthew noted, the mussel has emerged as a key role model in the development of bio-inspired self-healing polymers, underwater glues, surgical adhesives, and this study has provided critical new information concerning self-assembly mechanisms behind such functional behavior.

For those that would like to learn more or get involved in Harrington's line of research, he is co-organizing the second conference on **Mechanochemistry and Mechanobiology**, to be held in Montreal on July 29-31, 2019. More can be found on the conference webpage:
https://www.mcgill.ca/mechanochembio/ .

So much for this Summer's update on crystallography in Canada. As always, please feel free to contact me on my e-mail address, **tomislav.friscic@mcgill.ca**, with any comments, critiques or suggestions of topics, events or people that you think should be highlighted in this column. Keep warm this Winter!

Tomislav Friščić

What's on the Cover



The **Bertram E. Warren Award** for 2018 was presented to **Simon Billinge**, Professor of Applied Physics, Applied Mathematics and Materials Science, Columbia University, at the ACA Annual Meeting in Toronto in a ceremony following his award lecture. The 2018 Warren Award Committee consisted of: Lawrence Marks (Chair), Louise Dawe, Paul Langan, and Brian Toby.

The cover image depicts recent work done by Simon and his student, Soham Banerjee to create a highly automated database infrastructure for obtaining the core structures of metallic nanoparticles, called ClusterMining. PDFs obtained from high quality synchrotron x-ray data from different sources may be compared to computer calculated PDFs from algorithmically generated metallic nanoparticle cores to find the best fitting structural candidates from among hundreds to thousands of candidates computed from among dozens of cluster families.

The Award was established in 1970 by students and friends of Professor B. E. Warren on the occasion of his retirement from the Massachusetts Institute of Technology. It recognizes important recent contributions to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques. Works published within a six-year period ending June 30 of the year preceding the Award may be nominated. A monetary award, travel expenses to accept the award at the ACA Annual Meeding, and a certificate are awarded every third year.

The cover image was created by Soham Banerjee (Columbia University). Transmission Electron Microscopy (TEM) images of metallic nanoparticles were collected in the group of Christopher Murray (Department of Chemistry, University of Pennsylvania). Adapted with permission from Doan-Nguyen, V. V. T. et al. *ACS Nano 8*, 6163–6170 (**2014**). Copyright 2014 American Chemical Society; Unpublished images courtesy of Jennifer Lee. The HRTEM image of a representative metallic nanoparticle is from Yang, H. *et al.*, *Nat. Commun. 7*, 12809 (**2016**). Adapted under license CC BY 4.0. The TEM image of metallic nanowires is adapted with permission from Liu, H., Koenigsmann, C., Adzic, R. R. & Wong, S. S., *ACS Catal. 4*, 2544–2555 (**2014**). Copyright 2014 American Chemical Society.

Connie Rajnak

2018 ACA Fellows

Andrew J. Allen

Andrew Allen's research on truly difficult materials, many used in construction such as cement and surface coatings, beautifully demonstrates the impact that basic research can make on unsolved technical problems. One example is his investigation of the microstructure of cement pastes, complex mixtures of mineral and gel phases. Answering the important questions regarding in-service properties of such materials requires that one understand and quantify the relationship between the many phases that are present and water. Many years of work resulted in a highly-cited 2007 Nature Materials paper – the first one on cement to appear in this journal - in which he successfully defined the chemically active gel surface area within the cement paste.

In his earliest work, Andrew focused on both the development of a small-angle neutron scattering instrument and its application to complex problems in materials science. He is now Physicist at the National Institute of Standards and Technology (NIST) in the Materials Measurement Science Division. His approach to the characterization of complex microstructures continues to combine neutron scattering, x-ray scattering and imaging with the insightful development of quantitative analysis methodology.

His professional service to the scientific community has been extensive and excellent. His broad base of knowledge has made him a journal editor many times over. Currently he is one of three Main Editors for the Journal of Applied Crystallography and has recently been a Guest Editor for a Special Issue on Neutron Instrumentation and for the SAS2015 Special Issue. In 2002 he became a member of the IUCr Commission on SAS (CSAS) and served as Chair from 2011-2014 and, since 2014, as a consultant to the CSAS. Another major role he has played has been in the development of reference materials for small-angle scattering. His service to the American Crystallographic Association includes serving as Chair of the SAS Special Interest Group.

Andrew is among the leading experts in the analysis of structure and microstructures of inhomogeneous materials. His scholarly work has represented breakthroughs in technologically and economically important research fields and his service to the international crystallographic community as an editor and Commission Chair are just two of the indications of the immense impact he has had in the scientific community.

Kay Onan

James F. Britten

James Britten has made major contributions to crystallography in Canada and abroad by his many professional activities. Jim looks forward. He is generous with his time and expertise, especially as it relates to the teaching of the next generation of structural scientists and using his scientific vision to help expand technical possibilities for his colleagues.

Jim is currently the Manager and Scientific Director of the McMaster Analytical X-Ray (MAX) Diffraction Facility for the Chemistry and Chemical Biology Department and the Brockhouse Institute for Materials Research. Besides providing x-ray diffraction assistance, Jim provides access to synchrotron data collection, as necessary. In fact, he was the Principal Investigator for the Small Molecule Crystallography Beamline Proposal at the Canadian Light Source (CLS) and is currently a member of the Canadian Institute for Synchrotron Radiation.

ACA Fellows

The ACA Fellows program recognizes a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of cyrstallography and science. The program celebrates the excellence of ACA members, and promotes their recognition worldwide to constituencies outside of the ACA. ACA Fellows serve as ambassadors to the broader science community and the general public to advance science education, research, knowledge, interaction, and collaboration. This program allows the ACA to significantly recognize and honor a broader cross-section of the membership than was previously possible with other, more specific awards. Nominations are collected year-round with the deadline being April 1 of each year.

Besides the management and maintenance of this facility, Jim teaches graduate courses on crystallography and on 2D/3D powder diffraction techniques. His interest in spreading knowledge of crystallography is exemplified by his founding, in 2009, of an intensive, multi-day workshop called the Canadian Chemical Crystallography Workshop that he continues to organize annually. This kind of teaching has effects that will ripple into the future. His teaching knows no earthly bounds; in 2016 he was invited to be an instructor at a Committee on Space Research international school entitled Crystallography for Space Sciences.

Jim's service to the scientific community can be seen in his many professional activities. He was Chair of the Canadian National Committee for Crystallography (2010-2015), Chair of the Canadian Division of the American Crystallographic Association (ACA) (2003-2006), Canadian Representative on the ACA Council (2008-2010) and program chair for the 2009 ACA meeting in Toronto. He has also taken roles in the three most recent International Union of Crystallography (IUCr) congresses. He was on the International Program Committee for the 2011 and 2017 IUCr congresses and he was the Chair of the International Program Committee and Local Chair for the 2014 IUCr Congress in Montreal.

At the beginning of his career Jim received a Killam post-doctoral fellowship. One of the criteria was that "A Killam scholar should not be a one-sided person…" Jim has shown by his many contributions, scientific and professional, that he is not one-sided but rather looks to the future, teaching the next generation, utilizing new technologies and engaging with the entire world.

Kay Onan

Majed Chergui

Majed Chergui is a leader of the chemical physics research community for his work utilizing ultrafast spectroscopies to study the dynamics of a variety of chemical and biological systems as well as solid-state materials. He was educated in Paris, France, studying math and physics and, in 1987-1988, he was an Alexander von Humboldt Fellow at the Freie Universitat Berlin, Germany. He is currently Professor of Chemistry and Physics at the Ecole Polytechnique de Lausanne (EPFL), Switzerland, and has been a Professor of Experimental Condensed Matter Physics at the Universite de Lausanne and Guest Professor at both the National University of Quilmes-Bueno Aires, Argentina, and at the Max-Born-Institut and Helmholtz-Zentrum, Berlin, Germany. He is also currently the head of EPFL's Laboratory of Ultrafast Spectroscopy.

Majed's leadership in the field of ultrafast structural studies is evidenced by his being invited to write a review article on the topic (Picosecond and femtosecond X-ray absorption spectroscopy of molecular systems, *Acta Cryst.* **2010**, *A66*, 229-239) as well as his chairing many conferences and committees on the topic. He has played a prominent role in the utilization of synchrotron facilities and, more recently, free-electron lasers in his cutting-edge ultrafast dynamics research.

The respect that others have for Majed's research is reflected in his many prestigious awards, including the Rammal Medal of the Euroscience Foundation (2007), the Humboldt Research Award (2009), the Kuwait Prize for Physics (2010), the Plyler Prize of the American Physical Society (2015) and the Edward Stern Award of the International X-ray Absorption Society (2015). He is also a Fellow of the Royal Society of Chemistry.

Given his research, it is no surprise that he was an early and strong supporter of the concept of the ACA journal, *Structural Dynamics*. He became its Founding Editor-in-Chief and was instrumental in putting together an excellent advisory board and slate of associate editors. He was a leader in the development of the journal and has worked tirelessly to make the journal a success. Majed recognized early on that the journal provided a great opportunity for the ACA to be directly involved in subject areas of prime importance and growth to the Association.

Majed is a superb spokesman and dynamic ambassador for science. Fluent in seven languages and possessed of unusually wide-ranging interests, he is a true "citizen of the world."

Kay Onan

Wladek Minor

Wladek Minor holds the Harrison Distinguished Professorship in the Department of Molecular Physiology and Biological Physics at the University of Virginia. His work comprises both structural biology and methodology development. He is perhaps best known for the development of Scalepack, the analysis software which, combined with Zbyzek Otwinowski's DENZO, formed the basis of x-ray data reduction for over 90% of structures deposited in the Protein Data Bank (PDB) during the 1990's. He is co-author (with Z. Otwinowski) of a *Methods in Enzymology* article on processing of x-ray diffraction data that ranked as the 23rd most cited paper ever in the 2014 Nature analysis. Later he developed the integrated system HKL3000 for protein structure solution, refinement and interpretation. This software was one of the first user-friendly and comprehensive integrated packages available for this purpose.

Several other programs, dedicated to various stages of crystal structure solution and interpretation, were created in Wladek's laboratory and made available to the community. Two practical examples are CheckMyMetal and CheckMyBlobs which have proved helpful in the interpretation of metals and small molecule ligands in electron density maps.

Wladek has been a key contributor to the field of structural genomics, working with several structural genomics consortia whose general missions are "to rapidly determine the structures of strategically selected and biomedically important targets…" One of his contributions is the development of an integrated database system that is among the very most well-developed in the structural genomics field. While his nominal role in the NIH structural genomics centers has been database development and management, his own laboratory has contributed an amazing 512 depositions to the PDB. During the last several years Wladek has been one of the major contributors to efforts aimed at maintaining the highest quality of crystallographic structures and of the resulting publications. To this end, Wladek's laboratory has carried out many detailed analyses of structures in the PDB.

Serving the crystallographic community has been important to Wladek. Since 2014 he has served as a US representative on the Commission of Biological Macromolecules of the IUCr and in 2017 became its chair. That year, he also became a member of the IUCr Data Committee.

Kay Onan

Thomas Proffen

Thomas Proffen has been a leader in the development of what has become known as the Pair Distribution Function (PDF) scattering technique. However, his early work involved single-crystal work

on disordered materials. At that point he entered into a long-term collaboration with Reinhard Neder to develop a software package (DISCUS) to simulate disordered systems. He was interested in making the software accessible and useful to a large body of scientists so he and Neder promoted it at workshops and at national and international conferences. The package has matured and is widely used by a broad cross-section of scientists.

Moving to Michigan State University to work with Simon Billinge, Thomas became involved with the embryonic PDF work. At this time, Billinge and Egami had figured out the fundamentals of PDF analysis of disordered crystalline materials but it was something that only they could apply since there was no software available to the community. Thomas took the opportunity to develop software that non-experts could use to carry out this type of analysis (PDFFIT, predecessor to the current PDFGui). He was one of a few people who started organizing sessions on PDF-related science at ACA meetings. In large measure because of his early and sustained conference organization efforts, the ACA is the home for structural science on locally ordered, disordered and even amorphous materials.

Next Thomas moved to the Lujan Center at Los Alamos National Laboratory where he was responsible for upgrading the neutron powder diffraction (NPDF) instrument. He continued to grow the PDF community and focused on developing user-friendly software to simplify the process of determining a pair distribution function from a neutron diffraction powder diffraction.

He is currently Director of the High Performance Computing and Data Analytics Science Initiative of the Neutron Science Directorate at Oak Ridge National Laboratory. He was previously the Neutron Data Analysis and Visualization Division Director and Group Leader for Diffraction there. His research interests are at the cutting-edge overlap between structural characterization and theoretical modeling of materials.

Thomas has contributed to the ACA and IUCr by serving on a variety of committees and commissions and was the Chair of the Neutron Scattering ACA SIG. He has served the scientific community by being an editor of Zeitschrift for Kristallographie and co-editor of the Journal of Applied Crystallography. In addition Thomas mentors middle-school girls interested in computer science and was the founder and director of the nonprofit Oak Ridge Computer Science Girls.

Thomas has contributed to science by his research; his providing, and teaching about, software that is user-friendly; and developing a STEM mentoring program for young girls.

Kay Onan

Janet L. Smith

Janet Smith is a distinguished structural biologist who has provided leadership in the development of macromolecular crystallography in ways that have had a major impact worldwide. Her belief in the importance of structure in biology originated while working with her PhD advisor, M. Sundaralingam. She pursued this growing interest in protein structure by joining Wayne Hendrickson at the Naval Research Laboratory as a National Research Council Research Fellow. She then moved to Columbia University and held positions as associate research scientist in the Hendrickson lab and as associate research scientist at the Howard Hughes Medical Institute.

Janet moved to the Department of Biological Sciences at Purdue and established her own research program in structural biology. Here her interest in the crystallographic phase problem and the relatively small anomalous effect caused her to become interested in accurate X-ray diffraction data collection. This led to her accepting a position of Director of the Collaborative Access Team for NIGMS and NCI at the Advanced Photon Source (APS) synchrotron at the Argonne National Laboratory. In 2012 she became Scientific Director of NIGMS & NCI beamlines at the APS, a position she continues to hold. Janet has been very effective in improving the facilities available for structural biologists. For instance, she was responsible for developing micro-crystallography beamlines enabling many data sets to be taken with a single crystal. The beamline she directs is arguably the best protein crystallography beamline in the world providing a very small, intense beam for the study of very small crystals using single wavelength or multiple wavelengths anomalous dispersion. Her work there has had an impact on the scientific lives of thousands of crystallographic scientists from around the world.

In 2005 Janet moved to the University of Michigan as Professor of Biological Chemistry and Director of

the Center for Structural Biology in the Life Sciences Institute (LSI). The University recognized her by appointing her to the prestigious Martha L. Ludwig Professorship of Protein Structure & Function where she provided an outstanding role model for young aspiring women crystallographers, as had Martha. In 2013 she was named Margaret J. Hunter Collegiate Professor at the LSI.

Besides her very strong publication record in top journals, Janet has been an outstanding citizen of crystallography. Her deep knowledge of structural biology ranging from methods development to structural biology to functional analysis, combined with her wise persona, has made her very effective on a broad range of policy committees. As an example, she took a key role in helping to develop the recommendations for how best to validate structures determined by x-ray crystallography for use by the Protein Data Bank.

Janet's abiding interest in analyzing the mechanisms of enzymes using crystallography and her leadership at the APS to aid in data collection, along with her contributions on many national committees shows her to be a great contributor to the crystallographic community. *Kay Onan*

Robert B. Von Dreele

Robert Von Dreele's research illustrates the fearlessness with which he approaches science. He carried out ground-breaking experimental work demonstrating that superb powder diffraction data could be obtained from protein diffraction data. His deep insight into what was possible with the relatively limited data provided by powder diffraction combined with his amazing code development skills resulted in the first solution and refinement of a protein structure using powder diffraction data.

Bob, who is currently Senior Scientist at the Advanced Photon Source (APS) at Argonne National Laboratory, completed his PhD work at Cornell with a specialization in inorganic chemistry and an interest in crystallography. He joined the faculty at Arizona State University and, within a year, took a leave and went to the Inorganic Chemistry Laboratory at Oxford University where he began his pursuit of powder diffraction crystallography. This event has proved to be a great benefit to the crystallographic community. After a decade at ASU, he moved to Los Alamos National Laboratory to pursue his interest in neutron scattering and its use with powder diffraction. He designed and constructed the High Pressure Preferred Orientation (HIPPO) powder diffractometer. After 17 years, he moved to Argonne National Laboratory where he co-authored the proposal that funded the APS 11 – BM powder diffractometer, an instrument that has revolutionized the use of synchrotron powder diffraction.

Perhaps Bob is best known for his creation of the General Structure Analysis System (GSAS) software package, initially co-authored by Allen Larson, that can be used for analysis of both neutron and x-ray powder diffraction data. Bob, working with Brian Toby, has continued to develop this package. GSAS-II is now used by much of the powder diffraction community for data reduction, powder diffraction indexing, parametric fitting, structure determination, and small-angle scattering reflectometry.

An important aspect of Bob's contribution to the ACA was his service as Vice-President, President and Past-President. He has served as local organizer, has organized conference sessions and has been an instructor at numerous powder diffraction data analysis workshops. He is also a regular contributor to the ACA Summer School. He was elected to the US National Committee for Crystallography. Bob received the 2009 Barrett Award from the Denver X-ray Conference and the 2013 J.D. Hanawalt Powder Diffraction Award from JCPDS – International Centre for Diffraction Data.

Perhaps less known but arguably the most important part of Bob's contribution has been his educational outreach. He almost never declines an invitation to teach at a workshop or tutorial and he is always ready to answer questions from other scientists whether in person or via e-mail – and people know this so he is constantly answering questions or discussing others' issues.

Not only has Bob played a major, pioneering role in developing the powder diffraction crystallography instrumentation and methodology used around the world, he has contributed greatly to the ACA and the wider scientific community. *Kay Onan*

Andrew Allen Appointed as Editor-in-Chief of IUCr Journals

Andrew Allen will begin his new duties as Editor-in Chief of the International Union of Crystallography journals in mid-September 2018. He has been called an "editor's editor." He has served on the Editorial Board of the Journal of Applied Crystallography (JAC) since 2002 as a Co-editor (2002-2013), Deputy Editor (2011-2013) and as a Main Editor (one of three) from 2013 to the present. During this time he was one of the Conference Issue Co-editors for the SAS 2006 Conference (2006-2007) and since then has taken a leading role as Guest Editor for several Special Issues, specifically the SAS 2012 (2012-2014) and SAS 2015 (2015-2016) Special Issues and currently the Neutron Instrumentation Special Issue. Previously, from 1991 – 1996, Andrew served on the editorial board of the Journal of Physics: Condensed Matter.

Through his editorial work, and despite challenging times for all scientific research journals, Andrew has continued to strive to raise the publication standard and reach of JAC to meet the needs of authors and readers alike, across the whole range of applied crystallography. He will no doubt bring these qualities of leadership and optimism, as well as his well-developed judgement in matters of scientific publishing, to his new, broader role.

Andrew's excellence in scientific research and service to the crystallographic community has been noted in his being named an ACA Fellow (*vide supra*).

Kay Onan

ACA Judy Flippen-Anderson Structural Dynamics Poster Prizewinner at ECM 31

Przemyslaw Nogly

The 31st European Crystallographic Meeting (ECM31) was held in Oviedo in Asturias, in the north of Spain. A judging panel was convened for this poster prize comprising John R Helliwell (Chairman), Ana Gonzalez, Andrey Kovalesky, Anders Madsen and Brent Nannenga. The winner was Dr. Przemyslaw Nogly of the Institute for Molecular Biology and Biophysics, Zürich with the poster entitled "Retinal isomerization in bacteriorhodopsin captured by a femtosecond X-ray laser".

John Helliwell

ACA member elected Fellow of the American Academy of Arts and Sciences

In April 2018, election of **Helen Berman**, Board of Governors Distinguished Professor Emerita of Chemistry and Chemical Biology at Rutgers University as a Fellow in the American Academy of Arts and Sciences was announced. Founded in 1780, the American Academy of Arts and Letters is one of the oldest academic societies in the United States. It admits leaders in the humanities, arts and education as well as science, engineering, and technology. Among the Academy's Fellows are more than 250 Nobel Laureates and 60 Pulitzer Prize winners.

Ed Stevens

2018 Margaret C. Etter Student Lecturer Awards

BioMac	**Jessica Thomaston, UC San Francisco**	**Materials Science**	**Juby Varghese, Clarkson U**
Canadian	**Raúl Castañeda, U Ottawa**	**Neutron Scattering**	**Stephanie Gnewuch, U Maryland**
Cryo-EM	**William Thomas, Princeton U**	**Powder Diffraction**	**Matthew Logan, U Central Florida**
Data Analysis & Archiving	**Maxwell Day, U Manitoba**	**Small Angle Scattering**	**Maxwell Watkins, Princeton U**
General Interest	**David Moreau, Cornell U**	**Small Molecule**	**Cara Vennari, UC Santa Cruz**
Industrial	**Luzia Germann, MPI Stuttgart**	**Service Crystallography**	**Seth Cory, Texas A & M U**
		Young Scientist	**Emilia Arturo, Fox Chase Cancer Center**

New ACA website to "go live" in October

Kristin Stevens

Photo by Richard H. Bromund

Many members and ACA Council requested a new website. The primary complaints were that the old site was dated and confusing. Furthermore, many members were looking for a more in-depth membership experience that allowed for a way to manage membership, contact information and contacts online. Thanks to all those who donated to the website redesign fund!

We were excited to discover that a member management system (MMS) offers a cost-effective website design/hosting service as well as a member management portal. This created a wonderful window of opportunity that the ACA excitedly took advantage of. After I researched a dozen different solutions and made a recommendation, the ACA Council chose MemberClicks.

With MemberClicks the new site will be streamlined and organized. It will allow our members to autonomously control their preferences and contact information. The portal will allow members to access "members only" pages and communication tools. It will increase the ability of the SIGs and committees to host and encourage communication. It will automate the dues process, streamlining things for not only our members, but ACA headquarters as well.

I feel confident in saying that this is probably the biggest change the ACA has implemented in a number of years. It will take the cooperation of MemberClicks, ACA headquarters and ACA members. Transitioning to the new MMS is not complicated; however, we do expect that there will be a few bumps along the way and we ask for patience from the membership during the move. Here at the Buffalo office Kristina Vitale and I are ready to assist members with their new logins and any questions or problems that might come up.

Currently the site is scheduled to be launched in October of 2018. We are very excited and believe that this transition will benefit our members tremendously.

Kristin Stevens

ACA History Project News

Simon Billinge (Columbia University and Brookhaven National Laboratory) received the Warren Award at the Toronto meeting. Billinge emphasized that studying and designing modern materials requires going beyond single-crystal studies. He characterizes nanocrystalline materials using powder diffraction, capturing both the Bragg peaks and the diffuse scattering; he analyzes the total diffraction using the atomic pair distribution function – he calls this "crystallography for the 21st century" – to obtain information on the local order in the material.

Image credit: Richard H. Bromund.

As Billinge pointed out, **Bertram Eugene Warren** (1902-1991) was a pioneer in the study of non-crystalline materials. Early in his career at MIT he became interested in the short-range order in glass, carbon black, and binary alloys, and he found that diffuse scattering gave the information he sought. Warren famously said, "As with humans, it is the deviations from regularity that are more interesting." This comment could apply not only to the non-crystalline or disordered materials he was studying but also to the non-Bragg diffraction intensities that turned out to be so useful in studying these materials. He was also known as a meticulous and caring teacher.

Emilio Segrè Visual Archives, Physics Today collection.

The late **Judith Flippen-Anderson** left the ACA a treasure trove of photographs. Do you enjoy looking at historical pictures from meetings and conferences and recalling ACA friends? If so, you are in for a real treat and also an opportunity to play an important role in the ACA History Project. Thanks to Paul Anderson, we now have access to hundreds of photos that document decades of ACA history. The photo of Clara Shoemaker to the right is one example.

Clara Brink Shoemaker (1921–2009). For more about Clara Shoemaker, see her obituary on the ACA History page https://bit.ly/2BIk9GV.

The people in most of the photos are not identified. In order to make this important database searchable, please contact me to volunteer to look at part of Judy's collection and to identify as many of the people as possible. Below are some samples for your enjoyment. (There will be a prize for the person who correctly identifies the most people in both of these photos. Extra credit for knowing the place and date.)

Virginia Pett
pett@wooster.edu

2018 Margret C Etter Early Career Award to Jason McLellan

Jason McLellan receives Etter Early Carrer Award from Lisa Keefe.

The McLellan lab is part of the Molecular Biosciences Department at the University of Texas at Austin. They are interested in elucidating the molecular mechanisms of host-pathogen interactions, particularly those involving viral glycoproteins. The synergy that exists between basic and translational science is exploited - for example the determination of structures and the development of tools needed to answer basic science questions can be translated into therapeutic interventions that can be used to illuminate biological processes.

Before beginning the discussion, some conflicts of interest are: 1) the lab is an inventor on patents related to prefusion RSV (respiratory syncytial virus) F and its uses; 2) the lab is an inventor on patents related to RSV prefusion F-specific monoclonal antibodies and camelid nanobodies; 3) the lab has received funding from Janssen and Medimmune for projects related to prefusion RSV F and monoclonal antibodies; and 4) the lab consults for MedImmune.

Pneumoviruses cause substantial morbidity and mortality in infants and the elderly; RSV is responsible for 6.7% of all-cause global mortality in children 1 month to 1 year of age.[1] Human metapneumovirus (hMPV) is a leading cause of hospitalizations in the US; for adults ≥ 50 years old rates are similar to RSV and influenza, and for children < 5 years of age, rates are similar to influenza.[2,13] Seropositivity to RSV and hMPV is universal after early childhood and reinfection throughout life is common[2].

Prophylactic RSV treatment with the humanized murine monoclonal antibody Synagis® reduces hospitalization in high-risk infants.

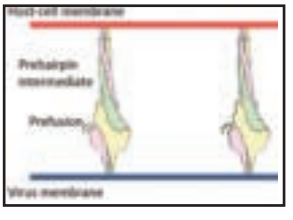
MED18897 is a potential once-per-season prophylactic anitbody.Although a few RSVb strains are less sensitive to MED18897 there is a structural basis for enhanced potency and reduced sensitivity of MED18897.[4] Prefusion-specific antibodies are extremely potent.

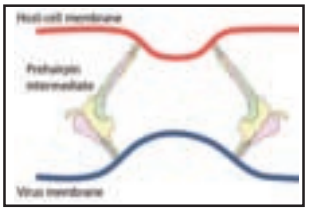
RSV and hMPV belong to the Pneumoviridae (non-segmented ssRNA (-)) family.

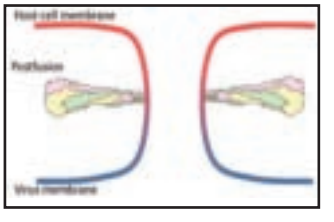
Genus:	Orthopneumovirus	Metapneumovirus
	Human RSV	Human metapneumovirus
	Bovine RSV	Avian metapneumovirus
	Murine pneumonia virus	

RSV and hMPV F glycoprotein is required for virus entry. F is a class 1 fusion protein which is synthesized as a single-chain inactive precursor, F 0. The N- and C-termini of the RSV F_1 undergo a dramatic conformational rearrangement.[5,7,8,9] F1 contains the 4 elements needed to promote fusion: fusion peptide, HRA, HRB, and transmembrane domain. Interfering with any stage of the fusion process blocks viral entry. Metastability leads to refolding of prefusion RSV F. It may also be triggered.

Collapse of the prehairpin intermediate brings the two membranes into close proximity. Membrane fusion occurs as F adopts the extremely stable postfusion conformation. A disulfide bond, cavity-filling mutations and foldon stabilize the soluble ectodomain in the prefusion state.[6]

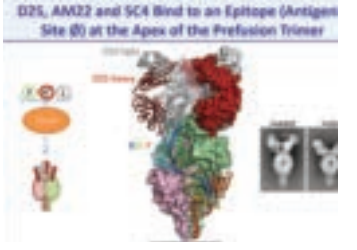


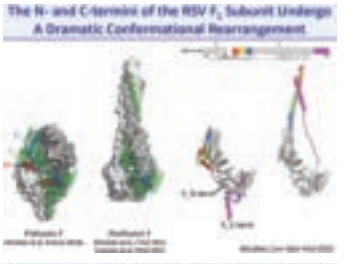


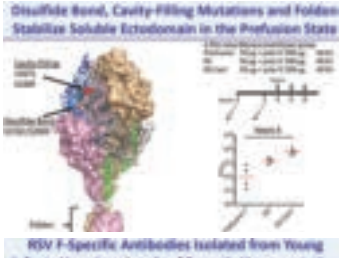


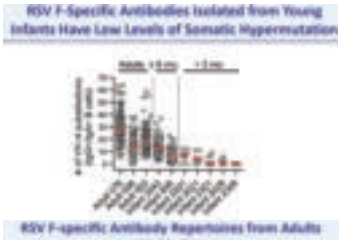
RSV F-specific antibodies from adults are highly diverse, bind to prefusion F[10,11], and are neutralizing. Site III-directed antibodies preferentially recognize PreF and are neutralizing.

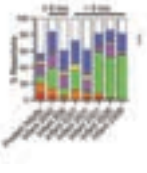
RSV F ΔFP adopts the postfusion conformation and elicits neutralizing antibodies in mice.[5,6] The most potent are PreF-specific.[10] They do not require SHM to potently neutralize RSV.

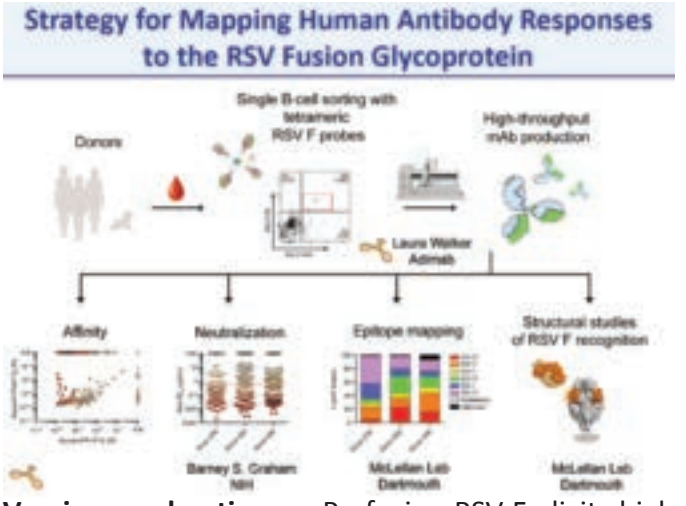












Vaccines and antigens: Prefusion RSV F elicits high titers of neutralizing antibodies. To date, postfusion F-based antigens have not fared well in clinical trials. hMPV F can be stabilized in the prefusion conformation using strategies that worked for RSV F. Initial mouse experiments suggest that prefusion and postfusion hMPV F elicit similar neutralizing antibody titers.

Antibodies: Natural infection with RSV induces clonally diverse antibody repertoires in adults, but more restricted repertoires in infants. Antibodies that target sites Ø and v are the most potent; (vaccine antigens should contain these sites, particularly for pregnant women or elderly populations). RSV neutralization does not require somatic hypermutation. Infants may benefit from age-specific RSV vaccination strategies that focus on antigenic site III.

Small molecule RSV Fusion inhibitors comprise diverse compounds isolated by many companies in the early 2000s which have been screened for neutralization of RSV infection of immortalized cells. These compounds were potent when administered prophylactically. Two fusion inhibitors cross-link the F1 subunit.[14] The crystal structure of TMC-353121 bound to HRA-HRB peptides confirmed the predicted binding mode.[15] All of the resistance mutations are clustered together in the prefusion conformation. Resistance mutations for fusion inhibitors are found in 3 regions of F_1: fusion peptides F1401, L141W, G143S, and V144A; the cysteine-rich region: D392G, K394R, S398L, K399I, and T400A/I; and HRB (D486N/E, E487D, F488I/V, and D489Y). The HRA-binding site doesn't explain mutations in the fusion peptide or cysteine-rich regions. Crystal structures reveal a single small molecule bound in the PreF cavity on the trimeric 3-fold axis[16]. Inhibitors are antagonists that stabilize the prefusion conformation. RSV F is expressed on cells, inhibitors are added and then they are heat-shocked at 55° C[16]. The internal fusion peptide location suggests a druggable target for both orthomyxoviruses and pneumoviruses.[17] All small-molecule RSV fusion inhibitors likely utilize the same binding mode.[18]

Concluding remarks: Structural biology has made a major impact on the development of vaccines, antibodies, and small molecules against RSV. The McLellan lab, as well as others, are now using these reagents as tools to answer fundamental questions about RSV biology, with particular regard to cell entry. Lessons learned from work on RSV are now being applied to other viral pathogens, such as coronaviruses and hMPV.

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Connie Rajnak

"Well, to be perfectly honest, we weren't going to revive you.

However, the rest of your species is extinct, and we are in desperate need of someone to throw us a stick."

Courtesy of Nick D. Kim, an analytical environmental chemist who currently works for Waikato Regional Council. He is an honarary lecturer at the University of Waikato in New Zealand.

ACA Toronto 2018
Notes – From the Program Co-Chairs

The 2018 ACA annual meeting was held in Toronto, Canada, this year. We started off as usual with a day of workshops before the opening ceremonies and reception. We were excited that the workshops were very well attended and hope that the trend continues!

Left to Right: Gerald Audette, John Polanyi, and Tiffany Kinnibrugh.

Our plenary speaker to open the meeting was Professor John Polanyi, Nobel Laureate and University Professor in the Department of Chemistry at the University of Toronto. The title of his talk was "Order in Crystals, Order in Society". Prof. Polanyi gave a lively and engaging lecture, starting with his personal and scientific recollections of Max von Laue and Sir William Lawrence "Willie" Bragg. He presented recent work into some studies they are currently engaged in exploring reaction dynamics at surfaces and a novel way of aiming colliding molecules at one another across crystalline surfaces. Prof. Polanyi concluded his talk with a "call to arms", that is how we as scientists can engage the public with our passion and excitement for science, and through this engagement we can make a better and more peaceful world.

Buerger Award winner, Frank Hawthorne (left), and Warren Award winner, Simon Bilinge (right)

We would like to extend our congratulations to this year's award winners: Simon Bilinge (Warren Award), Frank Hawthorne (Buerger Award) and Jason McLellan (Etter Early Career Award); and to our incoming "Class of 2018" ACA Fellows (Andrew Allen, James Britten, Majed Chergul, Wladek Minor, Thomas Proffen, Janet Smith, and Robert Von Dreele).

New to the meeting this year was a session that was open to the public. This session was focused on science on the International Space Station (see the session review later in the meeting summary), and was hosted by CASIS. The first portion of the meeting included a series of more general talks targeted towards the students and general public in attendance. An extended coffee break allowed for our guests to engage with several of our vendors and the ISS folks who brought some VR gear to let us experience the ISS, if not first hand, then in virtual reality! The session continued with more research oriented talks after our guests left. Thanks to all for providing such a welcoming environment to the students and their families!

A meetup with coffee for family and friends accompanying conference attendees was held on the first day of the meeting. Thanks to Tina Rose, who helped coordinate sightseeing events for the families that attended, and for her help at the registration desk.

As at every meeting, our vendor exhibition and poster sessions were very well attended. Thanks to all the vendors for attending and contributing to making the meeting a success. We tried something a bit different this year, a vendor passport, to hopefully allow more attendees to engage with the vendors (even if just for the stamp). This year we had 7 vendors who joined in the fun; two winners were drawn from all submitted (complete) passports, with the prize of a small gift card of their choice. The two winners of our vendor passport draw were Prinsa Boonkon Haller and Joe Haller, a Mother-Son duo affiliated with the School of Chemistry, Suranaree University of Technology, Thailand. Very Nice! (We promise we didn't rig the draw). And we understand

Left to Right: Joe Haller, Prinsa Boonkon Hallrt, Gerald Audette.

that Joe convinced his Mom to let him spend their winnings on a VR setup from Nanome (one of the vendors); we think this is much better than a simple Amazon gift card!

Natasha Myers (center) with Gerald Audette and Tiffany Kinnibrugh.

Following 4 days of exciting scientific sessions, engaging posters, beverages and lively discussions, we gathered for the annual banquet. Our dinner speaker this year was Natasha Myers from York University, who gave an outstanding lecture examining how macromolecular crystallographers render three-dimensional, atomic-resolution of proteins not only by informed scientific data, but with a modeler's entire sensorium. Dr. Myers spoke about her time embedded in a macromolecular laboratory exploring the influence of crystallographers' gestures and intuition combined with scientific knowledge to develop protein models. She observed through the process of protein purification, crystallization, and structure determination that the scientists became the subjects of the molecules that they were working with; they were at the whims of the molecules. Her study is described in the book *Rendering Life Molecular: Models, Modelers, and Excitable Matter*, which received the 2016 Robert K. Merton Award from the Science, Knowledge and Technology Section of the American Sociological Association.

Dr. Myers delighted us with a story of how a crystallographer animated her body to describe a protein structure to a student; she would twist and strain her body to mimic the folding of the protein. She explained that as crystallographers gained experience, they could recognized the misshapen proteins with both the knowledge of bond angles, laws of chemicals and physics, molecule interacts with water, surface tensions, and their senses. A short interpretative film of how molecules move was shown to illustrate how scientists use their bodies to animate biological phenomena. Later on the dance floor, many attendees did their own interpretive dance of different molecules.

Following our dinner speaker, the Poster Prizes were handed out. Congratulations to all the winners on your excellent science and your presentation of it to everyone! We ended the evening with music and dance, courtesy of a local band, The Stringhoppers. A great way to end a meeting!

Andreea Gheorghita (right), U of Toronto, with Lynne Howell after receiving the award for the best Three Minute Thesis presentation.

A quick note on the meeting's metrics. This year's meeting had 663 attendees from 26 different countries! Thank you all for making the trip to join us for the meeting! We really do hope that you all had a productive and engaging meeting, and a wonderful time in Toronto.

Certificates of appreciation and gifts presented to Kristin Stevens and Kristina Vitale (right).

Thank you to Council for the opportunity (and trust) to organize the conference. Many thanks to all the session chairs for their hard work, to Louise Dawe and David Rose for their coordinating the Poster Sessions, Dick Bromund for photography, and to our student volunteers for their efforts. And of course a big thank you to Kristin and Kristina, our stalwart and dynamic duo at ACA HQ, for all their on-going help and encouragement for the meeting!

We look forward to seeing everyone again in 2019!

Gerald & Tiffany

(Photos by Richard H. Bromund)

2018 ACA Transactions Symposium: Shining a Light on Structure-Based Drug Discovery

The objective of this transactions symposium was to guide the audience through the current approaches to structure-based drug design from data acquisition, analysis all the way through to new technologies with exciting case study examples of application with a focus on drug discovery. **Steve Soisson**, Merck, set the stage for the symposium with an excellent overview of the history of "Rational Drug Design" demonstrating that the field has matured to a plateau of productivity that is represented by a plethora of clinical candidates and marketed drugs that owe their origin to structure-based drug design. The recent advances from how data are collected, the challenging targets we are now succeeding on such as membrane proteins and how new technologies such as cryo-electron microscopy and small angle X-ray scattering are now impacting how we leverage structure were described. Steve ended his introduction with a forward looking view of how we should be thinking about leveraging all the data we have assembled over the years and the potential of machine learning and artificial intelligence to improve our predictive power in the future.

Lisa Keefe, Industrial MacroMolecular Crystallography Association (IMCA), began the symposium with an exciting overview of one of the cutting edge beamlines for high-throughput crystallography specifically tailored to the needs of drug discovery. The description of the unique history of the IMCA consortium set the stage for what the critical considerations are for a beamline supporting drug discovery and how that translates into the strategy for the IMCA beamline. The key needs of the IMCA members are routine access, absolute reliability and high quality data. In addition, she compared and contrasted IMCA's need for effectively unlimited capacity and how that is a different paradigm than how traditional beamlines operate. The drive of the evolution of the IMCA beamline has been to meet these critical needs through operational efficiency, capacity with uncompromising reliability. The goal of this is to achieve a capacity of 1,000 data sets/day over the course of the next 5 years. IMCA has also expanded access to other beamlines during normal APS shutdown periods to ensure weekly access to robust data collection throughout the year and is beginning to offer access to other structural techniques such as small angle X-ray scattering to it's members. With this focus and strategy, IMCA has been able to sustain for more than 25 years and is well positioned to be a leading industrial beamline well into the future.

The next presentation by **Matthieu Schapira**, Structural Genomics Consortium, highlighted efforts to start to really mine and leverage the tremendous amount of structural data that has been accumulated in the public pdb (RCSB). Matthieu's interest was to investigate the merit of deep learning of structural information on ligand binding and interactions. The first step was to mine the pdb indentifying over 15,000 unique ligands and categorizing nearly 1 million interactions. Quality controls were used to curate the data with a resolution of 2.5 Å resulting in approximately 11,000 suitable structures for analysis. Through this analysis they were able to tabulate and rank interactions that are observed. Not surprisingly, hydrophobic interactions dominated the list followed by hydrogen bonds, pi-stacking and salt bridges. When focusing specifically on fragments however, the data show that they are more polar and salt bridges are more highly represented. The observation is consistent with the literature on fragment based drug discovery is that by the small nature and increased degrees of freedom to optimize binding in a pocket, they are better able to make good hydrogen bonds and salt bridges and therefore often have high binding efficiency (BEI). What was somewhat surprising was that in the analysis of all compounds, the ones with the highest BEI were making more hydrophobic interactions. His overall conclusion was that the best compounds derive from the polarity and high efficiency of fragments, but end through optimization by adding hydrophobic interactions. Having now curated and categorized nearly a million interactions, the next steps will be to use deep learning to begin moving towards more predictive use of this information.

Continuing with the theme of data collection, **Michael Hennig**, LeadXpro AG, provided an excellent overview of X-ray Free Electron Laser (XFEL) technology, specifically at the Paul Scherrer Institute (PSI) neighboring the SLS in Switzerland. The emphasis at LeadXpro AG is on gene to lead generation with a focus on the use of XFEL. Michael described the evolution of the XFEL at the PSI which is now beginning to look at protein samples. Michael pointed out that XFELS are approximately 10^9 times more brilliant than the average synchrotron which brings some great advantages as well as new technical challenges for doing protein X-ray crystallography. As a result of the high brilliance of XFELS, radiation damage is a major challenge and the solution to that challenge is to collect single images per crystal with very short pulses of X-rays. To accomplish this, new methods

of delivering samples to the beam must be invented, these methods include crystal injectors, acoustic levitation and solid support fixed target methods. All of these approaches rely on generating large numbers of microcrystals, which in itself can be a challenge. It was pointed out that no single technology solves all problems and therefore having multiple techniques is a benefit. The advantage of crystal injectors is that you can stream crystal slurries through your beam, but the challenge is to get the crystal density right so that you have a high hit rate of beam to crystal which can take significant optimization. Acoustic levitation is growing in interest where crystals in a plate can be acoustically ejected into the beam at a regular rate. Once again, condition optimization is a challenge but Michael described that this approach can even be used for crystals in lipidic cubic phase (LCP). Plate based, or solid support enables both room temperature and cryo capabilities. In this case micro crystals are grown in a plate that can be placed in the beam and 10o wedges can be collected. Michael also discussed the advantages of room temperature data collection providing greater insight into protein dynamics than cryo-crystallography which is of growing interest in general in the field of protein X-ray crystallography. Finally, time resolved crystallography is a real vision for XFELS where data can be collected on the order of 16 nanoseconds to 1.7 milliseconds. While still in the relatively early days, XFELS continues to expand and overcome the technical challenges resulting from the extreme brightness afforded by XFELS.

The next question addressed at the symposium was how to collect the very best data. **Gerard Bricogne**, Global Phasing Consortium, described the data collection revolution, the move towards serial crystallography, and the challenge of merging partial data sets from XFELS. Gerard described this as the Humpty Dumpty problem, how do you put it all back together? Gerard's argument is that we are better off collecting what he termed "club class" data. He pointed out that in many of the data collection strategies today we are missing key cusps of data such as detector edges, seams between modules on a pixel array or merging partial data sets. *Staraniso* is a program designed to help crystallographers evaluate their data to visualize missing data. At a minimum the recommendation is to collect more data from the same crystal in multiple orientations to ensure that all data cusps are eventually covered and accounted for, resulting in the highest quality starting model. One of the challenges is the need for high throughput data collection to which Gerard described work at Diamond with Armin Wagner using an inverse kappa goniostat interfaced with GDA and MxCube to capture orientation and symmetry of each crystal and efficiently collect highly redundant data. He also gave another example from EMBL at Grenoble using the Arinax robot for high throughput crystallization, soaking and automated mounting of crystals. At EMBL, pipedream was used for taking raw images to map and fit. Gerard described the advantages of club class structures in improving the success of fragment screening. Using a standard model and PANDAA for processing and map calculation, no fragment hits were identified. Using the same data but starting with a club class starting model many fragment hits were successfully identified from the same data. His recommendation is to collect club class data on all crystals and a dramatic improvement should be seen in the number of successful hits identified and the quality of interpretation.

While, earlier we examined the information in the protein data bank, **Jason Cole**, Cambridge Crystallographic Data Center, described their work on small molecule crystal structure data mining. Using the data in the CSD, tools such as Mogul have been developed for geometry analysis to understand affinity, comformations and probabilities to identify non-optimal conformations that can be modified through chemistry to improve activity of future molecules. He described the rational, with examples of rigidifying molecules to improve affinity or selectivity. IsoStar is a tool designed to analyze interactions of molecules in the CSD. It creates propensity maps of what interactions atoms make in the CSD, their frequency and geometry. This can help inform drug designers on the types of interactions favored by their molecules. CSD Cross finder builds on IsoStar to evaluate which structural features bind in similar environments. Jason described the ability to do pharmacophore searches of both the CSD and the PDB, going from features to pharmacophore. The pharmacophore can be constrained to match the PDB or CSD for inter or intra molecular interactions, and this was exemplified by an example of scaffold hoping for a kinase target. In this case they were able to identify new cores that were selective for Aurora kinase. There is a wealth of information in the CSD and the PDB, and we are now beginning to learn how to best leverage that information to design better compounds.

We began case studies with **Joe Wedekind**, U of Rochester School of Medicine and Dentistry, discussing his work on the HIV-1 Translocation Response (TAR), which is needed to transcribe proviral DNA into RNA, in an effort to target latent

viral reservoirs. Joe's work focused on finding TAR binding proteins (TBP) and complex with TAR-RNA's. They were successfully able to get the structure of the complex with TBP6.7 which binds TAR with 2.5 nM affinity to 1.8 Å resolution. Their results were really quite surprising because TBP6.7 bound to the RNA major groove where most related proteins bind to the minor groove. In this case they found that TBP6.7 binding was mediated by 3 arginine residues and using a combination of alanine mutations and molecular dynamics identified which arginines were critical to binding and that the loop they were located on was very stable. They confirmed this finding by inserting the loop into unrelated proteins and demonstrated that they could still bind TAR. They then designed constrained peptides of this loop with disulfide linkers that retained 1.8 µM affinity and demonstrated in HELA nuclear lysate that they could still bind and attenuate TAR transcription.

The next case study was a fragment based approach to a protein/protein interaction target, WDR5 by **Thomas Peat**, CSIRO. WDR5 functions to bring other proteins (MLL1 and Mycn) together in a complex and disregulation of this protein can lead to leukemia. A surface plasmon resonance (SPR) fragment screen was done which yielded a rich supply of fragment hits. While the crystals were not particularly nice looking, they diffracted to <2.0 Å, providing excellent structural insight on the fragment leads. The fragment hits ranged in affinity from 4 mM to 300 µM with excellent ligand efficiency. The lead series they pursued was an imidazole series that despite being a challenge for chemistry they were able to quickly optimize from 100 µM to 5 µM. Interestingly Steven Fesik from Vanderbilt University was also working on this target and had independently identified similar fragment leads. The Fesik team was able to optimize their series to pM binders but unfortunately was still unable to demonstrate robust cellular activity and the project was terminated.

Anna Gardberg, Constellation Pharmaceuticals, described the importance of making the right measurement to identify novel allosteric inhibitors of the p300-HAT domain. P300 is an epigenetic target and is highly homologous with CBP, another histone acetyl transferase. There is a cryo-EM structure of the entire P300 complex but in the X-ray studies, just the HAT domain was used. In their high throughput screening campaign, an antibody TRFRET assay was used as well as a tritiated acetyl group assay. From this screen they were able to identify a set of compounds that showed an allosteric mechanism profile. They overcame challenges of self acetylation of the protein using several mutants to obtain structures of the P300-HAT domain in complex with their ligands, which they found binding in a pocket neighboring the Acetyl-COA site. They evaluated several fragment binders and found one series they could advance to a K_i of 0.3 µM. Interestingly, despite good affinity, cellular assays did not give good activity and in the end it was concluded that using commercially purchased protein was the source of the discrepancy. Once full length protein was generated in house, assays began to align and significant progress was then made. This is an ongoing discovery effort.

The role of structural biology is extending beyond traditional small molecule support and now includes significant efforts in understanding biologics structure and function. To give the audience some understanding of the role of structure in biologics, **Mark Chiu**, Janssen Research and Development, provided an exciting overview of what they have done on OX40 agonists. The challenge in immune-oncology is tuning the immune system appropriately. For immune disease you want to turn down the immune system and hit the brakes, and for immune-oncology you want to ramp up the immune system and remove the brakes. For the OX40 agonist antibody project, they found that it was critical to find an OX40 epitope that allowed antibodies, particularly the Fc portions, to cluster together. Clustering of Fc's enhanced Fc receptor binding and therefore signaling. The Janssen strategy was to look at structures of the Fc and Fc/Rgama, and they identified a hexabody complex of Fc's clustered together. They then screened for OX40 antibodies that had increased agonism and found two Fc mutations, T437R and K248E that promoted clustering of the Fc's and thereby increasing agonism. Fortunately these mutations do not drive aggregation in solution, but do promote clustering in the cellular environment in high receptor density. This talk highlighted the power of bringing in structure and functional insight together to drive progress on a biologic target.

The final project discussed was on B-cell Lymphoma and the role of Bcl6, which is required for germ cell B-cell maturation, and critical to the survival of DBLC cells. **Gil Prive**, Princess Margaret Cancer Centre, described his team's structure-based drug design work on the BTB domain of Bcl-6. They performed a virtual library screen (VLS) of 5 million virtual compounds which resulted in 6 leads validated by both a fluorescence polarization and SPR assays. Their hits ranged in affinity from 300 µM to 130 µM and with some limited structural information they were able to drive to 20 µM. Once they achieved 20 µM, crystal structures became much more robust and

high resolution, as high as 1.17 Å. The BTB domain of Bcl6 forms a homo dimer and the compounds were found to bind across the dimer interface making direct interactions with both chains of the dimer. The core was the critical bridge across the dimer interface and was therefore very sensitive to modification. Armed with robust, high resolution crystal structures (over 250 were obtained), the chemistry team was able to optimize compounds from 20µM down to 4 nM. While the compounds have good cellular activity, they do not kill cells, but do inhibit their growth. No effect was observed in non-Bcl6 containing cell lines indicating that compounds were indeed specific to Bcl6. More recent chemistry efforts have improved potency, microsomal stability and removed a glucuronidation issue with a phenol in the compounds. Boehringer Ingelheim, Takeda and Astra Zeneca have been working on similar chemical matter for this target independently.

Our final presentation was from **Giovanna Scapin**, Merck, who described her experience and perspectives on cryo-electron microscopy (Cryo-EM). She described the evolution of a structure-based program starting with your first early crystal structures which provide critical insight to the need for robust and high turnaround of iterative structures in the optimization phase of a program. The key question is where does cryo-EM fit into this paradigm. The resolution revolution of cryo-EM has been exciting and is driven largely by development of electron counting cameras with beam induced motion correction technology. Nevertheless, despite all the excitement, there are very few structures (a handful) that are actually useful for drug design. Cryo-EM remains very slow at this point. Giovanna described the challenges of putting your protein effectively on grids, and the painful process of obtaining any useful grids. She also highlighted the importance of dedicated expertise. Going from a good grid to a good model can take a real expert hours to days, for most scientists it can be 8 days to 8 months. So what is being done to try to speed and improve the process? Giovanna described new innovations to speed the process. The "Spotiton" robotic system sprays your sample on the grid and moves it rapidly to liquid ethane. It is highly reproducible with very minimal ice thickness. This is a significant advance in grid preparation. There is still a need to improve the turnaround time and resolution. Continued emphasis on better cameras, better stages and better software is still needed. Currently data processing involves classification of molecules and if they are good, particle selection, to evaluate heterogeneity. What is needed are general particle pickers for 2D and 3D classes. If your EM data are better than 3.5 Å, you are able to use standard X-ray data to fit your maps. If you are below 5 Å, you may still be able to do molecular replacement, but if you are lower, it is much more challenging. There is a need for a real map to structure pipeline. Another issue is the lack of validation tools to avoid over fitting of data. With dedicated resources and microscopes, a few structures per week or month is feasible, but as described above, there is a lot more technology improvement needed to make cryo-EM quality and throughput a robust part of the drug discovery process. This is a rapidly growing field and with a lot of enthusiasm and interest, and one should expect rapid progress on many of the existing bottlenecks.

Steve Soisson and Vincent Stoll

TMT 1 & 2: Three Minute Thesis

1) Kenneth Childers, 2) Mariusz Krawiec, 3) Yue Zhao, 4) Victor Young, 5) Chelsy Chesterman, 6) Pavol Juhas, 7) Elspeth Garman, 8) Thomas Fitzgibbons, 9) Vanessa Kristina Seiler, 10) Johnathan Labriola, 11) Andreea Gheorghita, 12) Diane Dickie, and 13) Morgan Gilman. Judges from morning sessions not pictured: Andy Howard, George Lountos, and Carla Slebodnick.

At the 2018 Annual Meeting in Toronto we saw the inauguration of the Three-Minute Thesis Session. This was a major revamping for the Poster Preview Session that was held in previous years. The Three-Minute Thesis concept is inspired by the elevator speech where a person briefly explains what they do for research and their motivation for pursuing it. There were 19 graduate students and postdoctoral students who participated in the two preliminary sessions early Saturday morning. These were chaired by Pavol Juhas and Victor Young. Each participant was given three minutes' time to present their Three-Minute Thesis along with one PowerPoint slide. Our morning judges George Lountos, Carla Slebodnick, Andy Howard, and Diane Dickie selected three participants from each preliminary session for the finals session held during the noon hour. The finals session judges Elspeth Garman, Mariusz Krawiec, and Thomas Fitzgibbons selected Andreea Gheorghita as the winner. Andreea also gave a wonderful encore presentation at the annual awards banquet. The Three Minute Session is here to stay so please plan to attend it at the Covington ACA meeting in 2019.

Victor Young

1.1.1: Closing the R-Factor Gap in Protein Crystallography

Left to Right(Front row): David Case, Helen Ginn, Henry van den Bedem, Steve Meisburger, (Back row): Randy Reid, James Holton, Garib Murshudov, Pavel Afonine, and Robert Thorne. Photo courtesy of Nozomi Ando.

Session 1.1.1, *Closing the R-Factor Gap in Protein Crystallography*, focused on approaches that might lead to improved agreement between structural models and experimental diffraction data. Model errors, as measured by R_{cryst} and R_{free}, are seldom better than 20%, much larger than the estimate of experimental error (R_{merge}), and an order of magnitude worse than in small-molecule crystallography. This poor agreement is not due to experimental noise or inaccurate model phases.

Randy Read, Cambridge Institute for Medical Research, discussed the use of measures of information content to assess and weight experimental observations of diffraction intensities in constructing models. Some strong reflections may contain little information, while weak reflections (especially for crystals with strongly anisotropic diffraction or translational non-crystallographic symmetry) may be information rich. Using the Kullback-Leibler divergence as a measure of information added by a measurement, a significant number of reflections can be eliminated, while some weak reflections that might be eliminated by a local I/σ cutoff are retained. However, the total K-L information content of a data set is not as predictive of potential model quality as resolution or reflections per atom, as the latter give more weight to the short wavelength Fourier components that constrain atomic positions. An alternative metric, the Fisher information, may be more predictive.

David Case, Rutgers University, discussed how chemical restraints used in refinement of crystallographic models can be improved using force field energies computed with Amber molecular dynamics, now integrated into Phenix. This approach aids in weighting different restraints, gives more restrictive restraints at low resolution than conventional geometric restraints, and can be used when good geometric restraints are not available. Application of this approach to over 13,000 paired protein refinements yielded improved MolProbity and clash scores, and (with modelling of electrostatics) more modeled hydrogen bonds, and similar R_{free} values but with less overfitting.

Garib Murshudov, MRC Cambridge, discussed issues that arise when using *R* factors and correlation coefficients to compare different data sets and models derived from different crystals. Differences in crystal structure (e.g., due to twinning), order (e.g., anisotropy of *B* factors), and shape affect the probability distribution of the intensities/amplitudes. Alternative indicators of agreement were presented,

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and their impact on maximum likelihood refinement in combination with other common refinement tools were discussed.

James Holton, UCSF/LBNL/SSRL and **Henry van den Bedem**,SLAC/UCSF, discussed how models may be improved by including multiple side chain conformers. Starting with an MD simulation of a protein in a crystal lattice, Holton found that the calculated side chain conformational heterogeneity could typically be modeled to within experimental error using no more than two conformers, with no more than 14 conformers required to describe the most disordered side chains. The resulting models yield low R_{free} values for the protein atoms alone, but inclusion of solvent atoms leads to unstable refinements. van den Bedem described his modeling tool, qFit, which automatically selects a parsimonious set of side chain conformers to minimally account for the experimental data, and CONTACT, which uses qFit-generated models to identify allosteric networks of overlapping conformations within the protein. A new tool, qFitLigand, has been developed to automatically model ligand conformational heterogeneity. Analysis of over 2000 ligand-bound PDB structures with drug-like ligands identified widespread conformational heterogeneity, and in many cases alternative conformers can be exploited to guide compound design to improve potency or selectivity.

Protein crystals typically contain between 30% and 80% solvent, only some of which is structured and can be atomically modeled. **Pavel Afonine**, LBNL, described attempts to extend the standard flat (uniform density) model for the disordered, bulk solvent, to account for internal voids, unmodeled and partially occupied regions, *etc*. A bulk solvent model, constructed based on analysis of flat solvent mask connectivity and difference map density and having regions with different flat densities, consistently improved *R* factors in a test set of 90,000 PDB entries, with particularly large improvements at resolutions below ~6 Å.

Steve Meisburger, Princeton/Cornell, discussed new efforts to extract information about correlated protein motions from the diffuse scatter between and underneath the Bragg peaks. Complete high-resolution 3D diffuse scattering maps in reciprocal space were determined from room temperature measurements of several single-domain proteins spanning a wide range of unit cell volumes, solvent content, and space group symmetries. Halos of intensity surrounding Bragg peaks were shown, in the case of triclinic lysozyme, to have a power law decay characteristic of acoustic phonons. All-atom MD simulations of triclinic lysozyme show that a large number of unit cells is required to capture the features in the experimental map, suggesting that phonon-like, long-range correlations are important contributors to diffuse scattering in these crystals.

In a beautifully hand-illustrated talk, **Helen Ginn**, Oxford University, described Vagabond, an alternative model refinement approach. Vagabond defines the model using bond lengths, angles, and torsion angles rather than atomic x, y, and z values and associated *B* factors. This approach reduces the number of parameters required to describe most of the structure, describes side chain flexibility/motions in a more chemically sensible way, and can describe some electron density distributions that can't be captured using anisotropic *B* factors. In test cases, the approach reduced overfitting and yielded cleaner maps.

Taken individually and together, the various approaches discussed in this excellent session appear to yield only modest improvements in *R* factors. So how can the *R* factor gap be closed? Are static crystal disorder, disorder caused by radiation damage, and/or errors in converting measured diffraction frames into structure factor amplitudes the key? Do we have evidence that the *R*-factor gap for high resolution structures involves biologically relevant information, and can this guide model improvements? Is there some, more fundamental obstacle that may not involve fixable errors in data interpretation and modeling?

This session raised more questions than it answered. There seem to be as many theories about the dominant source of error that leads to the R-factor Gap as there are investigators looking into it. Fortunately, in science, that is a good thing.

James Holton and Robert Thorne

Editor's Note: Unless otherwise noted, all photos in the *Toronto ACA Meeting Scientific Sessions* section are either by Richard H. Bromund or student volunteer session monitors.

1.1.2: Structural Biology of Nucleic Acids and Protein-Nucleic Acid Complexes

Left to right: Soumya Remesh, Clara Kielkopf, Eric Montemayor, Wen Zhang, Yun-xing Wang, Ailong Ke, Rui Zhao, Joseph Wedekind.

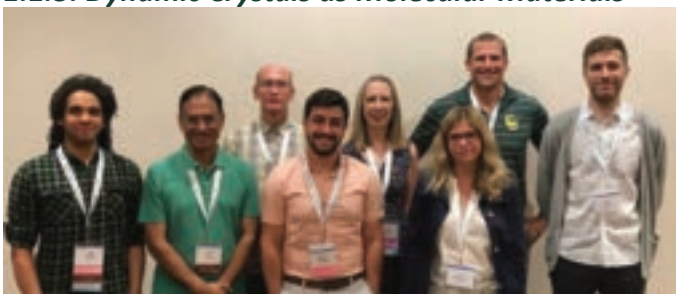
Session 1.1.2 provided many new insights into the form and function of nucleic acids. **Wen Zhang,** Harvard University, presented mechanistic studies of non-enzymatic RNA polymerization using custom phosphoramidites with imidazole leaving groups that were caught in the act of catalysis by crystallographic snapshots. This work has implications for catalysis in a pre-biotic RNA world. **Sun Cheol Park**, Kangwon National University, Korea, described DNA recognition by the PadR repressor. Binding of phenolic acid blocks DNA binding to relieve PadR repression, activating downstream detoxification genes.

Yun-Xing Wang, NIH/NCI, described use of an X-ray free electron laser to capture conformational changes of the adenine riboswitch during effector binding, providing insights into RNA-mediated translational regulation. **Clara Kielkopf**, University of Rochester, described progress to decode the basis of 3´-splice site recognition of pre-mRNA by U2AF proteins, including polypyrimidine tract recognition and binding to degenerate splice-sites. The work has implications for correction of splicing defects found in human diseases.

Eric Montemayor, University of Wisconsin, described later steps of pre-mRNA splicing, including a model for U6 snRNA remodeling by contacts to the Lsm2-8 ring protein and the Prp24 chaperone. **Soumya Remesh**, Lawrence Berkeley National Lab, used small angle scattering and soft X-ray tomography to reveal how small molecules interact with the abundant HU protein to alter DNA supercoiling. The work has implications for controlling bacterial gene expression. The session was anchored by **Ailong Ke**, Cornell University, who presented structural snapshots that contribute a novel mechanistic framework to describe how bacterial type II-A CRISPR systems create new molecular memories of short, foreign 'spacer' DNAs that invade bacterial cells.

Joseph Wedekind, Rui Zhao and Aaron Robart

1.1.3: Dynamic Crystals as Molecular Materials



Left to Right: (Front) Travis Mitchell, Jagadese Vittal, Demetrius Vazquez-Molina, Yael Diskin-Posner, Filip Topić , (Rear) Dmitriy Soldatov, Louise Dawe, Mario Wreidt.

This session introduced a new topic of dynamic crystals into the ACA meetings agenda. Dynamic crystals are seen as a first step towards a next generation of molecular materials where the internal motion or externally forced displacement of molecules within the crystal structure induces changes in macroscopic properties or chemical nature of a material. The session was organized by Dmitriy Soldatov, U Guelph, and Louise Dawe, Wilfrid-Laurier U, and supported by Proto Manufacturing and *Crystals*, an MDPI journal. Six speakers illustrated various ways that the dynamic nature of crystals may affect the properties of bulk materials.

Jagadese Vittal, National U Singapore, introduced the field of mechanically responsive materials and specifically dynamic molecular crystals that respond with various movements when exposed to heat or light. In some examples, the movements resulted from a solid state chemical reaction occurring inside the crystals! **Demetrius Vazquez-Molina**, U Central Florida, reported on crystals where a rigid covalent organic framework has been decorated with flexible side-chains exhibiting dynamic behavior. **Yael Diskin-Posner**, Weizmann Institute of Science in Israel, presented a series of crystals with molecular-size cages. The inclusion of guest species in the cages, or light-induced isomerization of the guest molecules included, causes dramatic changes in the crystal structure as the cage adapts to a new shape. **Mario Wriedt**, Clarkson U, demonstrated how absorption properties of metal-organic frameworks can be efficiently controlled by reversibly changing the charge distribution within the framework with photo- or electrochemical external stimuli. **Filip Topić**, McGill U, reported on a number of intermediate co-crystalline phases formed on the way to the final product of a "mechanochemical cocrystallization". Finally, **Travis Mitchell**, U Buffalo, showed how the incorporation of photochromic molecular fragments into metal organic frameworks makes it possible to

alter the local chemical environment around the pores in the crystals with light.

Dmitriy V. Soldatov and Louise Dawe

1.1.4: Neutron and X-ray Scattering of Correlated and Quantum Materials

This session dealt with current topics in correlated and quantum materials in which the power of neutron scattering techniques, both elastic and inelastic, was emphasized. Participants included both solid state chemists and condensed matter physicists from universities and national laboratories. Two students and a postdoctoral fellow were among the speakers. **Efrain Rodriguez**, Univ. of Maryland, began with an introduction to the concept of ferrotoroidicity and the requirements for candidate materials which might exhibit this unusual effect. The technique of Spherical Neutron Polarimetry was introduced along with a progress report on the development of relevant instruments at North American neutron sources. **Stephanie Gnewuch**, Univ. of Maryland, described the magnetic structures of candidate ferrotoroidic materials with the olivine structure. Stephanie was the recipient of the Etter Student Award from the Neutron Scattering SIG. **Mirela Dragomir**, McMaster Univ., described the remarkable differences in magnetic properties between the isostructural phases $Sr_{0.8}La_{1.2}MnO_4$ and $Ba_{0.8}La_{1.2}MnO_4$, the former showing the expected two dimensional short range order followed by long range antiferromagnetic order below 95K, while the latter is a highly unusual anisotropic spin glass below 26K. Perovskites and related oxides based on Ir in various oxidation states were discussed by **H.C. zur Loye**, Univ. of South Carolina. This was followed by **Adam Aczel**,ORNL, who described double perovskite oxides based on Ir^{4+} and the effects of very strong spin orbit coupling on magnetic properties. The session concluded with two papers on frustrated pyrochlore oxides. **Chris Wiebe**, Univ. of Winnipeg, described the search for new spin liquid materials with the example of Nd_2ScNbO_7. Studies of the candidate spin ice material, Dy_2ScNbO_7, were presented by Megan Rutherford, Univ. of Winnipeg,.

J. E. Greedan and Craig Bridges

1.2.1: Structural Dynamics - In Honor of Phil Coppens

Left to right: Yu-Sheng Chen, Filip Topic, Majed Chergui, Tomislav Friščić, Lin Chen, Jim Britten, Gage Bateman, Wilfred Fullagar, Marc Messerschmidt, Jason Benedict.

This special session was dedicated to the late Professor Philip Coppens for his lifetime of outstanding scientific achievements and dedication to serving the broader scientific community. His contributions impacted every aspect of charge density theory and application as well as the development and application of time-resolved X-ray diffraction methods to monitor light-induced structural transformations in small molecule systems. Presenters in this special session described recent advances in structural science using X-ray diffraction that highlight the exciting developments in this area, many of which were directly inspired by Philip's impactful scientific legacy.

The symposium began with a brief remembrance of Philip given by the organizers, Jason Benedict and Yu-Sheng Chen. Primarily consisting of photos from friends, family, colleagues, and collaborators, the audience was treated to heartwarming highlights of Philip's life. Perhaps most notable were those that included his late wife, Marguerite, who was also well-known and loved by many who were present.

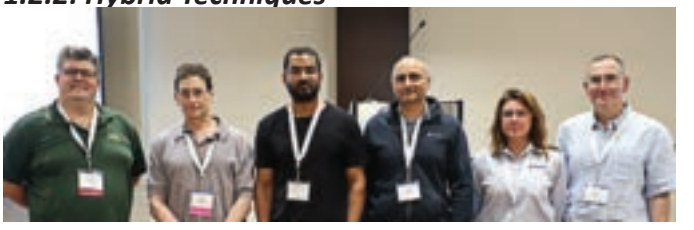
The science portion of the symposium began with **Majed Chergui**, Ecole Polytechnique Lausanne, highlighting some recent synchrotron-based studies of light-induced charge carrier trapping in transition metal oxides which have important applications in solar energy research. He also presented recent work on myoglobin dynamics performed by his group using X-ray free electron lasers (XFELs). The next speaker was **Marc Messerschmidt**, BioXFEL, who shared details of the earliest experiments being performed at the European XFEL. The presentation included exciting results of commissioning runs that showcased the high repetition rates and other features of this unique light source. And just before the coffee break, **Lin Chen**, Northwestern U, presented an investigation of excited state pathways and electronic structural

dynamics during photodissociation of CO from heme in myoglobin using ultrafast X-ray transient absorption (XTA) spectroscopy at the Linac Coherent Light Source (LCLS). Her results revealed earliest electronic and nuclear dynamics atomic movements, and energetics from which one can modify the binding site of heme to adapt new capabilities of binding other small molecules for substance transport in biological systems.

After the break, the science was back in full swing with **Jim Britten**, McMaster U, presenting on some updates to MAX3D, a program used to visualize 3D-diffraction data. The program helped identify strain properties in alloys and was used to monitor phase transitions in a variety of materials. Next to speak was **Tomislav Friščić**, McGill U, who continues to demonstrate that synthesis via mechanochemistry is capable of producing products in high yield over a surprisingly broad scope of reactions. He continues to provide important insight into these reactions using in situ powder X-ray diffraction methods developed in his laboratory. The theme of solid-state structural transformations continued with **Gage Bateman**, U at Buffalo. He shared recent results in which the guest exchange reactions occurring in a flexible metal-organic framework were monitored using in situ single crystal X-ray diffraction. These experiments revealed key structural intermediates and reversibility in a reaction previously reported as irreversible. The penultimate talk by **Wilfred Fullagar**, Australian National U, outlined how the energy of quanta received by an integrating detector is related to the ratio of observable noise to intensity. These observations played a critical role in the success of the laser-driven, detector-based tabletop ultrafast X-ray pump-probe experiments recently perfomed at NIST. The final speaker of the session was **Filip Topic**, McGill U, who described two ternary cocrystals assembled from crown ether, thiourea and an iodoperfluorocarbon, both exhibiting rich polymorphic behavior. The underlying robust hydrogen and halogen bonding interaction were preserved in all cases, in both high- and low-temperature polymorphs as well as in polymorphs with different framework topologies.

Jason Benedict

1.2.2: Hybrid Techniques



Left to Right: Chris Colbert, Tobin Sosnick, Srinivas Chakravarty, Bhushan Nagar, Angela Criswell, and Osman Bilsel.

Small angle X-ray scattering (SAXS) has rapidly emerged as a valuable biophysical tool widely recognized as a powerful complement to other structural, biophysical and biochemical techniques and the session titled “Hybrid Methods” highlighted this in the context of a variety of bio-medically significant projects. There were also instances of increased sophistication in analysis tools that have enhanced the scope of SAXS in bio-molecular research.

The session started with a talk by **Thomas Grant**, Hauptman-Woodward Institute, in which he discussed the use of methods developed for image reconstruction algorithms and their application to the problem of density reconstruction in solution scattering. The new algorithm he developed is capable of reconstructing *ab initio* 3D electron density maps from the 1D solution scattering profiles without modeling. This algorithm avoids many of the assumptions limiting the resolution of traditional modeling algorithms and is capable of reconstructing complex shapes of particles containing multiple density components.

Osman Bilsel, U of Massachusetts Medical School at Worcester, gave a presentation that shed light on recent advances in time-resolved SAXS. He showed that SAXS offers a number of advantages for probing kinetics because it is label-free, sensitive to a wide range of length scales and also to the oligomeric state of macromolecular complexes. He also demonstrated the capabilities of microfluidic mixers fabricated in his lab which were critical for optimizing the duty cycle of continuous-flow time-resolved SAXS experiments used to study the properties of protein chains under folding conditions.

To end the first half of the session, **Xu Zhen**, U of Iowa at Iowa City, talked about how advances in liquid handling, integrated workflows and software, and SAXS coupled with other methods rapidly provide accurate characterization of shapes, conformations, and oligomeric states of proteins. In his case, size exclusion chromatography and in-line collection of

multi-angle light scattering (MALS) and SAXS data was critical in a variety of contexts such as – 1) Determining a protein's novel oligomeric states in solution based on crystal structure and hypothesized models, and 2) helping solve the crystal structure by differentiating the protein oligomeric states in solution.

To start the second half of the session, **Angela Criswell**, Rigaku, introduced SAXS as a means to study atypical bio-molecular samples. Specifically, these are high concentration and high viscosity samples where SAXS data are used for the purposes of optimization of biological pharmaceuticals, for characterizing crystallization suspensions prior to measurement at an X-Ray Free-Electron Laser Facility (XFEL), and for characterizing structural changes in response to solution conditions. Dr. Criswell presented the latest capabilities of the Rigaku Oxford Diffraction's BioSAXS-2000 nano system which has been shown to be well suited for analysis of all types of biological samples, independent of concentration, viscosity and phase.

Proteins adopt non-native geometries during their synthesis, folding, transport, and turnover and a significant fraction of the proteome is intrinsically disordered. **Tobin Sosnick**, U of Chicago, talked about a method developed to extract the dimensions and solvent quality of a polymer from a single SAXS measurement, applicable to intrinsically disordered proteins (IDPs). Studies using this technique found IDPs to be expanded in water, which behaves as a good solvent. Additionally, discrepancies between SAXS and FRET data were discussed and it was demonstrated that fluorescent dye labelling induced contraction of IDPs.

To end the session, **Christopher Colbert**, N Dakota State U, reported his findings from sequence analyses, structural modeling, mutagenesis combined with pull-down assays, crystal structure determination and SAXS, which were used to investigate the interaction between Beclin 1 (a key component of the autophagosome nucleation complex) and GAPR-1 (Golgi-associated plant pathogenesis-related protein 1, a negative autophagy regulator). Singular value decomposition analysis of SAXS data was used to detect monomer and dimer species of a mutant construct of GAPR-1 and the role of the 5 mutated residues in altering monomer-dimer equilibrium and in disruption of the GAPR-1:Beclin 1 interaction was determined. Overall, the session was successful in showing the power and versatility of SAXS.

Srinivas Chakravarty

1.2.3: Neutrons as Complimentary Probes for Crystals and Scattering

The session on Neutrons as Complimentary Probes for Crystals and Scattering highlighted the powerful research being performed at our remarkable neutron sources and beamlines that have become increasingly available over the last five years.

Zimei Bu, City College of New York, began the session with an impressive talk entitled "Controllable Activation of Nanoscale Dynamics in a Disordered Protein Alters Binding Kinetics." The adapter proteins NHERF1 and Ezrin are of interest because they regulate transmembrane signaling complex assembly, trafficking and signaling by linking the cell membrane to the F-actin cytoskeleton. Dr. Bu is using neutron spin echo spectroscopy (NSE) to study the effect of phosphorylation on nanoscale motion of the C-terminal tail of NHERF1. The binding to ezrin activates inter-domain motions in NHERF1 of more than 100 Å. The data were all interpreted with beautiful small angle neutron scattering (SANS) envelopes with the help of phase contrast methods.

The following two talks demonstrated how neutron crystallography is finding potential errors in textbook biochemical mechanisms. **Dagmar Ringe**, Brandeis U, delivered a fascinating lecture on "The Missing Atom in function: reliability of the determination of hydrogen positions in protein structures". The most important atom in a protein is the smallest one, hydrogen, and it is also the most difficult to visualize. To identify hydrogen positions with X-ray crystallography 0.7 Å is required but with neutrons only moderate resolution is needed (<2.5 Å), opening the door for many structural mechanistic studies. Using chymotrypsin as a test system, Dr. Ringe is exploring how the pKa's of amino acid residues are influenced by the active site environment, by soaking crystals at pH 5, 7 and 9 before collecting neutron diffraction data. Surprisingly, some histidine residues remained doubly protonated even at pH 9. Then **Timothy Mueser**, U of Toledo, spoke about "Neutron diffraction studies of pyridoxal-5'-phosphate dependent (PLP) enzymes". Neutron crystallography was used to visualize the positions of hydrogen atoms in aspartate aminotransferase (AAT) and then theoretical calculations were performed. Before neutron diffraction data collection the AAT crystal was reacted in situ with α-methylaspartate. In one monomer, the PLP remained as an internal

aldimine with a deprotonated Schiff base. In the second monomer, the external aldimine formed with the substrate analog. A deuterium was observed equidistant between the Schiff base and the C-terminal carboxylate of the substrate, a position indicative of a low-barrier hydrogen bond. Dr. Mueser pointed out the importance of having the hydrogens in the right place before performing theoretical calculations. He also described how neutron crystallography unexpectedly revealed that Bohr effect protons, that decrease O_2 affinity in hemoglobin, are also located in the $\alpha_1\beta_1$ interface.

Jahaun Azadmanesh, U of Nebraska Medical Center, then told us about his progress on "Structural investigations into the catalytic mechanism of human manganese superoxide dismutase (MnSOD) using neutron and X-ray crystallography". Mitochondrial MnSOD protects from excessive amounts of reactive oxygen species by converting superoxide to peroxide and oxygen. By using the Bio-Deuteration Laboratory at Oak Ridge National Laboratory (ORNL) they have been able to perdeuterate MnSOD for relatively large volume crystal growth (~0.2 mm^3). Perdeuteration reduced the background in neutron diffraction experiments at the MaNDi beamline at ORNL, and 2.1 Å neutron data was collected. This was the largest unit cell to date for neutron diffraction (a=b=80 Å, c=240 Å) that revealed hydrogen positions. Data has been collected on chemically reduced and oxidized MnSOD crystals that provide snapshots of the proton environment during the catalytic mechanism. It is noteworthy that oxidized structures are not possible with X-ray crystallography due to reduction of the active site metal by X-rays. The resulting structures are highly anticipated and expected to unveil a proton relay for proton-assisted electron transfer.

Drew Marquardt, U of Windsor, gave a sampling of his new projects on "Vitamin E, bilayer asymmetry and siloxane lipids: neutrons and X-rays probing different membrane problems". He is using neutron methods to answer basic questions about membrane systems. By using SANS and contrast matching between hydrogen and deuterium he has found that vitamin E does not destabilize lipid rafts, a surprising result. SANS is also useful for studying how protein insertion impacts asymmetric liposomes through lipid-protein interactions. Dr. Marquardt also discussed some unique siloxane lipids they have synthesized and measurements of lamellarity dependency on hydrocarbon chain length. These self-assembling nanoparticles have possible pharmaceutical applications.

Thomas Cleveland, NIST, described "Observing membrane proteins via SANS during lipidic cubic phase crystallization". By using a deuterated cubic lipid phase and contrast matching he is able to watch how the hydrogenated protein, bacteriorhodopsin, responds to precipitating agents. He was able to see the particles repel at low salt concentrations and then become attracted to each other as salt increased. The clustering of particles into a crystal nucleus was detected when Bragg peaks appear in the SANS spectrum. It is expected that these results and methods will have significant impact on the crystallization of G protein-coupled receptors (GPCRs), a large family of receptors that are important medical targets.

The session finished when **Brendan Sullivan**, ORNL, explained how he has "Improved Bragg peak integration for neutron crystallography by 3D profile fitting". The 3D reflection profile is created by using an Ikeda-Carpenter function to describe the time-of-flight coordinate and a bivariate Gaussian to fit the remaining two directions. Adjacent and overlapping peaks can be deconvoluted properly and weak peaks can be fit by applying the profile of a nearest neighbor strong peak. Peaks at detector edges can be recovered, important for beamlines like MaNDi with lots of detector edges (detector edges can affect 20% of all peak intensities). Datasets show improved merge statistics, lower R_{free} and improved nuclear density maps. These exciting improvements will dramatically increase not only the completeness of neutron data but also the measured resolution of neutron diffraction (as much as 0.3 Å). It is anticipated this software will be very helpful to neutron diffraction and will further push the envelope on what can be achieved with neutron crystallography by making higher resolution structural features and larger unit cells accessible. These algorithms have been are incorporated into the *Mantid* software package and it is available to the user community.

Gloria Borgstahl and Leighton Coates

1.2.4: Forefront of Electron Scattering for Nanoscale and Metastable Materials / Electron Diffraction

This half-day session was focused on the latest developments and applications of electron probes with multimodal and ultrafast techniques. Research studies using electron scattering techniques were demonstrated with quantitative structural analysis visualized in more-than-three dimensions, with 3D in crystallography and additional dimensions in the time-domain, energy-space and/or chemical mapping. This session was chaired by Jing Tao, Brookhaven National Laboratory.

Invited speaker **Jim Ciston**, Lawrence Berkeley National Laboratory, gave the first lecture about the development of 4D scanning electron diffraction experiments to understand the structural origin of many functional materials. The method integrates high-quality electron sources, advanced electron scattering techniques and state-of-art direct-detection cameras as a big-data processing and smart data-analysis tool to confront a variety of challenges, such as probing bonding details in a crystal, in quantum materials and materials with engineered heterostructures.

After a few talks, **Jianming Cao**, Shanghai Jiao Tong U and Florida State U, presented a recent study of laser-induced spin relaxation in nanoparticles using ultrafast electron diffraction techniques. Dynamics of demagnetization was obtained by probing the electron-phonon coupling via lattice variation. The findings advance the previous interpretation of the energy pathway from electronic system to the lattice/spin counterpart in materials during laser pumping.

The session was closed with a talk from **Bradley Siwick**, McGill U, on observations of ultrafast electron diffuse scattering from a 2D material. Taking advantage of the sensitivity of ultrafast electron diffraction in both the time-domain and momentum-space, phonon excitations to specific branches in graphene were observed and analyzed through the relaxation of non-equilibrium states. Such processes were found to be non-thermal and will shed light on a better understanding of structural dynamics and laser-pumping mechanisms.

Jing Tao

2.1.1 & 2.2.1: Special Sessions in Honour of Richard E. Marsh

Left to Right: (Front) Paul Boyle, Michael Takase, Alexander Filatov, Jenny Glusker, Suzanna Ward, Carolyn Brock (Rear), B. C. Wang, Sue Byram, Victor Young, Jim Kaduk, Bernard Santarsiero, George Sheldrick, Louise Dawe, Ton Spek (Missing: Frank Fronzek)

In January 2017, Richard (Dick) E. Marsh passed away. This session, in his memory, combined presentations on his contributions to the crystallographic community, as a scientist, educator, and someone who made significant contributions to the American Crystallographic Association community. His former colleagues and mentees presented on the impact of structure "Marshing" – that is, the detecting and correcting of structures with missed symmetry in the published literature. Others focused on modern methods used to prevent these problems prior to publication (talks by Ton Spek and George Sheldrick), with emphasis on the educational aspect of these methods. Finally, speakers recalled personal interactions in honor and memory of Dick Marsh (B.C. Wang and Bernard Santarsiero). The education aspect of this session was present throughout, consistent with the lasting impact that Dick Marsh had on our larger community, and Suzanna Ward demonstrated how this is preserved and curated in the Cambridge Structural Database. For those that could not attend, his autobiographical memoir from 2013 can be read here: **http://www.amercrystalassn.org/h-Marsh**.

Paul Boyle, Louise Dawe, Alexander Filatov, and Michael Takase

Session 2.1.2: Current State of Instrumentation, Automation, Status and Future. Focus on Practical Aspects

Left to right: Janet Newman, Didier Nurizzo, Mayank Aggarwal, Jean-Luc Ferrer, Debanu Das, Clemens Vonrhein, Nigel Moriarty, Matthew Clifton, Jan Abendroth. Not present in the picture: Alexi Soares. Photo courtesy of Matt Clifton.

Session 2.1.2 focused on the current state of instrumentation, automation, status and the future; focusing on practical aspects. **Alexi Soares**, Brookhaven National Laboratory, started the session talking about high-throughput fragment screening at the nano-scale utilizing laboratory miniaturization integrated with the beam-line. **Janet Newman,** Collaborative Crystallization Centre (C3), presented on refining the interface between automation and crystallization. **Debanu Das,** Accelero Biostructures, discussed their recent fragment-based drug discovery efforts utilizing crystal soaking and high-throughput data collection.

Didier Nurizzo, EMBL, presented on the automated data collection services at the ESRF. **Nigel Moriarty**, Lawrence Berkeley National Laboratory, presented on utilizing Phenix for high-throughput protein-ligand complex structure determination. **Jean-Luc Ferrer,** IBS University Grenoble Alpes, discussed automated robot-based systems for crystallography on beamlines and in laboratories, and other developments performed on FIP-BM30A at the ESRF. **Mayank Aggarwal,** Formulatrix, discussed recent advancements in automated drop setting and imaging for high throughput crystallization. **Clemens Vonrhein,** Global Phasing Ltd., wrapped up the session presenting advances in automated data analysis and processing with autoPROC, and utilizing STARANISO to improve characterization, mitigation and visualization of the anisotropy of diffraction limits.

Matthew Clifton and Jan Abendroth

2.1.3: NMR Crystallography

Figure 1. (a) David Bryce, U of Ottawa, first speaker; (b) Paul Hodgkinson, Durham U, discussing the use of solid-state NMR in addressing disordered structures of organic solids; (c) Robert Schurko presenting the basics of NMR Crystallography; (d) Philip Grandinetti, Ohio State U, discussing problems of structure solution for transition metal salts using solid-state NMR; (e) Yining Huang, Western University, is presenting on benefits of solid-state NMR in understanding the dynamic of guest molecules in metal-organic frameworks. (e) Left to Right: Tomislav Friscic, Yining Huang, Darren Brouwer, David Bryce, Philip Grandinetti, Robert Schurko, Paul Hodgkinson, Manish Mehta.

Session 2.1.3 was the second session dedicated to NMR Crystallography at an ACA Annual Meeting. This session was a follow-up of the highly successful first one held last year in New Orleans, and it was organized by **Manish Mehta**, Oberlin College, and **Tomislav Friščić** from McGill University. The session involved six speakers from three countries, covering a number of topics in this rapidly developing field.

Overall, the session was well attended, with around 50 attendees throughout both morning sets of talks. The opening remarks on the increasing importance of the field, as well as the complementary nature of NMR spectroscopy and X-ray diffraction in structural analysis was given by Tomislav Friščić, who was followed by **David L. Bryce**, U of Ottawa, with a presentation focusing on the use of solid-state NMR spectroscopy in obtaining not only structural information of organic cocrystals, but also on the course of their formation through solid-state reactivity (*Chem. Commun.* **2017**, *53*, 9930). **Paul Hodgkinson**, U of Durham (UK), provided a

number of excellent examples where the use of NMR spectroscopy in the solid state enables correcting limited structural information obtained through X-ray diffraction, improving and sometimes correcting the structures of organic compounds, such as furosemide cocrystals. Some of that work can be found in his paper *Chem. Commun.* **2016**, *52*, 6685.

Following a brief coffee break, the session continued with **Robert Schurko**, U of Windsor, who gave an illustration of structural information available on a range of metal-organic framework (MOF) and pharmaceutical materials through the use of solid-state NMR spectroscopy of different nuclei, including ^{111}Cd, ^{35}Cl and ^{14}N (*Acc. Chem. Res.* **2013**, *46*, 1985–1995). **Philip Grandinetti**, Ohio State University, presented an outstanding demonstration of the ability of solid-state NMR to provide full structural characterization of paramagnetic hydrated salts (J. Chem. Phys. 2018, 149, 084503). Next, **Yining Huang** from Western U (Canada) gave a lecture addressing the use of solid-state NMR spectroscopy in structural characterization of not only MOF materials, but also of the arrangement and dynamics of molecular guests located in their pores (*ACS Appl. Mater. Int.* **2018**, *138*, 28582).

The final talk was by **Darren Brouwer**, Redeemer U (Canada), who gave an overview of a methodology that he is developing for using solid-state NMR crystallography in elucidating the topologies of two- and three-dimensional framework structures (*Acta Cryst.* **2017**, *C73*, 184, in a recent special issue of *Acta Cryst., Section C*, dedicated to NMR Crystallography and edited by David Bryce and Francis Talleule from Université de Versailles, France). Overall, we are happy to report that this second NMR Crystallography session was dynamic and clearly demonstrated the current breadth and direction of future growth of the field. We are looking forward to welcoming you to the third edition of this emerging ACA session!

Tomislav Friščić

2.1.4 & 2.2.4: Advances in Biological Cryo-Electron Microscopy 1 & 2

Over the past five years, cryo-EM has become increasingly popular and is often the method of choice for structure determination of proteins larger than ~200 kDa. It has been particularly successful for proteins that are difficult to crystallize, including membrane proteins, large assemblies and multi-protein complexes. This pair of sessions co-chaired by Lori Passmore, MRC-LMB, and Wah Chiu, Stanford U, featured recent structures determined using cryo-EM.

The morning session focused on membrane proteins. It was clear from listening to the many excellent talks in this session that cryo-EM is making a huge impact on our fundamental understanding of membrane-bound complexes, including those involved in lipopolysaccharide transport (**Liao Maofu**, Harvard U), insulin recognition (**Giovana Scapin**, Merck), protein secretion (**Justin Deme**, U Oxford and **Natalie Strynadka**, UBC), and sterol-sensing domain transmembrane proteins (**Xin Gong**, Princeton U), owing to advances in sample preparation (e.g.,nanodiscs), image detection, and computational algorithms. Efforts to automate cryo-EM image processing and reconstruction that repurpose software management practices developed for synchrotron experiments are also underway (**Alun Ashton**, Diamond).

Several of the talks in the afternoon session focused on investigations of challenging macromolecules including dynamic complexes and smaller proteins. These included studies of RNA-protein complexes: spliceosome (**Kiyoshi Nagai**, MRC-LMB) and U1 snRNP (**Rui Zhao**, U Colorado), and transcription activation complexes (**Xiaodong Zhang**, Imperial College). A method to improve analysis when multiple conformations are present was also presented (**Javier Vargas**, McGill). Two talks discussed challenges in comparing and validating models derived from cryo-EM, making use of models submitted to the recent CryoEM Model Challenge (**Andriy Kryshtafovych**, UC Davis; **Jane Richardson**, Duke U). **Gabe Lander** (Scripps) ended the session by giving many excellent tips on how to squeeze the most out of a cryoEM imaging experiment, enabling high resolution visualization for complexes even as small as hemoglobin.

Cathy Lawson

2.1.5 Materials for a Sustainable Future

Left to Right: Jeremiah Gassensmith, Tomislav Friscic, Uta Ruett, Matthew Logan, Juby Varghese, Wesley Newsome, Mario Wriedt, Fernando Uribe-Romo.

Uta Ruett, APS, discussed the Structural Science (SRS) group which she heads composed of 4 beamlines specializing in in situ and operando structural analysis using high energy X-rays. She stressed the advantages of using X-rays 30 keV and above which provides high penetration power and better precision in structural determination making this technique further accessible to energy related applications. She also discussed additional experimental opportunities offered at their beamlines such as laser pump, X-ray probe and operando electrochemical cell experiments further highlighting the versatility of investigations that can be carried out with the help of the SRS group.

Tomislav Friščić, McGill U, highlighted solid state MOF synthesis, specifically of zeolitic imidazolate materials, using ball milling mechanochemistry which is advantageous in that it allows for the construction of complex materials using a simple, rapid and inexpensive technique. He affirmed that due to the ease of the nature of this technique, the intermediates, kinetics, stabilities and enthalpies behind each of the materials can be simultaneously investigated. The combination of experiments and density functional theory calculations bring this field one step closer to theoretical prediction and stability evaluation.

Juby Varghese, Clarkson U, received the Margaret C. Etter Student Lecturer Award and discussed the use of high-resolution transmission electron microscopy to, for the first time within the field of MOFs, directly see a guest, specifically a single-molecule magnet (SMM), within the cavities of a MOF host for the application of data storage. Furthermore, the composite material formed by the loading of the SMM into the MOF pores retained the unique magnetic properties of the SMM and provided enhanced stability afforded by the encapsulation within the MOF. She also highlighted the next step this investigation in thin film formation and analysis of the composite film closing in the gap between experimental investigations and device fabrication for read-and-write processes.

Wesley Newsome, U of Central Florida, presented the talk "Tunable Solid State Fluorescence in Isoreticular MOFs," where he discussed a synthetic strategy to prepare MOFs that emit white light using mixed linkers of red, green, and blue fluorescence as the organic part of the MOFs. The mixed linker approach allowed varying the ratios of phenanthroimidazole fluorophores present in the MOFs obtaining isoreticular materials that vary in composition, but retain the crystal structure of the parent MOF. Depending on this ratio of fluorophores, different white light temperatures were obtained, including cool and warm white light in a predictable and controllable fashion.

Fernando Uribe-Romo, U of Central Florida, in his talk "Structure-property relationships in titanium-based MOFs for the photocatalytic reduction of carbon dioxide" discussed how the photophysical and photocatalytic properties of titanium based MOFs can be tuned depending on the molecular and electronic structure of the organic building blocks. By utilizing seven different N-alkyl functionalized building blocks in MIL-125 MOF, a systematic decrease in the bandgap and an increase in the excited-state lifetime were observed, enabling increased photoreduction of CO_2 to formate under blue LED light. These new MOFs exhibited high CO_2 reduction rates under open ambient conditions without decomposition of the MOFs.

Matthew Logan, U of Central Florida, presented the talk "Systematic Isoreticular Expansion of Titanium MOFs" where he presented the crystal structure solution of a new family of three isoreticular MOFs based on titanium and biphenyl, terphenyl,and quaterphenyl dicarboxylate organic linkers, utilizing high-resolution powder diffraction, solid-state NMR spectroscopy, and total scattering methods (pair-distribution). These new MOFs are candidates for a new generation of photoredox catalyts with tunable reactivity. For his talk, Matthew received the 2018 Margaret C. Etter Student Lecturer Award on Powder Diffraction.

Juby Varghese from Clarkson University receives the Margaret C. Etter Student Lecturer Award, presented by her research advisor Mario Wriedt.

Mario Wriedt

2.2.2: New Advances in Fiber Diffraction

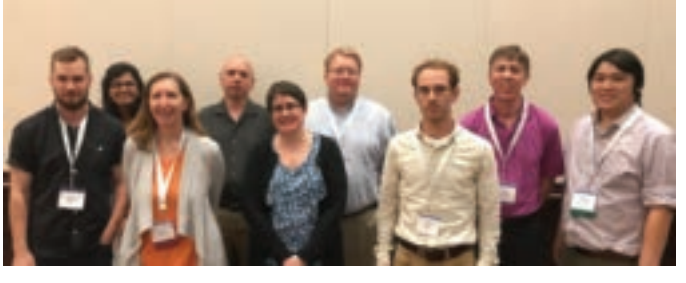
Left to Right: Joseph Orgel, Tom Irving, Volker Urban.
Photo courtesy of Joseph Orgel.

The fiber SIG conducted the "New Advances in Fiber Diffraction" session this year, co-chaired by Paul Langan and Joseph Orgel. The talks were picked from the abstracts submitted for the session and were of the customary outstanding quality drawing some wider discussions (including a press release of "Contemporary and ancient tissues give modern insights into biomedical engineering"). A new and much needed contribution to data analysis in fiber diffraction 'MuscleX' was demonstrated in addition to outstanding contributions in biomass treatment of wood and understanding the process of diabetic pathological tissue transformations.

At the SIG meeting, it was determined that the nominations for the coming Fiber schedule (which meets once every two years rather than every year as per other ACA SIG's) would be: Secretary-elect nomination, Thomas Irving. Chair-elect nomination Joseph Orgel. The next Fiber SIG session/s will be in the year 2020.

Joseph Orgel

2.2.3: General Interest 1

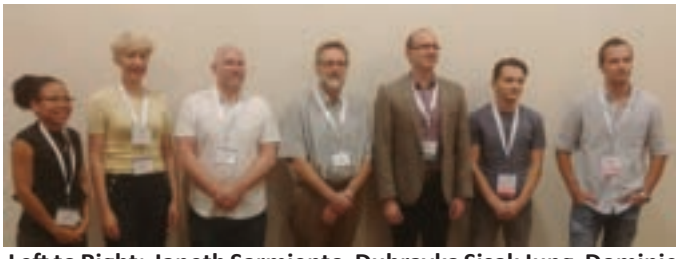


Left to Right (Front row): Matt McLeod, Catherine Lawson, Sarah Bowman, David Moreau, Michael Takase (Back row) Soumya Govinda Remesh, Lance Westerhoff, Jeffrey Lovelace, Dean Johnston.

The General Interest session this year focused on a variety of topics of broad interest to the crystallography community including improvements in small molecule and protein refinement protocols, challenges in protein crystallography and use of technology for teaching purposes. The first speaker of the session, **Alexander Y. Nazarenko**, SUNY College at Buffalo, presented the adaption of Independent Atom Model software (SHELXL-201X) in removing residual bond density in organic molecules. **Dean H. Johnston**, Otterbein U, followed by introducing the Temperature Validation tool for investigating the variation in the atomic displacement parameters using the Cambridge Structural Database Python API. **Mathew Brown**, Simon Fraser U, outlined ways to 3D print crystal data including anisotropic models and later assemble the printed models for classroom use. Next, **Matt McLeod**,U of Waterloo, presented cryo-cooling methods for investigating conformational landscapes for phosphoenolpyruvate carboxykinase. **Sarah Bowman**, Hauptman-Woodward Medical Research Institute, followed with a lively discussion on ways to enhance high-throughput detection of nanocrystals using Second Order Nonlinear Imaging of Chiral Crystals (SONICC) combined with UV-Two Photon Excited Fluorescence (UV-TPEF) and a photomultiplier detector implementation by Formulatrix. **Catherine Lawson**, RCSB, Rutgers U, then presented an overview of the new open access modular educational curriculum for developing and managing PDB pipeline and data archiving (Project website: http://edsb.rcsb.org/). **Masahiro Fujihashi**, Kyoto U, next presented a very interesting talk on using a crystallography derived signature pattern to discover novel pyrophosphate-dependent kinases. **Jeffrey Lovelace**, Eppley Institute for Research in Cancer, introduced hyper-restrains and use of supercells to improve refinements of incommensurately modulated proteins. **Lance Westerhoff**, Quantum Bio Inc., presented an overview and validation of a free energy based algorithm coupled with Phenix/DivCon package to address ligand placement problem. **Dmitriy Soldatov,** University of Guelph, presented strategies for template-directed assembly of short peptides to generate porous frameworks with desired structure and properties. The session concluded with a presentation by **David Moreau**, Cornell University, discussing practical importance of ice formation in protein crystals, their implications, and steps to ensure high quality ice free data sets.

Soumya Govinda Remesh and Michael Takase

2.2.5: The Diverse World of Materials Chemistry: From Deep Space to Titanium Dioxide Nanocomposites



Left to Right: Janeth Sarmiento, Dubravka Sisak Jung, Dominic Fortes, Philip Squattrito, Olaf Borkiewicz, Sergei Rigin, Georgii Bogdanov.

This symposium, a joint collaboration between the Powder Diffraction, Materials, and Neutron Scattering SIGs, provided an overview of topics related to the broad field of materials chemistry, with subjects ranging from deep space exploration to the properties of CdSe nanoparticles to computational analyses of charge-transfer within crystalline complexes.

Dominic Fortes, ISIS Neutron and Muon Source, presented results of a meticulously designed and executed study on the anisotropic thermal expansion of protonated, deuterated and fluorinated benzene crystals. While benzene is probably the most studied compound in the history of organic chemistry, the datasets discussed here by Dr. Fortes provided the first thermal expansion measurements on C_6F_6 and C_6Br_6. All of the benzene derivatives exhibit anisotropic expansion, but that of C_6F_6 is extreme. The expansion along the 2-fold axis is several times larger than the greatest linear expansion in any of the other analogues. Moreover, there is a dramatic variation in the linear expansion along the c-axis, indicating the onset of rotational disorder at this temperature. One striking preliminary result reported by Dr. Fortes that the relative change in unit-cell volumes, when normalized by the respective melting temperatures, are very similar for the low melting-point species C_6H_6, C_6D_6 and C_6F_6, whereas that of the higher melting-point species C_6Br_6 differs significantly.

Georgii Bogdanov, of the New Mexico Highlands U, reported on a custom-built novel setup for organic crystal growth by vapor deposition. His apparatus enables growth of soluble materials with much improved crystal structure characteristics, when compared to materials synthesized through traditional solution-growth mechanisms. This has been achieved through the implementation of a three-zone furnace, digital thermo-controller and turbo-molecular pump, allowing for a highly precise control of the experimental conditions within the growth chamber.

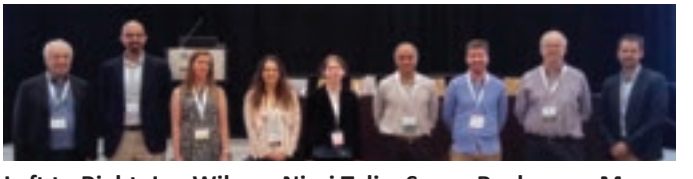
Olaf Borkiewicz

2.3.1: Would You Publish This?

This popular, less formal evening session was attended by over 70 scientists who discussed and debated a variety of questionable crystal structures. Some highlights included **Christine Beavers** (Advanced Light Source) presenting on 'tetrahedral carbonates' in a high-pressure crystal structure of an alkali/calcium carbonate shortite. Under pressure the typically planar CO_3 ions distort to be pyramidal, further examination shows that the distortion causes neighboring carbonates to interact via a long C···O interaction to form a C_2O_6 type moiety. **Joe Tanski** (Vassar College) presented on whole molecule disorder in 7-chloro and 7-methyl indole structures which elicited the most discussion of the evening. It focused on choosing the appropriate crystal system and space group when the seemingly isostructural 7-methyl indole refined in Monoclinic $P2_1/c$ with a beta angle almost exactly 90 degrees and the 7-chloro indole refined in Orthorhombic Pnma. Both structures showed whole molecule disorder, but the 7-chloro indole was disordered across a symmetry site. This presentation and subsequent discussion felt especially appropriate given that the session followed the day long special session honoring the late Dick Marsh. Other presenters included **Louise Dawe** (Wilfrid Laurier U.), **Victor Young** (U. of Minnesota), and **Danielle Gray** (U. of Illinois, Urbana-Champaign).

Danielle Gray and Jeff Bertke

Session 3.1.1 & 4.1.1: Structure Biology of Pathogens: Cellular Interactions, Drug Resistance, and Immune Responses



Left to Right: Ian Wilson, Niraj Tolia, Susan Buchanan, Megan Sjodt, Jessica Thomaston, B. V. V. Prasad, Stephen Scally, Michael Becker, Jean-Philippe Julien.

The speakers of the first Structural Biology of Pathogens session described applications of structure-based design to combat malaria, influenza, and pathogenic bacteria. To begin, **Niraj Tolia**, Washington U and NIAID, NIH) and **Stephen Scally**, Hospital for Sick Children, each recounted their efforts to characterize antibody-antigen interactions specific for malarial proteins, namely, *Plasmodium vivax* proteins, DBP and DARC, and *Plasmodium falciparum* circumsporozoite protein, respectively. Both researchers plan to use this structural data from their crystallographic studies, complemented

by biophysical techniques, to guide vaccine design.

After the coffee break, **Ian Wilson** (The Scripps Research Institute) presented work done by his group to design broadly-neutralizing small molecule inhibitors against influenza virus hemagglutinin, also by using the molecular basis of antibody-antigen binding as a guide. In contrast, using lipidic cubic phase-induced crystallization, **Jessica Thomaston** (U of California, San Francisco) targeted influenza by elucidating the mechanisms through which adamantane drugs inhibit the influenza virus M2 proton channel in order to use this knowledge to direct development of new inhibitors against emerging drug-resistant variants of the channel. Next, **Susan Buchanan** (NIDDK, NIH) shifted our attention towards the world of gram-negative bacteria, as she described her efforts to understand the Ton-B dependent transport system through X-ray crystallography, using seleno-methionine substitution and heavy atom soaking to overcome the phase problem, as well as preliminary low-resolution cryo-EM studies.

Finally, for the last talk of the session, **Megan Sjodt** (Harvard Medical School) introduced us to evolutionary coupling-enabled molecular replacement (EC-MR), a novel method in which evolutionary sequence covariation is used to produce models for molecular replacement. In this case, EC-MR provided a solution for the structure of RodA, a protein essential for synthesis of the bacterial cell wall, revealing potential target sites for small molecule inhibitors. Overall, this session demonstrated the valuable and diverse use of structural data for design of therapeutics in parasitology, virology and bacteriology.

The second Structural Biology of Pathogens session focused on the structural characterization of proteins from a variety of pathogens that are targets for therapeutic development. **Timothy Palzkill** (Baylor College of Medicine) started the session with an overview of resistance mechanisms that gram-negative bacteria employ to degrade β-lactam-based antibiotics. He focused on two β-lactamase enzymes, TEM1 and CTX-M, and extensively characterized the effect of key residues on acquired β-lactam resistance, describing several evolved mutations that confer wide selectivity for a range of broad-spectrum β-lactam antibiotics.

After this, **Ute Krengel** (U of Oslo) and **Liya Hu** (Baylor College of Medicine) both spoke about the importance of blood group antigens for pathogen infectivity and pathogenesis. Ute Krengel showed the specificity of cholera toxin to different blood group antigens, and structurally and biophysically characterized the preference of the toxin towards H group antigens, over A or B antigens. Based on this structural insight, she proposed the development of glycan mimetics that would be able to inhibit cholera pathogenesis by preventing binding of the toxin to blood group antigens on cells. Liya Hu described how rotavirus specifically interacts with blood group antigens, depending on the genotype of the virus. She provided insights into rotavirus host restriction and the susceptibility to specific strains depending on blood group antigens. This extensive characterization provides a useful pathway for the development of glycan-based therapeutics that would be able to inhibit rotavirus binding to cell surface glycans.

After the coffee break, **Lynne Howell** (Hospital for Sick Children) described her ongoing characterization of the *Pseudomonas aeruginosa* Pel pathway and the essential role that it plays in *P. aeruginosa* biofilm formation and survival. Through extensive structural and molecular biology studies, her group has elucidated the role of several key players of Pel polysaccharide synthesis and described an overall mechanism for Pel production for biofilms. Interestingly, she also characterized PelA, a surprising member of the Pel pathway that is capable of degrading Pel polymers, showing that this protein can be used to degrade Pel biofilms specifically, rendering the bacteria more sensitive to eradication through antibiotics. Next, **Michael Murphy** (U of British Columbia) provided a structural characterization of how the *Staphylococcus aureus* protein, IsdB, is capable of extracting heme from hemoglobin to promote bacterial survival. His structures provided insight into how heme is transferred to the IsdB receptor through receptor-induced unfolding of α-helix F in hemoglobin, shifting heme towards the IsdB receptor, where it can be coordinated by specific tyrosine residues to promote extraction.

Christopher Koth (Genentech) talked about two key projects; one focused on the structural characterization and development of inhibitors for Nav1.7, which is a voltage-gated sodium channel that is a key player in pain propagation, by cryo-EM. He also discussed the importance of MsbA, an ABC transporter essential for LPS transport to the outer leaflet of the outer membrane. By X-ray crystallography, he showed the characterization of a MsbA inhibitor that binds in the transmembrane portion of MsbA and is capable of preventing LPS transport, resulting in bactericidal activity.

Lastly, **Shuxia Peng** (Oklahoma State U) described the crystal structure of A6, a protein in poxviruses

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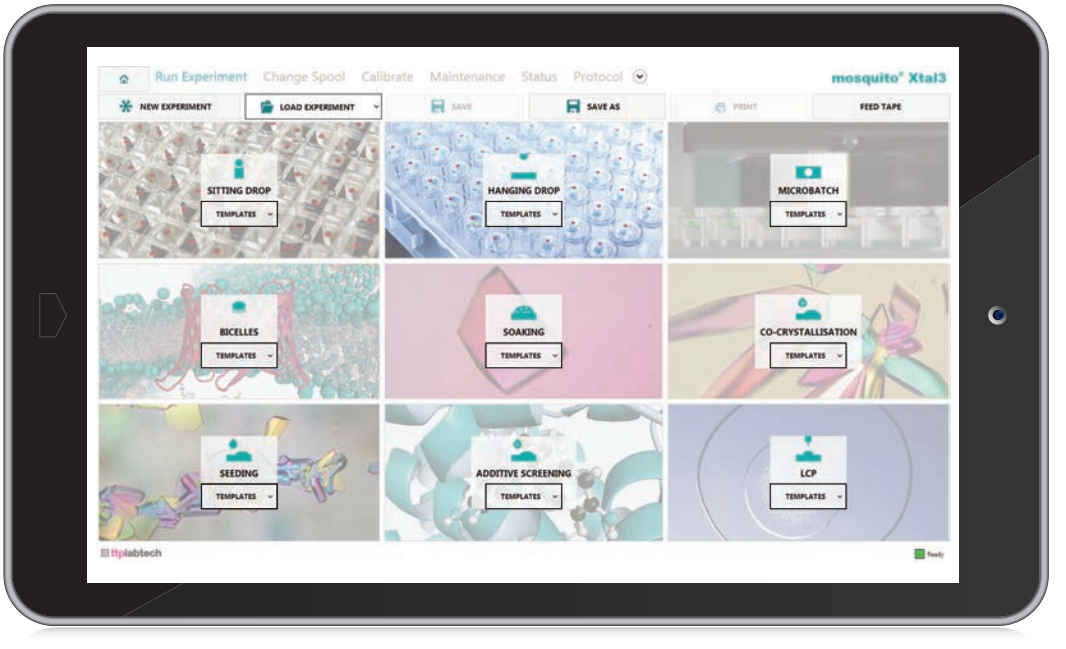

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that is essential for lipid transfer and membrane crescent formation. She provided structural evidence for how the different domains of the A6 protein may be involved in generating and stabilizing open-ended membranes that are important for viral membrane biogenesis. Overall, this diverse session provided insights into several thought-provoking studies of the therapeutically-relevant mechanisms for targeting and inhibiting clinically important pathogens, where the role of glycobiology was prominent in many of them. In addition, numerous impressive posters were presented related to both sessions.

Report by Taylor Sicard and Elaine Thai - the Hospital for Sick Children Research Institute and the University of Toronto.

3.1.2: Best Practices for Building, Refining, and Analyzing Ligands in Macromolecular Structures

Left to Rignt: Dorothee Liebschner, Thierry Fischmann, Anna Gardberg, Paul Emsley, Stephen Burley, Jack Tanner.
Photo courtesy of Anna Gardberg.

This session was chaired by Anna Gardberg, Constellation Pharmaceuticals, and Kurt Krause, University of Otago, NZ (although Kurt helped with planning, he was unable to attend so Jan Abendroth assisted with A/V and timing).

Jack Tanner, University of Missouri-Columbia, presented a case study for an incorrect ligand and highlighted the **https://pdb-redo.eu/** automated tool to find/fix strained regions, distorted geometry, and close contacts.

Stephen Burley, PDB, spoke about OneDep for validation during deposition. The new "versioning" system for deposited structures should simplify later corrections in the event that ligands need to be corrected.

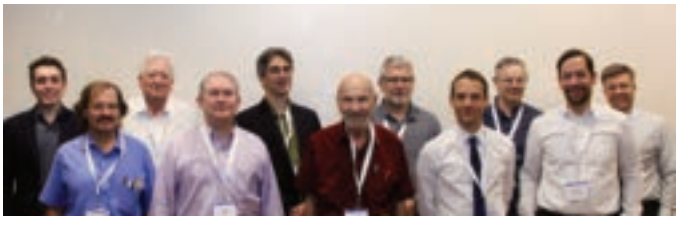
Thierry Fischmann, Merck (US), gave an overview of a workflow to generate and refine ligands correctly, highlighting GRADE to automate MOGUL for ligand CIF dictionary restraints, followed by Buster refinement. He mentioned that Buster outputs a report entitled "Ligand Mogul Analysis" which can further help with ligand validation. Thierry also spoke about radiation damage, with Br, Cl, and nitrile substituents most vulnerable, and suggested mitigation strategies for this problem.

Paul Emsley, MRC (UK), gave a useful COOT tip - for map display in bright rooms, resample the map and use "cut glass" mode. Then Paul moved on to describing COOT's tools for building and refining ligands: incorporating ACEDRG for dictionaries and computing a ligand distortion score.

Dorothee Liebschner, LBNL/Phenix, spoke about Polder maps as an improvement over OMIT maps for ligand validation, and which can also help to tease out ligands from bulk solvent.

Anna Gardberg

3.1.3 & 3.2.3: Theoretical and Computational Crystallography - Present and Future Opportunities at the Structural Interface of Experiment and Theory 1 & 2



Left to Right: John Dagdelen, Greg McColm, Michael O'Keefe, Branton Campbell, Peter Khalifah, Shelomo Ben-Abraham, Michael Ruf, Angelo Ziletti, Simon Billinge, Nils Zimmermann, Gus Hart. Speakers not included in the photo: Pavol Juhas, Stephan Lany, and Tania Gabriela Diaz Rodriguez.

The 2018 ACA meeting provided a special spotlight on the emerging applications of computational crystallography for the study of materials, with this double-length session covering both experimental and theoretical applications. Although this topic area is not commonly a part of ACA meeting, it was clear from the talks that computational tools are presently being developed to solve many challenging crystallographic problems that would otherwise be intractable.

Three morning talks feature research with a focus on topological analysis. While **Michael O'Keefe**, Arizona State U, is well-known for his classification of framework structures, his talk in this session focused on the classification and enumeration of the generally unexplored class of structural weavings in which linear chains may cross each other. This work was complemented by a presentation of **Greg McColm**, U South Florida, on the theoretical use of geometry and topology for structure prediction, as well as one by **Shelomo Ben-Abraham**, Ben-Gurion U, on some particularly intriguing aperiodic tilings.

More experimentally driven talks on structural analysis that spotlighted new computational

approaches included the work of **Simon Billinge**, Columbia U, on establishing the nature of the distribution of nanoparticle shapes from pair distribution function (PDF) data, the efforts of **Pavol Juhas**, Brookhaven National Lab, to develop the first routines for the search/match analysis of PDF patterns, and Peter Khalifah's combination of enumeration methods with high-throughput Rietveld refinement to solve large unit cell superstructures whose formation is driven by the ordering of mobile cations in battery cathodes at low temperatures.

Several talks focused on extending the precision with which structural analysis can be done. New Bruker single crystal diffraction software tools for modeling non-spherical electron densities around atoms using the Invariom-derived electron analysis (IDEAL) methodology were highlighted by **Michael Ruf**, Bruker AXS. On the powder diffraction side, **Peter Khalifah**, Brookhaven National Lab, presented a new general approach for visualizing the parameter space associated with occupancy defects through *f** diagrams, and demonstrated that using this approach powder diffraction data has sufficient sensitivity to identify problems with the X-ray atomic form factors routinely used in structural analysis, as well as to identify occupancy defects present at the 0.1% level. **Branton Campbell**, Brigham Young U, described the use of group representation theory to search for rigid-unit modes in networks of interconnected polyhedral, which has the dual advantages of allowing comprehensive searches to be carried out and of reducing the time needed for such searches by many orders of magnitude so that computational results are obtained nearly instantly.

The application of machine learning techniques to the high-throughput analysis of nanoscale electron diffraction data was presented by **Angelo Ziletti**, Fritz Haber Institute. In this study, deep-learning algorithms were able to automatically assign the orientations of different grains within 2D electron microscopy images after suitable training using a compact diffraction-based representation. **Gus Hart**, Brigham Young U, presented efforts to obtain quantum-accurate material energies at a small fraction of the computational cost, even for complex structures with many atom types. Additionally, it was demonstrated that commonly used cluster expansion methods are not suitable for certain classes of chemical compounds in which the size of the substituting atom modestly differs from the atom which it is replacing, thus overturning the conventional wisdom about this method. Complementary structure-based methods for continuously classifying the deviation from ideality of about two dozen local coordination environment were described by **Nils Zimmermann**, Lawrence Berkeley Lab, and these methods provide an important structural descriptor that can provide the basis for a variety of machine learning studies.

Last but not least, there were a series of talks on the application of density-functional theory (DFT) methods to make structure predictions and to explore structure-properties relationships. **Stephan Lany**, National Renewable Energy Lab, presented research aimed at discovering novel nitride compounds whose light absorbing properties have long been of interest, and this work was complemented by experimental studies to confirm the existence of predicted phases. **Tania Diaz Rodriguez**, U Autonoma Mexico, illuminated the electronic and atonic structures of a series of TiO_2 nanoclusters. Finally, **John Dagdelen**, UC Berkeley, discussed the computational screening of new auxetic materials (that when stretched expand perpendicular to the axis of elongation) with a negative Poisson's ratio in all directions. While some composite materials which exhibit these properties are known, single-phase materials with this type of behavior are exceptionally rare and high-throughput DFT methods have provided a new pathway to accelerate their discovery.

Peter Khalifah and Branton Campbell

3.1.5: Crystallography at Extreme Conditions

Crystallography coupled with an applied stimuli, like temperature, pressure or light, can reveal new phases and intriguing material properties. In our session, entitled "Crystallography at Extreme Conditions," an engaging group of speakers shared their experiences in *in-situ* diffraction. **Emma Ehrenreich-Petersen**, Aarhus U., gave an informative introduction to high pressure, high temperature work employing laser heating in diamond anvil cells (DACs), in addition to describing her research into rare earth metal nitrides. We commonly think of nitrogen gas as unreactive, but at high pressures and temperatures, this assumption breaks down, and nitrogen gas will react with metals to form metal nitrides. **Weizhao Cai**, U. Utah, described his work with lead bromide hybrid perovskites under pressure. Under pressure these potential photovoltaic materials undergo phase transformations, in addition to band gap shifts. **Martin Adam**, Bruker, described the impressive

in-house single crystal diffractometer, designed for high pressure diffraction, installed at the University of Hawaii, Manoa. Most practitioners of high pressure diffraction frequent synchrotron beamlines, but some prefer to have access to similar capabilities, albeit lower intensity, in their home lab.

Clemens Prescher, U.Cologne, asked the question of whether we are prepared for "Big Data" in high pressure science. Clemens is well known for his fast and user-friendly program Dioptas, which can calibrate and radially integrate 2-D diffraction patterns easily, and also includes functionality relevant to high pressure diffraction (http://github.com/Dioptas/Dioptas). With the arrival of brighter X-ray sources and faster detectors, we can collect more data faster than ever, but is more really better? Clemens argued that more will only equal better if we can take advantage the speed and analyze data on the fly. He also advocated for more scientists to write programs, because programmers lack the scientific knowledge to make science-relevant tools.

After the coffee break, we were joined by **Patricia Kalita**, Sandia National Lab, who has utilized the Dynamic Compression Sector(DCS) at the Advanced Photon Source (APS) at Argonne National Lab to explore the shock behavior of calcium fluoride. The DCS specializes in shock compression experiments, combining synchrotron X-rays with a gas gun that fires an impactor at the sample, and high speed diffraction images, which offer time resolution of the shock process. **Matthew Whitaker**, Stony Brook U., regaled us with his adventures in improving high pressure methodology. Matthew is a well-known innovator in high pressure work, employing large volume presses to study larger samples at high pressures and temperature. He has adapted his system at APS to offer ultrasonic interferometry as well as energy dispersive X-ray diffraction, with data rates 3 orders of magnitude faster than other competing systems. He also shared his highly exciting method for reproducing an amorphous phase, maskelynite, found in meteorites. Known as the SMACADAC method, a loaded DAC was dropped from height, which simulated the shock conditions necessary for the desired phase! **Carla Slebodnick**, Virginia Tech, detailed a high temperature exploration into the structural stability of datolie, which has potential as a nuclear waste sequestration agent.

Both **Melissa Sims** and **Melinda Rucks**, Stony Brook U., are interested in simulating geological impact conditions, but they employed distinct methods to investigate different aspects. Melissa employed a gas membrae DAC, to do precise pressure ramps, which allowed her to explore the effects of strain rate and kinetics. Melinda used a large volume press capable of spike heating while at high pressure, which created additional thermal pressure. **Cara Vennari**, UC Santa Cruz, was also investigating a geological process, the reaction of carbonate minerals to pressure. Cara shared a fun animated gif which set the tone: carbonitic magmas have very little viscosity compared to their silicate brethren. Carbonates aren't known to polymerize at ambient pressure, but Cara showed recent work on the mineral shortite, which does indicate that carbonates could polymerize at pressures found in the upper mantle. Cara was the Small Molecule SIG Margaret C. Etter Student Lecturer Awardee, and her talk was certainly worthy.

This session was well attended, and seemed enjoyed by those in attendance. We are thankful to our generous sponsors who funded invited speaker travel and supported students: Anton Parr, Dectris and Stoe. If you are doing crystallography at extreme conditions, keep this session in mind for ACA Northern Kentucky 2019.

Christine Beavers

Board on International Scientific Organizations
U.S. National Committee for Crystallography

Call for Proposals: Funding Support for Crystallographic Activities

The USNC/Cr supports crystallographic activities relating to the organization of conferences, workshops, and education outreach events. Applications are accepted and reviewed twice a year on a competitive basis. Your request should be submitted at least six months prior to your proposed activity.

Requests should be made by filling out and submitting the USNC/Cr Funding Request Form:

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The deadlines for each reviewing cycle are May 15 and November 15 of each year. If your proposed activity is funded, you will be required to submit a final report to the USNC/Cr within 30 days after the event.

3.2.1: Structural Biology of Inherited Metabolic Disorders: Personalized Biochemistry and Biophysics

Emily Arturo receives the Etter Student Lecturer Award from Jack Tanner.

This session was highly attended, with audiences above 70. The session featured four cornerstone presentations by senior PIs and four student presentations. **Wyatt Yue**, SGC/Oxford University, gave an overview of therapeutic strategies for inherited metabolic disorders using pyridoxine-related diseases as examples. **Julie Forman-Kay**, Univ. of Toronto, gave a comprehensive presentation about the structural biology of the cystic fibrosis transmembrane conductance regulator (CFTR), including a sneak-peek of a cryo-EM structure. **Eileen Jaffe**, Fox-Chase Cancer Center, discussed how alternative modes of oligomerization of phenylalanine hydroxylase underlie ALAD porphyria. The fourth cornerstone talk was by Mark Gerstein, Yale, who described computational methods his group has developed to understand the effects of genetic variations on protein function. Outstanding student presentations were delivered by **Kyle Stiers** (Univ. of Missouri), **Piotr Wilk** (Helmholtz-Zentrum Berlin), **Emily Arturo** (Fox-Chase Cancer Center), and **Matthew Whitley** (University of Pittsburgh School of Medicine). A unifying theme that emerged from the student talks is that genetic variations can "break" metabolic enzymes in a variety of ways, including modulating flexibility, producing steric clash in the active site, and altering oligomerization.

Jack Tanner

3.2.2: Crystallization on the International Space Station

Left to Right: Joseph Ng, Kristofer Gonzalez-DeWhitt, Ken Savin, Timothy Mueser, Gloria Borgstahl, Marc Giulianotti, Tanaka Hiroaki, Paul Reichert.

The use of microgravity to improve the quality and size of crystals for structural determination studies has been explored since the days of Mir and the Space Shuttle. Now with the availability of a long-duration microgravity environment aboard the International Space Station (ISS) these experiments have continued and expanded. This inaugural ACA session provided a forum for topics ranging from how to access the ISS for research purposes, best practices for microgravity crystal growth research, novel uses of microgravity for biological formulations, overview of different equipment, student STEAM engagement, as well as an overview of recent and upcoming experiments conducted on the ISS.

The session began with an introduction from **Ken Savin** and **Marc Giulianotti** both representing the Center for the Advancement of Science in Space (CASIS). Their talk described the role CASIS plays in managing the US National Laboratory aboard the ISS. They provided a historical overview of microgravity crystal growth, summarized the recent work onboard the ISS, and introduced a new Request for Proposals, www.iss-casis.org/mmcg, to support crystal growth experiments on the ISS. **Joseph Ng** (University of Alabama, Huntsville and iXpressGenes, Inc.) presented a case for utilizing the ISS to grow large crystals for neutron diffraction studies. **Paul Reichert** (Merck Research Laboratories) presented work with monoclonal antibodies, including Keytruda (pembrolizumab), onboard the ISS. This work covered the use of the microgravity environment for potential structure, purification, and drug delivery applications. **Ilia Guzei** (University of Wisconsin Madison) followed by describing how he has expanded his successful statewide STEAM program focused on crystal growth to now include an ISS experiment component.

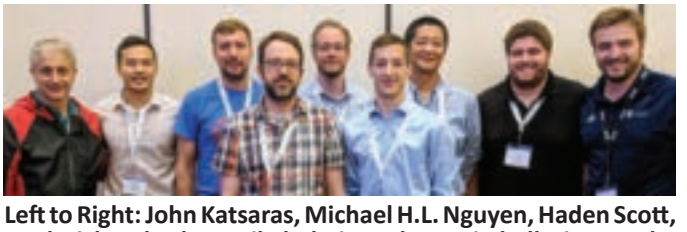
The session was open to the public and before the coffee break the audience, including students from the local area, were invited to participate in hands-on activities. These activities included two different virtual reality (VR) experiences. Nanome

Inc. provided attendees a VR experience at the atomic level while CASIS allowed people the opportunity to virtually explore the International Space Station. Anatrace/Molecular Dimensions gave attendees the chance to utilize the same hardware that has been to space.

The second half of the session began with a talk from **Kristofer Gonzalez-DeWhitt** (Bionetics Corp.) describing the use of commercial off-the-shelf crystallization products for expediting crystal growth experiments onboard the ISS. This was followed by two separate talks from **Timothy Mueser** (University of Toledo) and **Gloria Borgstahl** (University of Nebraska Medical Center). Each described how they are utilizing the ISS to grow large high quality crystals for neutron diffraction studies. The session closed with a talk from **Tanaka Hiroaki** (Confocal Sciences Inc.) where he described a novel device for growing large crystals both in an Earth-based laboratory as well as aboard the ISS.

Ken Savin and Marc Giulianotti

3.2.4 Scattering Strategies in Biomembrane Research



Left to Right: John Katsaras, Michael H.L. Nguyen, Haden Scott, Frederick Heberle, Maikel Rheinstadter, Mitchell DiPasquale, Michihiro Nagao, Brett Rickeard and Drew Marquardt.
Photo curtesy of Maikel Rheinstadter.

The biomembrane session was a rousing success, with an effective balance of invited speakers and contributed talks. These included several contributed talks from students, which gave them an opportunity to present their findings and develop their soft skills. Half of the talks were from Canadian institutions.

The session began with a fantastic invited talk by a very jetlagged **Michihiro Nagao**, NIST Center for Neutron Research. Michi presented a brilliant overview of the neutron spin-echo (NSE) technique and how it can be applied to the study of biomembrane bending rigidities and membrane thickness fluctuations. He further discussed a new theory relating thickness fluctuations to membrane viscosity and lipid lateral diffusion.

Dr. Nagao's talk was followed by the first student contribution of the session from **Mitchell DiPasquale**, University of Windsor, discussing his research on vitamin E in lipid membranes. He reported on the use of small angle neutron scattering (SANS) to investigate perturbations to a lipid bilayer induced by various tocopherol species including α-tocopherol, γ-tocopherol, and α-tocopherylquinone. Using unilamellar vesicles composed of domain-forming lipids, Mitchell elucidated that an increase in the tocopherol concentration was correlated with a destabilization of ordered lipid domains. This effect was evident with α-tocopherol and γ-tocopherol but much less pronounced in the quinone-doped system.

Frederick Heberle, U of Tennessee, gave an update on methods for determining the transbilayer structure of lipid membranes using SANS, with an emphasis on the structure of asymmetric bilayers. Fred highlighted the challenges of investigating membrane asymmetry and noted recent advances in the preparation of asymmetric liposomes. He emphasized that neutron scattering is particularly well suited for determining membrane structure due to the strong contrast between the stable hydrogen isotopes protium (^{1}H) and deuterium (^{2}H), and how the combined use of protiated and deuterated lipids, together with NMR and GC-MS, can be used to generate interleaflet contrast and thereby elucidate the asymmetric matter distribution normal to the bilayer plane.

Continuing the theme of membrane asymmetry, the first half of the session ended with an engaging student contribution by **Michael Nguyen**, U of Windsor. Michael discussed his preliminary data showing that the method in which peptides are incorporated into lipid bilayers is critically important for the retention of lipid asymmetry, and in turn the ability to measure flip-flop using SANS. He highlighted that peptides added externally to asymmetric vesicles resulted in an almost instantaneous loss of the lipid asymmetry (i.e., fast flip-flop on a time-scale that cannot be resolved by SANS). In contrast, lipid asymmetry was retained when peptides were pre-incorporated into the bilayer before generation of the asymmetry.

The second half of the session was kicked off by invited speaker **John Katsaras**, Oak Ridge National Laboratory, who provided an update of his group's pioneering use of SANS and NSE to study nanoscopic lipid domains in biomimetic membranes. This exciting work has culminated in the first use of neutron scattering to observe lipid domains in a living cell, the Gram-positive bacterium *Bacillus subtilis*.

Maikel Rheinstadter, McMaster U, finished up the talks by faculty and senior scientists with an overview of his lab's research program. Maikel discussed alternative and novel ways to detect small and fluctuating heterogeneities in membranes by controlling the coherence length of neutron beams

in neutron diffraction experiments. By using this technique, he observed the formation of cholesterol rafts and plaques in lipid membranes containing cholesterol and discussed the effect of the common drug aspirin on these structures.

Brett Rickeard, student presenter from U of Windsor, discussed the structural characterization of novel synthetic phospholipids containing siloxane chains. He spoke about the self-assembly properties of these newly synthesized lipids when subjected to an aqueous environment. The morphology of the resulting bilayers was characterized using small angle X-ray scattering (SAXS). Interestingly, the different lipids showed different self-assembly properties that correlated with the volume of the siloxane moiety relative to the total volume of the alkyl chains in the fatty acid residue.

The session ended on an exciting student contribution from **Haden Scott**, U of Tennessee. Haden discussed his PhD studies of interactions between membranes and the pH-low insertion peptide (pHLIP), which can adopt either a surface-bound or inserted (transbilayer) state depending on the pH. In this work, NSE was used to measure membrane dynamics including bending rigidity and thickness fluctuations, and SANS and SAXS were employed to measure the average membrane thickness and area per lipid. Both SANS and SAXS showed that pHLIP conformation did not affect the average bilayer structure. In contrast, NSE detected significant differences in membrane dynamics between the two protein states. Specifically, pHLIP in the surface-associated state decreased the amplitude of the membrane's fluctuations while increasing their frequency. Strikingly, as a transmembrane helix, pHLIP dampened the membrane's fluctuations.

Drew Marquardt, Frederick Heberle, and Maikel Rheinstadter

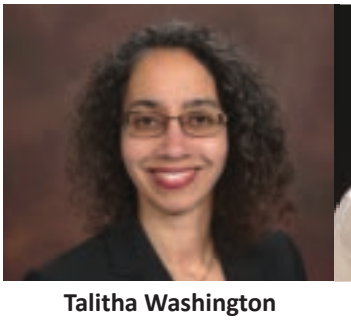
3.2.5: Mineralogical Crystallography

Left to right: Aaron Celestian, Camelia Stan, Adel Mesbah, J. Caleb Chappell, Nichole Valdez, Maxwell Day, Nancy Ross.

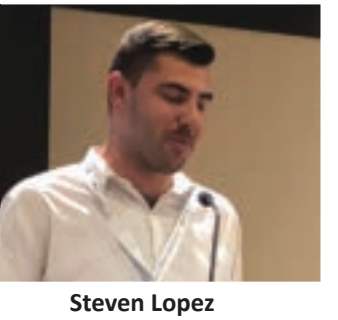
Session 3.2.5 brought together crystallographic researchers from all branches of mineralogy. Mineralogy is a broad science that encompasses aspects of material discovery, inspiring emerging technologies, understanding current and geological past of Earth, and the systematic classification of their structures. There were many interesting talks at this years meeting, but here are a few highlights. The mineral apatite has curious crystal chemistry that has confounded researchers for years. **J. Caleb Chappell,** Miami Univ. of Ohio, presented recent results of apatite structural distortion of its growth in Th-rich hydrothermal systems, with an eye toward understanding its structural stability and formation conditions. Xenotime is also a geological important mineral, as it has a wide P, T formation range and is often used for U-Pb geochronology. **Nancy Ross**, Virginia Tech, discussed the high-pressure crystallography and the equation of state for xenotime. **Maxwell Day**, U of Manitoba, presented the advancements he has made in developing a structural hierarchy for silicates that could be used for future methods of predicting mineral structure, their stability, and structural relationships.

Aaron Celestian

3.3.1: Diversity & Inclusivity



Talitha Washington



Steven Lopez

The session included two talks focused on historically underrepresented minority students. The session wished to explore how institutions get designated as minority serving institutions, what programs are available for funding in academic institutions, and what organizations are being formed to support URM students in science, technology, mathematics, and engineering, and especially in biomedical careers.

The first talk was by **Talitha Washington** who is a Program Director for the National Science Foundation (NSF). Her oversight includes the IUSE (Improving Undergraduate STEM Education) program, though he talked generally about funding for Hispanic Serving Institutions (HSIs) through the NSF. The NSF, like the NIH, seeks to improve the recruitment and retention of underrepresented minority (URM) students in science, engineering, mathematics, and biomedical fields. The approach is through the development of student support, faculty support, improvement of STEM curricula, greater participation in research, and partnerships with industry, government, and

communities. While much of the program seeks to improve access for URM students, the NSF also seeks to develop new strategies and best practices that can be exploited across the nation in both urban and rural universities, and non-research intensive colleges and universities. Increasingly, more institutions will be designated as minority serving institutions in the coming years with URM student communities over 25% of the total population. The priority will increasingly focus on greater retention of students from matriculation to graduation.

The second talk was by **Steven Lopez**, Assistant Professor of Chemistry at Northeastern University and Co-President and Co-Founder of the Alliance for Diversity in Science and Engineering (ADSE). Steven noted the lack of participation of URM groups in academic, industry, and government, and the focus of ADSE on mentorship and support of graduate student groups. At present, there are roughly a dozen student chapters across the US, which support visiting speakers, young scientist conferences, and networking among undergraduate and graduate students and postdoctoral research fellows. The organization grew from the merging of two graduate student groups, one at UCLA and a second at UCSB. He encourages faculty to help students form a local student group at their own institution.

Attendance, as it was last year, was poor since this was an evening event. The session chair encourages the ACA to move this session to the regular daytime session slot.

Bernard Santarsiero

4.1.2: Minding the Gap: MX to XFEL / Open Science

Left to Right: Ana Gonzalez, Marian Szebenyi, Aina Cohen, Nick Sauter, Elspeth Garman, Masaki Yamamoto, Qun Liu, Herbert Bernstein, Jennifer Wierman.

The first speaker was **Qun Liu**, NSLS-II, who gave updates on sample manipulation and data assembly at the FMX and AMX endstations. By raster scanning across polyimide micromounts from MiTeGen, their team is able to generate heat maps which can guide further data collection. Once a reference set is determined (perhaps through unit cell variation), on-the-fly analysis of serial microcrystal data sets can be obtained using correlation coefficients and Rmerge for crystal and/or frame rejection. Further data reduction using Rfree, Rsplit and Bijovet Fourier peaks. He also reported on work they've done at LCLS CXI looking at the anomalous signal in microcrystals with native SAD.

Nick Sauter, LBNL, presented on anomalous dispersion crystallography being performed at the LCLS. The talk consisted of an update to the photosystem II photocycle using the LCLS in a pump-probe configuration (in addition to collecting XES as in *In Situ* diagnostic tool!) to visualize when, how and where the O-O bond formation occurs. The team was also able to use two detectors to record both high and low resolution diffraction. Laser flashes separated by 2 ms (and probed via LCLS pulses) show the initial oxidation of Mn and subsequent reduction to observe all four states of photosystem II's photocycle. Using an omit map of oxygen, they show that it becomes a ligand to Ca and E189 moves away, while Ca maintains 8-coordination.

Elspeth Garman, Oxford University, reported on updates to RADDOSE 3D, where now the code will include photoelectrons and fluorescent photons into its algorithm for radiation damage within samples in addition to being adapted to SAXS and small molecule. She also shared the imminent release of RABDAM – which takes isolated PDB entries and gives them an index based off B-factor. Another unique tool her team will be releasing is RIDL, providing an objective assessment for damage from electron density loss in difference maps. She also revealed that most metallocenters are reduced in the PDB, and that re-evaluation must occur for correct deposits. For example, at 100K, 0.1 MGy is enough to reduce metal ions, and at 1MGy, the disulfide bond is cleaved. She reminded the audience that there are dose differences dependent on the shape of the beam (i.e. top hat versus Gaussian). Lastly, due to the nature of some of the light sources seeking higher energies, she explained how the photoelectric effect actually affects damage more at higher energies.

Aina Cohen, SLAC National Accelerator Lab, described the fixed target facility at the LCLS beamline MFX, capable of supporting different ways of data collection, including pseudo-oscillation helical data collection, and grid rastering on crystals both in undefined and defined positions. Several mounts for the crystals have been developed. Both cryo and room temperature experiments are supported, and a system to automate and optimize sample exchange at room temperature and controlled humidity is being

prototyped. Data processing is carried out on the fly, and the number of spots per image and number of indexed images are being displayed during the experiment. A facility to carry out SX experiments with a MESH injector also exists at the SSRL beamline BL12-2. The new SSRL beamline BL12-1, equipped with an Eiger 16M and multilayer optics will enhance SX capabilities.

Marian Szebenyi, MacCHESS, spoke about serial crystallography experiments at CHESS. The source is an undulator with a focusing capillary and a He path to decrease background. The Eiger 1M allows for a high speed of data collection and a reasonable resolution. The crystal mount developed at CHESS for fixed target experiments is based on a silicon chip with a surface layer of silicon nitride, covered with a thin Mylar tape to keep them hydrated at room temperature. Data collection is carried out by translating the chip and collecting a small oscillation at each point of the scan. XDS has been used to process the data. A new algorithm , Expand-Maximize-Compress or ECM increases the number of images indexed without degrading data quality. Plans for the future include the use of a new controller, growing the crystals on the chip and further automation of the experiment. She finished with a description of the ongoing upgrade to CHESS to convert it to a dedicated synchrotron source.

Masaki Yamamoto talked about the facilities at SPring8 and SACLA. Recently, SX data collected at SACLA have been used for a successful phasing experiment using SIRAS with data from a Hg derivative and a native, and, after better data processing from SAD data from the derivative alone. He then described the fixed target ZOO system installed on the SPring8 beamline BL32XU. The system uses a grid scan to locate the crystal before collecting data usually using a small oscillation. Several structures have been solved. Data set size varies between 14 and 600 crystals. The recommended data collection parameters are based on the results of an experiment exploring radiation damage and data quality when using different oscillation angles. Radiation damage was minimum for still images, but using oscillation decreased the number of images needed for SAD phasing. 3.2 MGy was the optimal dose per crystal for SAD signal. Finally, he mentioned plans to upgrade the BL41XU beamline to use pink beam and provide higher intensity for SX experiments.

The last speaker was **Herbert Bernstein,** NSLS-II. The subject of his talk was algorithms to identify unit cell clusters in a data set using different definitions of the distances between cells, as an initial step previous to doing a finer distinction between the cluster by comparing structure factors. Previous knowledge of the number of species in the data set is useful, but clustering can also be done based purely on the data. He reviewed several possible ways to reduce the cell to determine the distance. Compared to the Niggli reduction, used recently, the Selling reduction based S6 is less computation heavy and runs faster and gives same quality results. S6 uses the dot products b.c, a.c, a.b, a.d, b.d, c.d to define the space. He described to successful application of the algorithm to determine three crystals forms for NAG and benzamidine soaked crystals of lysozyme. *Jennifer Wierman*

4.1.4: Application of SAS to Complex Mixtures

Left to Right: Maxwell Watkins, Zimei Bu, Blaine Mooers, Thomas Weiss, Mattia Rocco, Nigel Kirby.

Photo courtesy of Tom Irving.

The session 4.1.4 "Application of SAS to Complex mixtures" focused on advances in experimental protocols such as size exclusion chromatography coupled to SAS (SEC-SAS) and data analysis methods to investigate samples containing different species in the solution using small angle scattering methods. The session started out with a presentation by **Thomas Weiss,** Stanford University / SSRL, who gave a general overview and introduction to the SEC-SAXS method and discussed major difficulties and pitfalls in the experimental implementation and execution. He then discussed potential solutions to handle such problems and showed how those are implemented at the optimized SEC-SAS setup available at the beam line BL4-2 at SSRL.

Then **Maxwell Watkins**, Princeton University, presented a talk on how he used SEC-SAXS together

Maxwell Watkins receives Etter Student Lecture Award from Thomas Weiss. Photo courtesy of Tom Irving.

with single-molecule Förster resonance energy transfer (smFRET) to characterize the solution structure and dynamics of highly flexible enzymes. He also explained how the method of evolving factor analysis (EFA) can be applied to the SEC-SAXS data to resolve the different conformational states in such highly flexible systems. For this excellent contributed talk, Maxwell also received the Etter student lecture award from the Small Angle Scattering SIG. Afterwards **Zimei Bu**, City College of New York, showed how SEC-SAXS was able to resolve the monomer and dimer form of α-catenin showing that the structures are much more open than expected from crystal structures. Neutron contrast matching was applied to look at α-catenin in complex with F-actin showing α-catenin even more open and flexible.

After the coffee break **Blaine Mooers**, University of Oklahoma, showed how the SEC-SAXS technique is essential in studying double stranded RNA due to the presence of aggregates that are readily formed in solution making it important to measure the sample directly after elution from the SEC column. After that **Nigel Kirby**, Australian Synchrotron, presented the co-flow methods for measuring SEC-SAXS data and how this method can be used to collect SEC-SAXS data at very high flux levels without significant capillary fouling issues. The last talk of the session was given by **Mattia Rocco**, Ospedale Policlinico San Martino, Genua, Italy, who presented a thorough introduction into the capabilities and recent developments of the SEC-SAXS module of the US-SOMO software that was specifically developed for analyzing SEC-SAXS data. Overall the session was very well attended by about 30 to 40 people throughout the whole morning session speaking to the general interest of this subject within the field of SAS and beyond. *Thomas Weiss and Nigel Kirby*

4.1.5 Operando & In-Situ Studies

Left to Right: Rebecca McAuliffe, Thomas Fitzgibbons, Andrew Allen, Michael Toney, Thomas Degen, Xiaoping Wang, and Wenqian Xu. Photo curtesy of Wenqian Xu.

In situ and operando methodology is broadly applied in modern chemistry and material science research to reveal structure-property relationships. This half-day session included seven presentations covering state of the art techniques and applications using neutron, synchrotron and lab X-ray instruments. **Michael Toney** from Stanford Synchrotron Light Source presented the opening talk of the session, on a topic of materials engineering. He showed how in situ X-ray scattering can be used to visualize crystallization pathways and to optimize synthesis of metastable phases of superior properties. An example was given on the hydrothermal synthesis of MnO_2 polymorphs. Under some chemical potential conditions, δ-MnO_2 directly transformed to the stable α-MnO_2 while skipping metastable γ and β phases predicted by theory. This apparent inconsistency was explained by size-dependent phase diagram and free energy differentials. Mike demonstrated a novel, predictive framework for materials synthesis by combining density functional theory and in situ X-ray scattering.

Andrew Allen from NIST, who presented after Mike, showed the instrumentation upgrade of Beamline 9-ID at the Advanced Photon Source (APS) to handle simultaneous ultra-small-angle, small-angle and wide-angle SAXS/SAXS/WAXS in situ measurements. This combination of scattering techniques is powerful in constructing a detailed picture of materials transformations. Allen used the technique to trace emergence and evolution of a deleterious δ-phase of nickel in an additive-manufactured nickel-based super alloy in traditional post-build heat treatments. Based on that, a further homogenization heat treatment was found to be effective in eradicating this phase. In a similar way, the combined in situ SAXS/WAXS technique was also employed by **Thomas Fitzgibbons** from Dow Chemical Company, who wanted to understand the function of polymer inhibitors in the deposition of wax from crude oil. Thomas presented his results later in the session.

After Andrew, **Xiaoping Wang** from Oak Ridge National Laboratory brought the audience to the neutron field. His talk discussed a multidimensional approach in both diffraction and parameter spaces with the use of a wavelength-resolved Laue technique. In his talk, Xiaoping gave examples of temperature slicing and time filtering of event-based single crystal neutron diffraction data, and illustrated how structural dynamics was probed in real time.

After the coffee break, **Nicholas Burtch** from Sandia National Laboratory showed his PhD work on decoding the impact of water on metal-organic framework (MOF) structures and generation of defects. This beautiful work employed *in situ* synchrotron powder and single-crystal diffraction measurements with dynamic humidity control.

Following Nick, **Rebecca McAuliffe** from University of Illinois at Urbana-Champaign showed her research on a potassium-tin-oxygen system. She showed her modification to a laboratory powder diffractometer and performance of environment-controlled temperature-resolved XRD measurements. Also based on lab diffractometers, in an earlier talk **Thomas Degen** from Malvern Panalytical showcased in situ battery testing capabilities and a cluster analysis method to boost the signal-to-noise ratio of lab data.

Wenqian Xu and Sanjit Ghose

4.2.1: Regulation of Protein Function by Shape Shifting

We originally chose the title "Regulation of Protein Function by Shape Shifting," and pointed to prototype examples (PBGS & VP40), to recruit speakers to discuss diverse ways in which protein function is regulated by what each speaker understood as a "shape shifting" phenomenon. Together, they covered a spectrum of biological processes that occur across different kingdoms of life. Many are proteins that can readily interconvert between alternate assemblies comprised of alternate subunit conformations, where this structural equilibrium is tunable. The functional distinctions were either the modulation of a single function (e.g. "on" vs. "off") or switching between alternate functions (as in moonlighting or multi-tasking).

The session began with an introduction by **Eileen K. Jaffe**, session co-chair and founder of the morpheein class of proteins. Jaffe's introduction led into a primer on the transformer VP40, delivered by **Michael Norris**, Scripps Research Institute, where VP40 is studied extensively by the Saphire group. VP40 can engage different surfaces to build different assemblies responsible for different essential functions in the Ebola virus lifecyle. Norris pointed out that VP40, and other such transformers, are a part of the "hidden proteome".

John Tainer, MD Anderson Cancer Center, described the allosteric modulation of Apoptosis-inducing Factor (AIF), by NADH. An NADH-controlled dimerization competency is proposed as the structural basis of cellular localization of AIF, where at the nucleus AIF is involved in parthanatos, while at the mitochondrial membrane it is involved in respiratory complex biogenesis. Tainer described designed dimeric variants of AIF that helped reveal the nature of the allosterically modulated multimer interface that is required for AIF's different functions.

Mark Saper, University of Michigan, reported on the shape rearrangements of LpoA, a multi-domain protein, and how different shapes are available across various species. Multiple crystal structures and solution measurements of full length or truncated LpoA demonstrate that shape changes governed by hinge motions between N- and C-terminal domains may be required to accommodate the expanse of intermembrane space that separates LpoA from its binding partner at the inner membrane space. This contributes to maintenance of the Gram negative bacterial cell wall. Saper stressed that processing and model building from archived datasets uncovered different shapes for the same primary sequence. These datasets had originally been deprioritized relative to other "better" datasets.

Yimon Aye reported remotely from her new academic home (Ecole Polytechnique Federale de Lausanne). Aye presented architecturally distinct assemblies of the alpha subunit of ribonucleotide reductase (RNR-α), which samples multiple assemblies dependent on the cellular nucleotide pool. That different RNA-α assemblies associate with different binding partners is proposed as a mechanism by which DNA replication is modulated. One assembly of RNR-α is susceptible to anti-lymphoma drugs that are proposed to leverage oligomer-specific binding sites. Rationally designed single residue substitutions afforded a dramatic shift in the equilibrium between hexameric and dimeric RNR-α assemblies allowing study of its different shape-specific capabilities.

David Korasick, University of Missouri-Columbia, reported on the dynamic oligomeric properties of aldehyde dehydrogenase 7A1 (ALDH7A1). The dimer ↔ teramer equilibrium sampled by wild-type ALDH7A1 is allosterically modulated by its co-substrate NAD+, which enhances formation of a more active tetrameric species. Interestingly, at least one single-residue variant of full length ALDH7A1, which is disease associated, samples a trimeric species that is likely the same trimeric species sampled by the C-terminal deletion variant of ALDH7A1. This result challenges the assumption that chains of a protein necessarily assemble in pairs.

Kushol Gupta, University of Pennsylvania, described the process of drug discovery that targets a multi-tasking protein, such as the viral HIV integrase, as "a Sisyphean task". He stressed that knowing the details of the different structures was critical to identifying a tractable target for drug discovery. HIV integrase can sample multiple oligomeric species, some of

which have identical molecular weight with different inter-subunit interfaces, while others can sample a gel that is selectively stabilized by an ALLINI class of antiviral drugs.

Jeffrey Watson, Gonzaga University, focused on HMG-CoA reductase from *B. cenocepacia* (BcHMGR). Unlike homologues of other organisms, this unusual HMG-CoA reductase likely does not participate in the mevalonate pathway. BcHMGR demonstrates the biphasic kinetic behavior consistent with it being a morpheein. This observation led Watson to use X-ray crystallography alongside multiple solution measurements to describe a dynamic oligomeric equilibrium including reversible assembly to a "big-mer" that maintains catalytic activity. This putative morpheein was also shown to catalyze a reaction not previously associated with HMG-CoA reductases, putting it among moonlighting proteins as well.

William Thomas during his Etter Student Lecturer Award Presentation

Graduate student, and winner of a Margaret C. Etter Student Lecturer Award, **William Thomas**, of the Ando lab (newly at Cornell University) presented his work on *B. subtilis* RNR, a class Ib RNR that was observed to assemble to a wide variety of oligomeric forms, including a helical fiber proposed to be a structural basis for inhibition. Different multimer-specific interfaces predicted by the structural equilibrium provide a rationale for the design of variants that would shift this equilibrium, ultimately allowing the detailed crystallographic structure of one of these multimers. He emphasized that without non-crystallographic measurements, there would have been no rationale to pursue other structures to which the same primary sequence could assemble; he described this as "hypothesis driven crystallography."

The discussion that followed the session stressed that neither allostery nor multi-tasking necessarily requires shape shifting. Nevertheless, the relatively large changes that characterize shape shifters, like hinge motions that rearrange domains or subunits relative to one another, are not currently well recognized as a structural basis for the tunability of protein function.

This was the inaugural public discussion of shape shifting proteins at an ACA meeting, and did not include such obvious examples at IMPDH, CTP synthase, or circadian clock proteins. There is a clear need for a common vocabulary to describe shape shifters and to improve upon how the community of structural biologists conceptualize the relationship among protein sequence, protein structure, and protein function.

Eileen K. Jaffe and Emilia C. Arturo

4.2.2: General Interest 2

Left to Right: Michael Sawaya, Markus Sutter, Wenqian Xu, Yan Kung, Nikolai R. Skrynnikov, Tengchuan Jin, Peter Y. Zavalij, Nicholas Schnicker, Bryan Chakoumakos, Travis Gallagher, Carla Slebodnick, Bruce Noll, Nick Gerasimchuk.

The General Interest 2 session started with **Travis Gallagher**, NIST/IBBR, who reported the structure of the Fab fragment of the NIST antibody standard RM8671, adding to over 20 other characterization methods and advancing RM8671's usefulness as an standard. **Yan Kung**, Bryn Mawr, presented structural data on HMG-CoA reductase that provides critical insight into NADPH cofactor specificity as well as the mechanism of cofactor and substrate binding and reactivity. **Markus Sutter**, Michigan State/LBNL, presented the crystal structure of a 6.5 MDa bacterial microcompartment protein shell. The 3.5 Å resolution structure shows highly conserved interactions between subunits, suggesting these functionally diverse organelles have similar construction. **Michael Sawaya**, UCLA, was able to drive a Green Fluorescent Protein to self-assemble into crystalline filaments by appending a protofilament of as few as 12 residues, raising the possibility of a relatively minor evolutionary pathway from globular protein to filaments. Additional talks in the macromolecular field included the use of chaperone proteins to assist with crystallization (**Tengchuan Jin**, U. Science and Technology, China), a new form of H-bonding between amino-acid ammonium group and carbonyl oxygens (**Nikolai Skrynnikov**, Purdue U.), and metalloprotein plasticity (**Nicholas Schnicker**, U. Iowa).

In the chemical crystallography area, presentations included technological advances toward electron density studies (**Bruce Noll**, Bruker AXS) and structure and metal-complexation of large-dipole azulenes. Two more unusual topics included **Brian Chakoumakas**, ORNL, and **Peter Zavalij**, U. Maryland. Brian Chakoumakas introduced vaterite, the least stable and least dense polymporh of $CaCO_3$, which forms in fish otoliths, i.e. fish ear bones. Vaterite from fish otoliths appears as spheroid clusters of particles that look amorphous based on visually inspection. Surprisingly, the round particulates are ordered with a principal optical axis and chirality. The spherical shape is generated by the packing of plates into "rosettes." The structure of the spherical fish otoliths can be used to determine the age and migration patterns of the fish. Peter Zavalij discussed Iron Gall Ink, the most common ink used between the 5th and 19th centuries. The structure of the main pigment, a variante of Fe^{III} Gallate, has remained elusive due to its amorphous nature. Five variants of Fe(III) Galate were identified, depending on iron oxidation state, pH, and temperature. The powder patterns and spectroscopic data from the structures were compared with those of the iron gall ink from historical documents and the main pigment identified as an amorphous form of an octahedral coordination polymer of Fe(gallate)•xH2O.

Carla Slebodnick and Wenqian Xu

4.2.3: Engaging Undergraduates with Crystallographic Research

Left to Right: Kraig Wheeler, Louise Dawe, William Ojala, Shao-Liang Zheng, George Lountos, Krystle McLaughlin, John Bender, and Karl Hagen.

Photo courtesy of Rachel Powers.

This half-day session included an engaging group of speakers who highlighted unique ways in which they involve undergraduates in crystallography at their institutions. **Shao-Liang Zheng,** Harvard University, discussed the development of a flexible lab module to integrate X-ray crystallography into the undergraduate curriculum at Harvard and also as a means of outreach to nearby colleges and high schools. **Karl Hagen**, Emory University, described how curriculum reform in the Chemistry department at Emory led to the design of lab modules to expose students to X-ray powder diffraction. **John Bender**, Grand Valley State University, described a productive collaboration with **Richard Staples** , Michigan State University, that allows him and several colleagues to incorporate small molecule X-ray crystallography into their research programs without having their own diffractometer. **Kraig Wheeler**, Whitworth University, told us about his successful journey to acquire an X-ray diffractometer at Whitworth under the NSF-MRI program and provided advice on the process to benefit faculty at other PUIs. **Krystle McLaughlin,** Vassar College, spoke about her experience of setting up a macromolecular crystallography research program at a predominantly undergraduate institution. She also provided advice to new faculty on balancing teaching and research. **William Ojala,** University of St. Thomas, told us about a three-week January term course he developed to expose students to concepts in crystallography. **George Lountos**, Frederick National Laboratory for Cancer Research, talked about his mentorship of a student in the NIH Summer Internship program and their project, which involved determining the structure of an enzyme from *Yersinia pestis*. **Louise Dawe,** Wilfrid Laurier University, ended the session with a talk that described her scaffolded approach to integrating crystallography into a chemical literature and scientific communication course, which culminated in a poster session attended by first year students in her general chemistry course.

Joe Tanski and Rachel Powers

4.2.4: Powder Diffraction of Industrial and Pharmaceutical Materials

This session focused on recent advances in methodology for solving crystal structures from powders and on results on industrially-relevant materials and processes. **Joel Reid**, Canadian Light Source, discussed the mail-in program for powder diffraction at the Canadian Light Source, using the Canadian Macromolecular Crystallography Facility (CMCF) bending magnet beamline (08B1-1 or CMCF-BM), available to industrial clients and academia. **Silvina Pagola**, Old Dominion University, discussed the use of the software WinPSSP for the crystal structure determination of organic materials from powders. **Elena Kabova**, University of Reading,

UK, discussed advances involving conformational restraints derived from crystal structures stored in the Cambridge Structural Database applied to the DASH software to solve crystal structures from powders.

Jim Kaduk, North Central College, Illinois Institute of Technology, and Poly Crystallography Inc., discussed the room temperature crystal structures of large-volume pharmaceuticals solved from synchrotron data collected at 11-BM APS, followed by **Amy Gindhart**, International Centre for Diffraction Data, ICDD, who discussed the incorporation of room temperature powder diffraction patterns of the top 200 pharmaceutical drugs by U.S. sales and prescription into the Powder Diffraction File databases, as part of the "Pharmaceutical Project". **Rajni Bhardwaj**, Eli Lilly & Company, discussed various case studies using X-ray powder diffraction for crystal structure determination, and as primary characterization tool during pharmaceutical solid form discovery and drug development. **Luzia Germann** (Max Planck Gesselschaft) talked about the use of in-situ monitoring methods to study the mechanisms and sequential mechanochemical formation of pharmaceutical co-crystals. **Peter Stephens** (Stony Brook University) discussed the crystal structure of iron(III)(deuteroporphyrin-IX), a material of interest toward the design of antimalarial drugs.

SIlvina Pagola & Jim Kaduk

Luzia Germann, Etter Student Lecturer Award winner, during her presentation.

4.2.5: Crystallography in Synergy with Computation, Spectroscopy and Synthesis

Left to Right: Chunhua Tony Hu, Victor Young, Nancy Ross, Joel Bernstein, Elizabeth Hillard, Larry Falvello, Lana Hiscock, Milagros Tomás, Wayne Pearson and Juergen Eckert.
Photo curtesy of Alberto Albinati.

This session was intended to address as wide a swath as possible of the problems that are addressed in structural science and the techniques that are applied to address them. The subjects covered include hydrogen location in materials and characterization of its motion; modeling of structural frameworks, under pressure; two flavors of synthetic chemistry, namely organic and organometallic; metal-metal bonds and stereochemistry; aspirin polymorphs; amide twisting; twin resolution; and one scientist's journey through important years in the development of chemical crystallography.

Location of hydrogen in host materials and identification of the state of the hydrogen and its interactions with the host continue to be a top priority in research related to a number of important applications, including hydrogen storage, proton transfer and catalysis. As explained by **Juergen Eckert**, Texas Tech U, the most sensitive experimental probes now available (inelastic and quasielastic neutron scattering, NMR) are producing high quality data that are difficult to analyze without help from theory. However, the studies that Juergen described, of H_2 in a number of MOF's and for coordinated hydrogen in a metal complex gave very good agreement only when very sophisticated ab-initio methods are employed, taking into account, in the coordinated hydrogen molecule for example, full motion in both the rotational degrees of freedom and treating the quantum dynamics explicitly.

The program opened with molecular dynamics and DFT calculations to search for structural changes in framework materials under pressure. As explained by **Nancy Ross**, Virginia Tech, the results of simulated compression and decompression were compared with selected experimental data, including diffraction patterns. The subject systems included inorganic zeolites and ZIF-8. [**https://geos.vt.edu/people/faculty/Nancy-Ross.html**].

In keeping with the spirit of the "Important Science...." program series, the presentation by **Lana Hiscock**, Wilfrid Laurier U, provided some real organic chemistry, about dicyanoheteropentacenes. The heteropentacenes are a hot area of research because some of them have been implicated in organic semiconductor development. Some background on the synthesis of penta- and higher acenes can be found in a recent review: *Eur. J. Org. Chem.* **2017**, 14-24. DOI: 10.1002/ejoc.201601129 .

Chunhua Tony Hu, New York U, recounted the remarkable process involving powder diffraction and crystal-structure prediction algorithms through which the structure of the third ambient phase of acetylsalicylic acid was analyzed. For more information, see *Cryst. Growth Des.* **2017**, *17*, 3562-3566, DOI 10.1021/acs.cgd.7b00673. Tony's animated presentation included music and images of swords.

Organometallic chemistry got its moment in the light in a presentation by **Milagros Tomás**, U Zaragoza, about a mixed-valence tetranuclear Pt(IV)Pt(II)3 compound with a distorted half-hexagram-shaped core. This compound is capable of hosting closed-shell (d10, s2) metals as was shown by the preparation of the disilver adduct, in which the original shape of the host is modified only slightly. More information can be found in *Chem. Comm*. **2017**, *53*, 13121-13124, DOI: 10.1039/c7cc07712b .

Wei Zhou, NIST Center for Neutron Research, presented a multi-technique approach to optimizing the separation of gases. A recent publication elaborates the approach used in the case of separating acetylene from carbon dioxide and ethylene. *J. Amer. Chem. Soc.* **2017**, *139*, 8022-8028. DOI: 10.1021/jacs.7b03850. Find more information on Wei Zhou's work here: https://www.ncnr.nist.gov/staff/wzhou/.

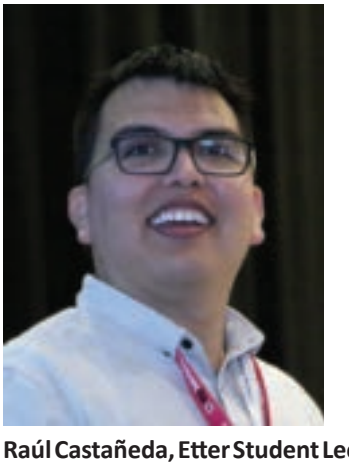
An interesting twist was presented in the talk by **Wayne Pearson**, US Naval Academy: A series of catalytically produced aryl amides was found to show torsion angles about the amide linkage ranging from nearly flat to as large as 46.2(1) degrees, and the upper limit was explored by a combination of x-ray diffraction and DFT calculations. The latter were used to gain insight into the favorable molecular conformations and their relative energies so as to estimate the energetic effects of crystal packing in the more twisted systems.

Elizabeth Hillard, CNRS, presented a multi-technique work on chemistry derived from the area of metal-metal bonds. During the 170th anniversary year of the discovery of spontaneous resolution, Elizabeth treated the audience to a panoply of spectroscopic techniques applied to the enantiomeric resolution of helicochiral paddlewheel complexes.

On twinning, **Bruce Foxman**, Brandeis U, and **Victor Young**, U of Minnesota, delivered an outstanding exposition of the history and function of Bruce's new program OMEGA, which calculates twin obliquity for an extensive set of possible twin laws. OMEGA and much more can be found on Bruce's web: http://people.brandeis.edu/~foxman1. The history of OMEGA began with Bruce's search for the program OBLIQUE by Yvon Le Page. The whole story is detailed in the distribution from Bruce's web.

Joel Bernstein, Ben Gurion U, related the fascinating history of several modern elements of molecular crystal chemistry, interwoven with his own experiences at the frontier of these developments. Beginning with the molecular and electronic structures of *trans*-azobenzene and *trans*-stilbene [*J. Amer. Chem. Soc.* **1972**, *94*, 3247-3249], and continuing through the ensuing decades up to Facts and Fictions about Polymorphism [Cruz-Cabeza, A. J.; Reutzel-Edens, S. M. & Bernstein, J., *Chem. Soc. Rev.* **2015**, *44*, 8619-8635]. Joel gave the audience a tour of modern chemical crystallography, in which he has been a principle protagonist.

Alberto Albinati and Larry Falvello



Raúl Castañeda, Etter Student Lecturer Award winner, during his presentation in Session 4.1.3.

Report on Poster Prizes, Toronto, 2018

Submitted by David R. Rose (U. Waterloo) and Louise N. Dawe (Wilfrid Laurier University)

As usual, the award committees were faced with a large number of worthy posters, making for intense discussions towards choosing the winners. A further feature this year was the presence of many posters from non-US laboratories, mostly, but not exclusively, Canadian, as reflected in the list of winners.

Pauling Poster Prizes

There were seven posters chosen for Pauling Poster Prizes. Students at the graduate or undergraduate levels (but not postdoctoral fellows) are eligible for Pauling Prizes, with no further stipulations. Of the seven, two prizes have further designations, as listed below. The posters selected were:

Tom Bateman, University of Toronto (Moraes Laboratory):

Investigation of a Novel Slam Dependent Heme Acquisition System in the Bacterial Pathogen Acinetobacter baumannii

Kenneth Childers, University of Maryland, Baltimore County:

Structural Determinants for the Activation of Soluble Guanylyl Cyclase

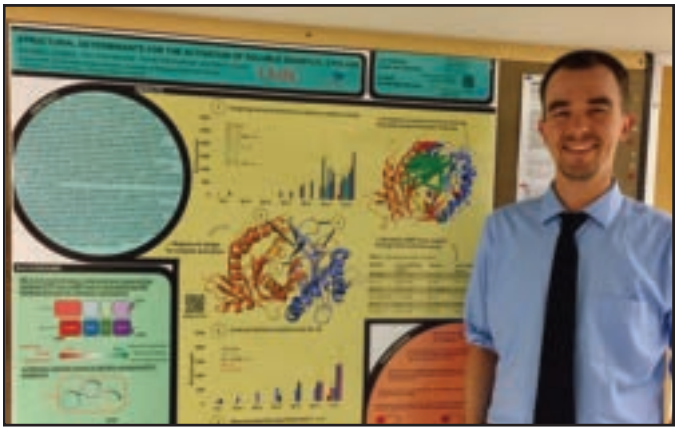


Photo curtesy of Kenneth Childers.

Andreea Gheorghita, Hospital for Sick Children and University of Toronto (Howell laboratory):

Role of AlgL in Pseudomonas aeruginosa Alginate Biosynthesis

Matthew McCallum, Hospital for Sick Children and University of Toronto (Howell laboratory):

The Molecular Mechanism of the Type IVa Pilus Motor

Tyler Vance, Queen's University, (Davies laboratory):

Diverse Ligand-Binding Domain Combinations at the Distal End of Bacterial RTX Adhesins are Postal Codes for Biofilm Formation

Louis Delbaere Pauling Poster Prize (top Canadian Poster)

Natalie Bamford, Hospital for Sick Children and University of Toronto (Howell laboratory):

Structural Insights into Biofilm Polysaccharide De-N-acetylation in the Fungi Aspergillus fumigatus

IUCr Pauling Poster Prize

Rachel Johnson, University of Leeds, UK (Stephen Muench, supervisor):

EM Studies of Cytochrome bc1 to Elucidate Inhibitor Binding

Journal of Structural Dynamics Prize

The Journal of Structural Dynamics Prize is given to a poster from a student or postdoc reporting results enabled by the emerging new instruments and new experimental and theoretical methodologies. This was awarded to:

Dmytro Guzenko, RCSB Protein Data Bank and Supercomputer Center, UC San Diego (supervised by Stephen Burley):

Complete 3D Zernike Moment Invariants: Applications to Electron Density Data

RCSB Protein Data Bank Poster Prize

The RCSB Protein Data Bank Poster Prize, awarded to a student working on macromolecular crystallography, was presented to:

Dean Lang, University of Calgary (Ken Ng laboratory):

Substrate Specificity in Three Groups of N-methyltransferases Important to Benzylisoquinoline Alkaloid Metabolism

Journal of Chemical Crystallography Prize

The Journal of Chemical Crystallography Prize is presented to a poster reporting chemical crystallography or small-molecule structure determination. It was awarded to:

Michael Guillot, Université Catholique de Louvain, Belgium (Olivier Ruant, supervisor):

Resolution of an Antifungal Compound Through Co-crystallisation

CrystEngComm Poster Prize

The CrystEngComm Poster Prize was established by the Royal Society of Chemistry for a poster in crystal engineering /supramolecular chemistry. This year's awardee was:

Aristyo Soecipto, The Hong Kong University of Science and Technology (Ian Williams, supervisor):
Chiral Segregation of Space by Anionic Assemblies found in Tartramide-based Spiroborate Salts

The next two prizes are open to participants at all levels of experience.

Oxford Cryosystems Low Temperature Poster Prize

The Oxford Cryosystems Low Temperature Poster Prize describes results making use of experiments at low temperature. The winner was:

Jin Kyun Kim, Ulsan National Institute of Science and Technology, South Korea (Chae Un Kim, supervisor):
Tracking Active-site Solvent in Human Carbonic Anhydrase II

Taylor & Francis Biomolecular Crystallography Poster Prize

The Taylor & Francis Biomolecular Crystallography Poster Prize specifies a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. It was awarded to:

Ondrej Halgas, University of Toronto (Emil Pai, supervisor):
First Experimental Visualization of the Gaseous Product CO_2 in the Active Site of ODCase Supports Substrate Strain as an Integral Part of the Catalytic Mechanism

MiTeGen-Society of Physics Students Undergraduate Poster Prize

Finally, the MiTeGen-Society of Physics Students Undergraduate Poster Prize is awarded to an undergraduate student poster. The awardee was:

Joseph Haller, home schooled, father Kenneth Haller affiliated with Suranaree University of Technology, Nakhon Ratchasima, Thailand:
Supramolecular Effects to Explain a Nonstatistical Disorder

The Poster Session Chairs would like to acknowledge all the presenters, who put considerable effort into producing posters of exceptionally high quality, making our jobs pleasantly difficult.

Many judges volunteered their time in evaluating the posters:

Gerald F. Audette, Christine M. Beavers, Robert A. Burrow, Matthew Clifton, Zygmunt S. Derewenda, Yael Diskin-Posner, James C. Fettinger, Katrina Forest, Marie E. Fraser, Ana G. Gonzalez, Danielle Gray, Todd Holyoak, Clara L. Kielkopf, Ute Krengel, Catherine Lawson, Jeffrey Lee, Adelaine K. Leung, Rebecca D. McAuliffe, Krystle J. McLaughlin, Eric J. Montemayor, Blaine Mooers, Kenneth Ng, Trushar Patel, Rachel A. Powers, Gil Prive, Soumya G. Remesh, Brian Shilton, Dmitriy Soldatov, Robyn Stanfield, Charles Stewart Jr., Edwin Stevens, Mariana Szebenyi, Wolfram Tempel, Filip Topic, Xiaoping Wang, and Kraig Wheeler.

Board on International Scientific Organizations
U.S. National Committee for Crystallography

USNC/Cr Recommendations for Crystallography Education

X-ray diffraction is an essential analytical technique used extensively in the physical and biological sciences for the determination of molecular structure with atomic scale resolution. The USNC/Cr encourages the incorporation of relevant crystallography topics into curricula at all educational levels in the US. The document below provides guidelines on recommended course content:

Crystallography Education Policies for the Physical and Life Sciences
Sustaining the Science of Molecular Structure in the 21st Century

Prepared by the American Crystallographic Association and the United States National Committee for Crystallography, ©2006.

http://www.amercrystalassn.org/documents/USNCCrPolicies.pdf

ACA Summer Course 2018. Left to Right: (Back Row) B. Pinheiro Bezerra, A. Sarjeant, S. Kandel, C. Stern, A. Rodriguez, R. Sommer, B. Noll, S. Shafeie, J. Luna, J. Newman, T. Yong, L. Mathivathanan; (Center Row) G. Pauly, S. Oliver, S. Chong, S. Morris, J. Rodriguez Henandez, G. Bogdanov, A. Peloquin, J. Reibenspies, C. Malliakas, K. Spielvogel, A. Ryan, A. Oliver; (Front Row) P. LeMagueres, S. Chornkrathok, C. Zeng, N. AlHaqbani, D. Gray, T. Watts, F. Khamespanah, S. Rigin, M. Padron Gomez, D. Patil, G. Diaz Delgado, L. Ohman, N. Wolford, R. Szlag, N. Byrne, A. Cardenas, R. Papoular.

The ***ACA Summer Course in Chemical Crystallography*** is a week long program that is now into its third decade of instruction here in the United States. Currently the course has components from both single crystal and powder diffraction techniques. The underpinning theory is applicable to both techniques and the course aims to cover both that theory as well as more practical aspects of the course as shown in the appended course curriculum.

The ACA Summer Course in Chemical Crystallography (***http://acasummercourse.net***) was hosted at the University of Notre Dame from June 10 to June 17, 2018. Course organizers were: Allen Oliver (Notre Dame), Charlotte Stern (Northwestern U) and Christos Malliakas (Northwestern U), and Amy Sarjeant (CCDC).

The course had 30 participants, covering all of the U.S. including the Hawaiian Islands and Puerto Rico and international attendees from Brazil, Saudi Arabia and Singapore. Amongst the domestic attendees were Faculty from several Universities (Air Force Academy, SUNY Fredonia and UC Santa Cruz) and industrial partners from Merck and the National Cancer Institute. The large majority of attendees were graduates and post-doctoral fellows from around the country along with one undergraduate.

The course had a total of 12 instructors with experts in both Single Crystal and Powder diffraction participating. Two vendors, Bruker and Rigaku, kindly donated time and expertise from their applications specialists towards the program. This enabled direct instruction of the various software packages by experts. This was appreciated by the course attendees.

Generous sponsorship was provided by The American Crystallographic Association, The US National Committee for Crystallography, Bruker AXS, Cambridge Crystallographic Data Centre, Pittsburgh Diffraction Society, MiTeGen and Rigaku Americas.

We have developed a curriculum that we feel covers the basic theory broadly and practical instruction more directly; we do not expect experts after one week of instruction. More critically is the networking that is enabled by having practicing crystallographers serve as instructors, directly interacting with the attendees. More modern practices are followed in the course, with a greater focus on the practical aspects of crystallography (data collection methodology, sample selection and software use). Course material was made available to all of the attendees. Particularly the lecture notes, but also recently developed software.

Each day of the week-long course was divided into 3 one-hour lectures covering diffraction theory, software, best practices and various methodologies while the afternoons were spent in practical workshops. For the first two days of the course, these workshops focused on sample preparation, and instructional tutorials. For the remainder of the week the workshops were spread over single crystal data collection, powder diffraction techniques. Lecture rooms, conference rooms, computer rooms and facility space for data collection were kindly donated by Notre Dame. Instrumentation accessible to the attendees included three single crystal diffractometers and one powder diffractometer.

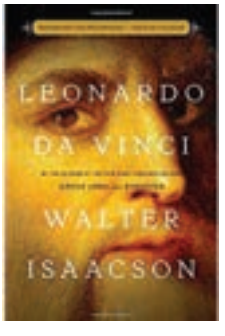
The International Center for Diffraction Data (ICDD) kindly provided temporary licenses for the Powder Diffraction File to allow instruction of this software. Notre Dame owns a site-license to the Cambridge Structural Database and the Inorganic Crystal Structure Database. Other software used and made available to students included: OLEX2, Platon, SHELX, GSAS2, APEX3, CrysAlisPro, FOX, Avogadro, WinPloTR, OpenBabel, EasyDIC and FullProf.

Participants were assigned to one of six groups based on research interests and experience level for purposes of the workshops on the first two afternoons/evenings. This helped promote networking among the attendees, especially for international attendees and helped facilitate SHELX workshops. We have also incorporated some challenging samples and structural problems that real-world crystallographers might encounter. This further promotes networking between the attendees and course faculty.

Attendees were encouraged to submit samples for data collection during the week. Fifteen successful single crystal data sets and five powder samples were submitted and were suitable for the participants to analyze. As in past years, we encouraged publication of these data with the request that an acknowledgment to the course be added.

Anecdotal feedback from the attendees was very positive and it was clear that this experience was valuable to them. This was especially highlighted on the final day when the attendees are requested to give a short presentation on their experience. It was clear that all had gained new, useful knowledge as well as having developed a network that they can contact.

Allen Oliver



Leonardo da Vinci, by Walter Isaacson, Simon & Schuster, New York, 2017, 599 pages, ISBN:978-1501139154.

Walter Isaacson's latest biography is an intimate venture into the life of Leonardo da Vinci: artist, sculptor, engineer, inventor, and even, one might argue, amateur coroner.

Isaacson includes some helpful guides for the reader at the beginning of the book. This includes, but is not limited to: a cast of characters with brief biographies; information about Italian currency circa 1500 and how it compares to the modern-day U.S. dollar; and, most importantly, a detailed timeline of Leonardo's life and work (complete with color images) juxtaposed with a timeline of important events around the world for context.

Leonardo, thanks to his painted masterpieces, namely The Last Supper and Mona Lisa, is first and foremost remembered as an artist. And Isaacson's da Vinci feels like an art history textbook, complete with thick, glossy pages and high-resolution color images of Leonardo's work (painted, sketched, and otherwise).

But despite textbook appearances, Isaacson's book is a true biography of the man—and an interesting, compelling one at that. Even if you think you know everything there is to know about da Vinci, you will definitely learn at least one new thing, if not more.

Isaacson starts with Leonardo's childhood in the small Italian town of Vinci, outside Florence. As the illegitimate child, Leonardo split his childhood between his mother's home and his father's parents. His illegitimacy was a blessing in disguise: it meant he could pursue his passions as a young man instead of following in his father's footsteps as a notary. It also meant Leonardo was never formally educated. Even in his old age, he considered himself a man of experience rather than a man of books.

When Leonardo was 12, he moved to Florence with his father. The city, then under the control of the Medici family, was a cultural center—a nexus for artists, architects, and sculptors. By the time Leonardo was 14, his father had arranged an apprenticeship for him in the workshop of a master artist: Andrea del Verrocchio. Some scholars even suspect that Leonardo was the model for Verrochio's David (as in David and Goliath). Under Verrocchio's tutelage, Leonardo developed two techniques that he would continue to use for the rest of his career: chiaroscuro and sfmuato. Da Vinci also contributed to several of Verocchio's painted works, such as Tobias and the Angel and Baptism of the Christ.

By the time Leonardo was twenty-four, he had moved out of Verrocchio's workshop and started his own. During this time, he only had three commissioned works—he never started one of them and left the other two unfinished—one of which was Adoration of the Magi.

Following his essential failure in Florence, at age thirty, da Vinci packed up and moved to Milan—he would stay there for seventeen years. In Milan, da Vinci was something of a cultural envoy. He worked on a tremendous number of inventions, such as the crossbow; acted as a court entertainer; and even perfected The Vitruivan Man.

Leonardo, though not often remembered or regarded as a sculptor (unlike his slightly-younger contemporary Michelangelo), actually spent five of his years in Milan on a massive horse sculpture for the Duke. The horse was never completed though, due to a series of unfortunate events that culminated in French invaders essentially melting his massive clay model down with flaming arrows.*

Despite the horse setback, da Vinci kept on. He conducted numerous experiments of scientific inquiry, seeking to understand why the sky is blue and how birds fly (spoiler alert: he figured both of these things out hundreds of years before modern particle physics or mechanical engineering). He drew incredible polyhedral figures for his friend Luca Pacioli's book On Divine Proportion. The skillful shading makes the illustrations seemingly leap off the page—they seem truly three-dimensional. He completed a series of commissioned portraits, such as Lady with an Ermine. And then he worked on one of his most famous pieces: The Last Supper.

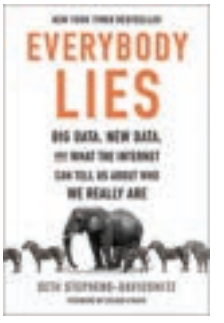
The death of Leonardo's mother brought him back to Florence, where he worked on numerous projects, including a failed attempt to redirect the Arno river. He also developed a rivalry with Michelangelo. Da Vinci eventually returned to Milan, where he continued his work dissecting corpses and studying human anatomy. He then spent some time in Rome before leaving the country for France, where he was widely revered as a master artist. It was there that he eventually died.

Isaacson ends the book with Mona Lisa, choosing to discuss the work out of chronological order. His point seems to be that the weight of this particular piece would overwhelm any discussion of any other work either before or after it.

One of the interesting segues in the book concerns modern efforts to authenticate works of Renaissance art that some seek to attribute to Leonardo. In da Vinci's time, artists often did not sign their work. Collectors have often sought a windfall from recognizing a work as da Vinci's that was not previously recognized as such—and naturally, chaos ensues. These anecdotes remind us that there is still quite a bit about Leonardo we cannot possibly know—the man lived 500 years ago after all. But it's quite thrilling to think maybe, just maybe, there is an unsigned masterpiece out there, hiding in plain sight, waiting for the right person to stumble upon it.

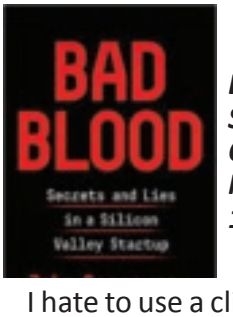
*Jean Fritz wrote a beautifully illustrated children's book, Leonardo's Horse, about the unfinished statue, and how an American airline pilot worked to help "finish" the piece. You can now see "Leonardo's Horse" in Milan.

Jeanette S. Ferrara, MA



Everybody Lies: Big Data, New Data, and What the Internet Can Tell Us About Who We Really Are, by Seth Stephens-Davidowitz, HarperCollins, New York, 2017, 352 pages, ISBN-13: 978-0062390851.

Seth Stephens-Davidowitz is a former Google data scientist and currently a lecturer at the Wharton School. He hypothesizes that surveys and Facebook do not reflect our true inner selves. The answers we provide in surveys and what we put on Facebook reflect what we want other people to think, not what we actually think. On the other hand, the anonymity of the Google search, and the ability to slice and dice the resultant data allows one skilled in the art of analytics to extract a true view of what we are thinking and feeling in near real-time. Stephens-Davidowitz provides many examples including tracking the flu, unemployment and racial slurs and how the results compare to Centers for Disease Control, Bureau of Labor Statistic and election results. He also demonstrates the ease with which hypotheses can be tested on the general population through big data in ways that would not pass ethics reviews otherwise. Warning: there is a lot of explicit language in this book – it is not for youngsters.

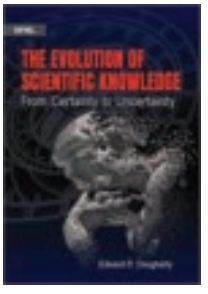


Bad Blood: Secrets and Lies in a Silicon Valley Startup, by John Carreyou, Penguin Random House, New York, 2018, 352 pages, ISBN-13: 978-1524731656.

I hate to use a cliché, but this book is a page-turner even though I already knew that the principals of Theranos, Elizabeth Holmes and Ramesh "Sunny" Balwani, were indicted on multiple charges of wire fraud and conspiracy to commit wire fraud. Carreyou does a superb job of narrative setup before he comes on the scene as a reporter for The Wall Street Journal then outlining the details of how he and the WSJ brought the facts to light, and kept going in spite of all manner of legal threats.

Theranos proposed using modern biochemistry and microfluidics to analyze a drop of blood using a small benchtop analyzer. It's a great idea, but Theranos could not execute it, failed to deliver on promises, and began to lie. The lies took many forms, but the most egregious was the production of false results on the

very blood tests that made them famous. Patients were being misdiagnosed. Imagine learning your potassium level is so high you could have a heart attack at any moment, when you previously thought you were not at risk? Here is an example of vaporware with the possibility of tragic consequences.



The Evolution of Scientific Knowledge: From Certainty to Uncertainty, Edward O. Dougherty, SPIE Press, Bellingham, 2016, 136 pages, ISBN: 978-1510607354.

I came across this title at the book shop at a conference for the International Society for Optics and Photonics (SPIE). The author is on the faculty of Texas A&M in the department of Electrical Engineering and Computer Science, as well as a SPIE fellow.

This book is about scientific epistemology-- the theory of scientific knowledge. As the title suggests, the book covers how scientific knowledge has evolved from the time of Aristotle to that of genomics.

In the first two chapters the author takes us through an introduction to epistemology. In the next chapter he explains pre-seventeenth century science.

The author posits the revolution in science occurs with the transition from the Copernican description of planetary motion to Kepler's three laws of planetary motion. Kepler's laws demonstrate the four basic components of a theory for the first time: observation, analysis, modeling and prediction of future events. This revolution culminates in the seventeenth century with Bacon, Galileo and Newton. The next step is determinism, in which Descartes, Laplace and Pascal all contribute greatly. Determinism is the paradigm that given enough information the future can be predicted.

Dougherty then spends a chapter looking at the philosophical changes brought about by the scientific revolution of the seventeenth century through the writings of Locke, Hume, Kant and Rousseau, as well some later philosophers. The age of uncertainty in science begins with Maxwell and continues into the quantum era with the particle/wave duality crisis.

The last two chapters focus on the problem of big data and the modeling of large systems with complicated interdependencies. The author provides a brief description of Bayesian statistics using a simple mammalian cell cycle as an example.

The book is short--only 136 pages--but demanding, especially the chapter on philosophy.

Joseph Ferrara

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

Organizers: Nicholas Sauter (LBNL; ***nksauter@lbl.gov***), **John Rose** (UGA; ***jprose@uga.edu***), and **Talapady Bhat** (NIST; ***talapady.bhat@nist.gov***)

Questions about data are common to many of the specialized interest groups within the ACA, whether focused on biological or small molecule X-ray crystallography, neutron or electron diffraction, or cryoEM. This symposium will be an opportunity to hear about current data challenges from lightsources, public data archives, and computational methods groups, and will provide a community forum to ask questions that will define future science in the upcoming years. How are big data experiments enabling new science? What do we expect from a good detector? Which data should be saved and which thrown away? How much of the data should be shared? Can my peers reproduce the results? Are the journals and databases serving present needs? What could beamlines do differently? What misconceptions have you noticed? Our hope is that the symposium will provide an informative and provocative platform for these topics.

Covington, KY, site of the 2019 ACA Meeting

ACA CINCINNATI/NORTHERN KENTUCKY

Saturday, July 20 - Wednesday, July 24, 2019

Travel Grant Application Deadline: March 29, 2019
Abstract Deadline: March 29, 2019
Early Registration Deadline: May 31, 2019
Hotel Reservation Deadline: June 28, 2019

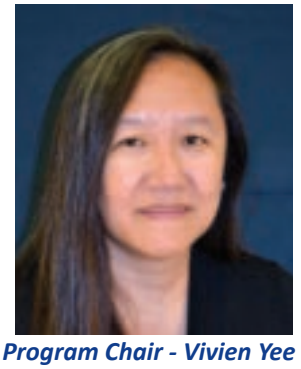
ACCESS UPDATED MEETING INFORMATION:

http://www.amercrystalassn.org

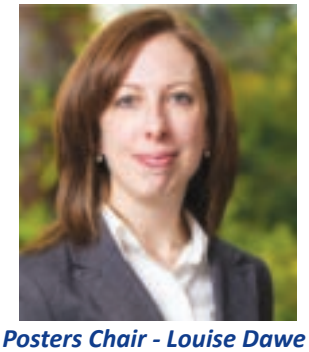
Abstract submission - Meeting registration - Full call for papers
Sponsorship opportunities
Information for exhibitors

Abstracts accepted online only
at least 40% of all talks will be from contributed abstracts

Program Chair - Stephan Ginell
slginell4aca@gmail.com



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



Posters Chair - Louise Dawe
ldawe@wlu.ca

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

WORKSHOPS

Advanced Structural Characterization of Nanomaterials
Accelerating your Career Development
Introduction to PHENIX for electron cryo-microscopists
Serial Crystallography: Obtaining Protein Structure from Many Crystals
CryoEM I : Image Processing II : Reconstruction

EDUCATIONAL SESSIONS & YSIG EVENTS

Three Minute Thesis Session
YSIG Orientation and Networking Mixer
Open Exchanges in Crystallographic Education
Sustaining Crystallography Education and Training
Diversity & Inclusion Session

ACA AWARDS

Robert Bau Award honoring Bryan Chakoumakos
I. Frankuchen Award honoring Eaton (Ed) Lattman
Kenneth Trueblood Award honoring Brian Toby and Robert Von Dreele
Margaret C. Etter Early Career Award honoring Efrain Rodriguez

SESSIONS

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

Solid State Supramolecular Chemistry and Crystal Engineering
Structure/Local Structure of Thin Films, Interphases and Surfaces
Locating and refining H atoms using X-rays, Neutrons, and Solid-State NMR
Cancer: Structure and Mechanics
Structure Without Structure
Diffuse Scattering in Crystals
Cutting Edge in CryoEM
Structure Based Drug Design
Time - Resolved @ XFELS
Radiation Damage in X-ray and EM
Understanding Polymer Dynamics
Structural Parameters of Porous Materials
SAS Contrast Methods in Biology and Soft Matter
Structural Biology Combining SAS and high resolution methods

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

General Meeting Information

Venue:

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

Hotel:

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

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

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

Travel:

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

Foreign Travelers:

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

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

If you require a participation letter to the conference to submit with your application, please e-mail your request to: **aca@hwi.buffalo.edu**. Please include your name, passport #, birth date, mailing address, e-mail address and the title(s) of any abstract(s) that you have submitted for the conference. A copy of the letter will be e-mailed to you.

Financial Support:

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

- Become a member! Discounted Meeting registration fees are available to members.
- ACA Travel support will be available for young scientists from the ACA. Applications for travel support will be available on the ACA's website and should be submitted to the ACA by March 31, 2019.
- More opportunities for travel support from ACA partners will be posted on the 2019 Annual Meeting website as they become available. The 2018 meeting provided over $10,000 of travel support from our partners and we hope to continue to provide the same level of support in the future.
- Become a session room volunteer! Registered students and post-docs attending the 2019 ACA Annual Meeting can apply to be session room monitors. Session room monitors operate audiovisual equipment, and room lighting, photograph the speakers (cameras provided), track and record attendance, and perform other tasks requested by the session chairs. Applications to be a session room volunteer will be available on the ACA's website and should be submitted to the ACA by May 1, 2019.
- Volunteer at the front desk! Registered students and post-docs attending the 2019 ACA Annual Meeting can help hand out registration packets and assist attendees with general questions and inquiries. Volunteer for one (1) full-day (7:00 a.m.–4:00 p.m.) and receive half-off regular student/post-doc registration.
- Share a room! This is an option facilitated by the ACA to help those looking to save money on their hotel accommodations by sharing the cost of a hotel room. The ACA only assists in facilitating contact between roommates and does not guarantee room availability. Further, attendees/roommates are responsible for making their own hotel reservations. Check out the ACA's website for information on sharing a room and to find a list of attendees looking for roommates.

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

BRUKER

PHOTON III – Capture More Reflections

The NEW PHOTON III

Speed provides the one genuinely modern pleasure - Aldous Huxley

Modern crystallography beamlines use large active area pixel array detectors to optimize the speed and efficiency of data collection. The new PHOTON III offers the same advantage for your home laboratory with an active area of up to 140 x 200 mm². The PHOTON III surpasses any laboratory detector in Detective Collection Efficiency (DCE) and guarantees the best data for your most challenging experiments.

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How AIP's TEAM-UP is Addressing Racial Diversity in the Physical Sciences

The number of physics degrees awarded to African Americans is stagnating, and AIP's TEAM-UP plans to find out why.

As the number of physics bachelor's degrees increases each year, one group remains consistently underrepresented. African Americans earn only four physics bachelor's degrees for every 100 that are awarded. This dilemma has many asking: why do so few African Americans pursue a degree in physics or astronomy? AIP's Task Force to Elevate the Representation of African Americans in Undergraduate Physics and Astronomy (TEAM-UP) intends to find out.

AIP has dedicated itself to ensuring that inclusion and diversity are represented in the physical sciences. In 2017, AIP launched TEAM-UP to examine and assess the persistent underrepresentation of African Americans in physics and astronomy at the bachelor's level. The goal of TEAM-UP is to eventually bring the rate of African Americans obtaining physics and astronomy degrees to parity with their overall graduation rate (from 4 percent to 9.5 percent).

AIP's Arlene Knowles, the project manager for TEAM-UP, graduated from Cornell with a degree in human development and pre-medical studies. At Cornell, Knowles enrolled in her first physics course and instantly felt the disparity.

"I came from a regular public school, and there were a lot of students who came from private schools that had a lot more resources. They just had better preparation. It was a little intimidating at some points," Knowles said. "There was a physics class where there was no instructor, so you had to teach yourself. I had major questions, and only had ten minutes with a grad student. That was discouraging. I believe I could have benefitted from some good teaching."

After school, Knowles spent many years at a member society doing diversity work in the physics community.

Reflecting on her diversity experience, Knowles believes the low participation of African Americans in physics and astronomy programs is in part due to bad PR, but also due to experiences once they have entered programs.

"People don't realize what you can do with a physics degree," Knowles said. "If you get an engineering degree, you're an engineer. If you get a law degree, you're a lawyer. When you get a physics degree, what are you? Nobody knows. Most people think you have to become a physics professor and that may not be what they want to be. Studies have shown that women and minorities are really motivated by helping their communities, and there's a disconnect between getting a physics degree and what you can really do to advance your community. I don't think we do a good job of educating people on that."

With regard to experiences in their departments, members of the physics and astronomy communities can do ordinary, everyday things to help close this racial gap, Knowles says.

"First, faculty have to build trust with students. Particularly students who are from different cultures and races… Letting students know that you believe in them and that they have what it takes to succeed, and that you're willing to support their success… Listen to what they have to say and what their motivations are. Figure out what they want to do and help them achieve that."

Knowles says that AIP Member Societies can shape the culture of physics and astronomy by prioritizing diversity and creating initiatives to uplift African American physicists, and society members can do the same by communicating the need for diversity to member societies.

"You can't solve problems with people who are all the same. You need different perspectives and ideas," Knowles said. "Diverse teams care about diverse problems."

TEAM-UP created a survey to measure the experiences of African Americans who are either studying physics or dropped out of their physics studies. This survey, which Knowles says is the first of its kind, seeks to uncover the factors that impede or encourage African American participation in physics and astronomy.

Once the survey's data has been collected and analyzed, TEAM-UP plans to visit institutions that produce higher levels of African American physics and astronomy bachelor's degrees. Afterward, the task force will develop evidence-based recommendations for the broader scientific community.

"My hope is that the broader community will see these recommendations and really feel it's important to act on them," Knowles said.

On Twitter, TEAM-UP hosts Twitterchats that are aimed at explaining their mission and showcasing the staff dedicated to accomplishing it. Follow @AIP_TEAMUP to stay updated on TEAM-UP's progress as they work to end the disparity in African American representation in physics and astronomy.

By: Skye Haynes, AIP Marketing and Communications Intern

The ACA is a Member Society of the American Institute of Physics, a federation of scientific societies in the physical sciences, representing scientists, engineers, educators, and students.

Puzzle Corner

This issue debuts a new kind of puzzle: a letter-substitution cipher Cryptoquote, er... ***Crystoquote***. Think Little Orphan Annie Secret Decoder Ring. The quotations will be by or about well-known crystallographers, past and present.

We also have a new DISORDERED puzzle, the solutions to the previous DISORDERED and Connections puzzles, and mention of those who provided solutions to previous ones.

DISORDERED

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

GRENTFAM	○○ ○
GLUMO	○○○
NAWGRID	○ ○
QUOSNECT	○ ○ ○○
CERASH	○ ○

Answer: ☐☐☐☐☐ ☐☐☐ - ☐☐☐☐☐

Crystoquote #1

G OZ KYV UYRJGEFM FUUMGEFKGZIJ, YV PZTHJ ZI KYV KYVZTVKGEFM. GK LFHVJ F AZZO KVFL. JEGVIEV TVBDGTVJ NZKY KRUVJ. *GJFNVMMF HFTMV*

Solution to Crystal Connections #14 – **Surnames of ACA committee members**

1) The Caltech Beavers baseball team won a game in 2013 after 228 straight losses. (*Christine Beavers*, Nominating)

2) Rose Mooney-Slater was the first female X-ray crystallographer in the USA. (*David Rose*, Nominating)

3) "In the middle of our walk of life, I found myself within a Forest dark, for the straightforward pathway had been lost." – Dante, *The Devine Comedy* (*Katrina Forest*, Communications)

4) "*The Picture of Dorian Gray*" by Oscar Wilde (*Danielle Gray*, Education)

5) "Ambition should be made of Sterner stuff." Julius Caesar, Act 3, Scene 2 (*Charlotte Stern*, Education)

6) Xylology is the study of the structure of Wood (*Pete Wood*, Education)

7) Average of particle size in fluid dynamics: Sauter Mean Diameter (*Nicholas Sauter,* Data, Standards & Computing)

8) The part of Capt. Jean-Luc Picard was played by Patrick Stewart (*Brian Patrick*, Communications)

Cynthia Day (Chemistry, Wake Forest) and **Diane Dickie** (Chemistry, U. of Virginia) provided the solution to the bar joke DISORDERED puzzle, and **Marian Szebenyi** (Cornell) provided the surnames for Connections #14. However, nobody made the connection that they were ACA committee members.

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

Frank Fronczek – ffroncz@lsu.edu

DISORDERED

Distill these smashed words down into sober ones

MITIVIPER	PRIMITIVE
COINRATH	ANOATHIC
WRECS	SCREW
LAXIBIA	BIAXIAL

Answer: IT WAS A P ONE BAR

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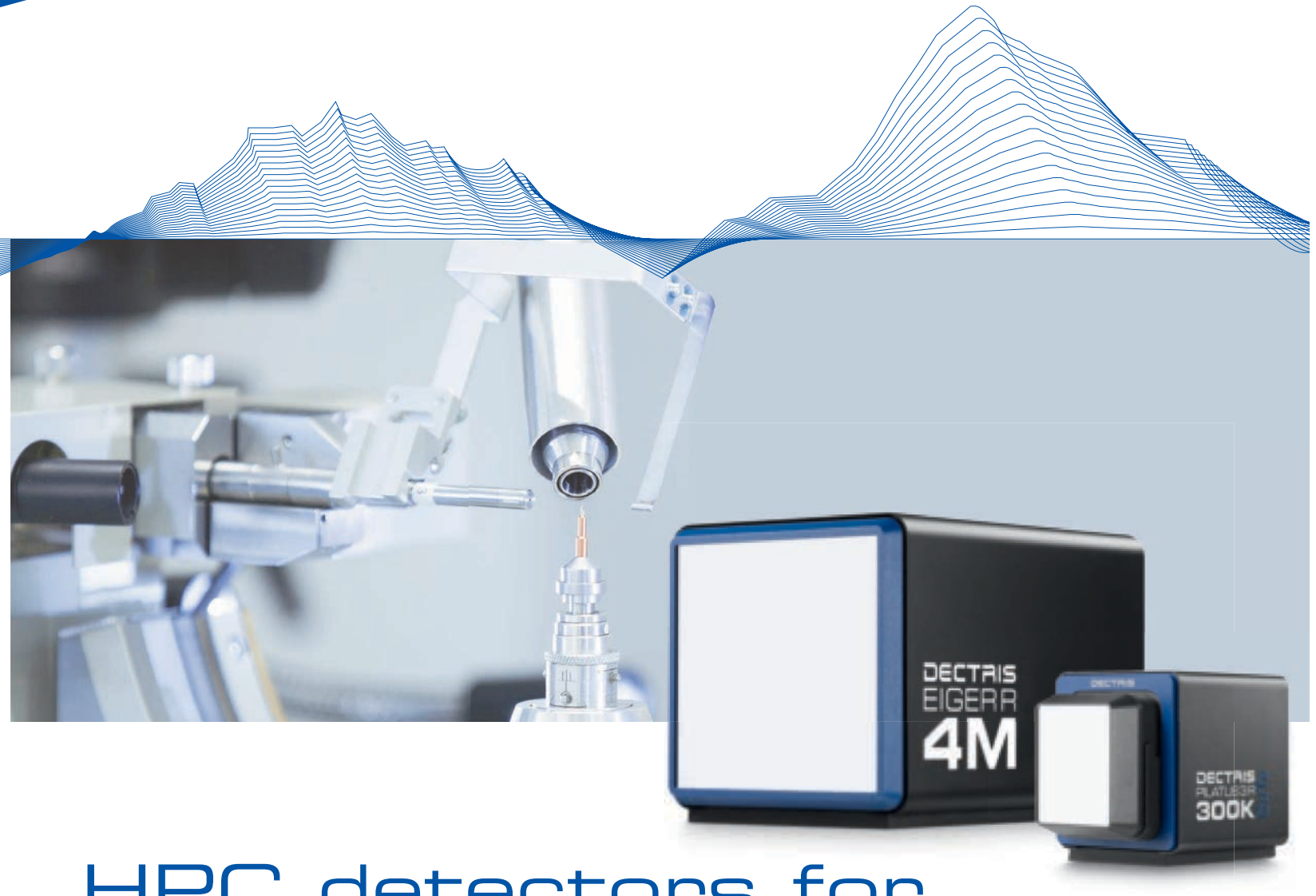

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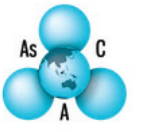
3-5 **III Meeting of the Latin American Crystallographic Association**. Valparaíso, Chile
https://cristalografia.cl/3rdlacameeting

14-16 **76th Annual Pittsburgh Diffraction Conference, Cleveland, OH**
http://www.pittdifsoc.org/pittsburgh_diffraction2018.pdf

15-30 **X-ray Methods in Structural Biology**. Cold Spring Harbor, NY
https://meetings.cshl.edu

DECEMBER 2018

25-30 **AsCA 2018**. Auckland, NZ
http://asca.iucr.org



Asian Crystallographic Association

JANUARY 2019

28-2 Feb **PCCr-2. 2nd Pan African Conference on Crystallograpy,** Accra, Ghana
http://www.pccrafrica.org

APRIL 2019

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

JULY 2019

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

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

AUGUST 2019

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

JULY 2020

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

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