ACA RefleXions

American Crystallographic Association
Structure Matters

Number 3

Fall 2016

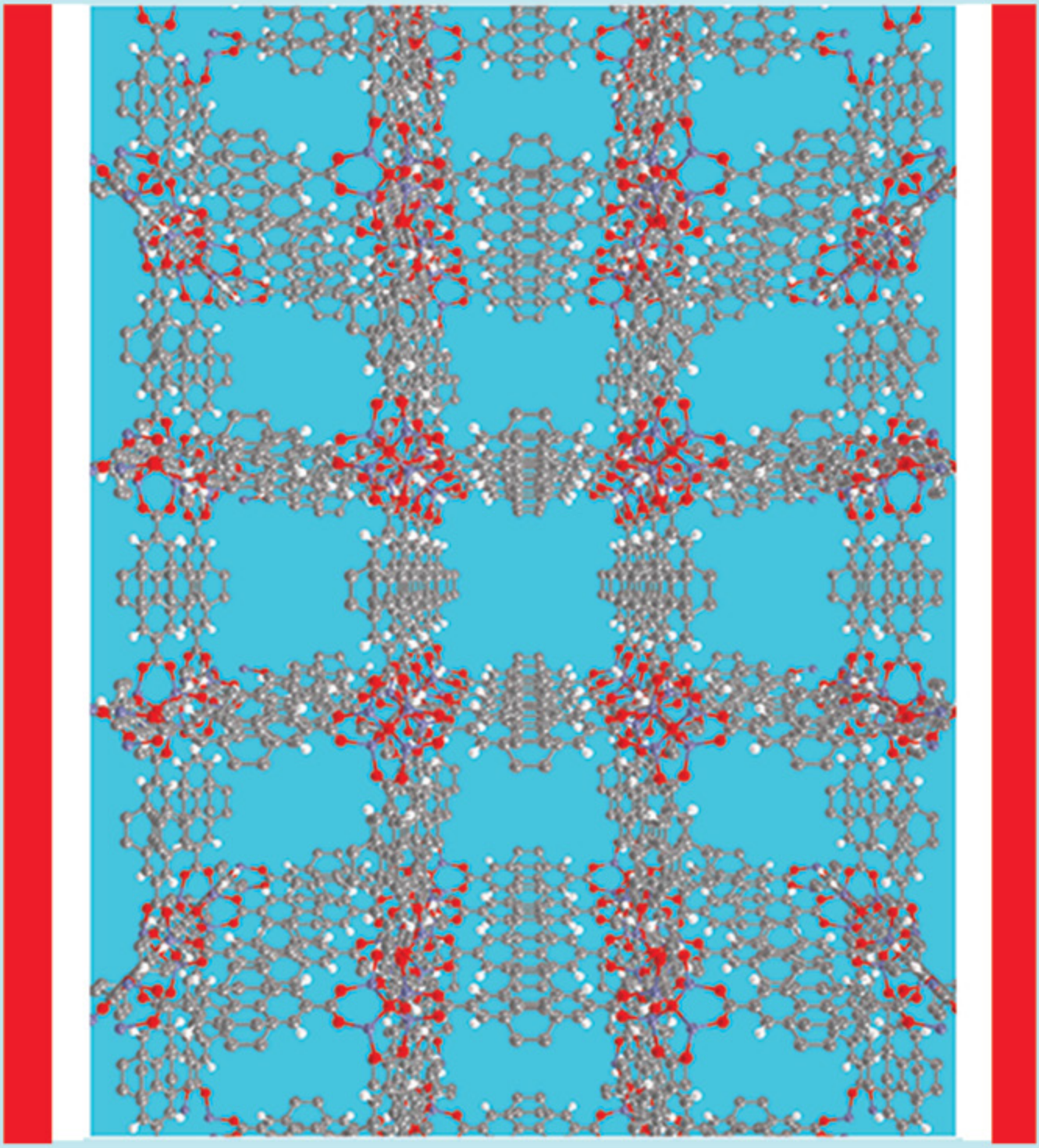

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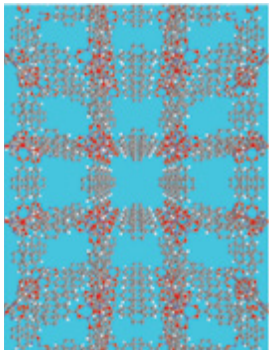
Table of Contents - Fall 2016

Tom Terwilliger
ACA President

The Bad Astronomer – Phil Plait
Awards Banquet Speaker in Denver



What's on the Cover. The image was supplied by Jason Benedict, our Etter Awardee. See p. 8.

Jason Benedict

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Tom Terwilliger

President's Column

Dear ACA members and friends,

I am so pleased that our ACA Annual Meeting in Denver was such a great success! I received many comments about how much my colleagues liked the meeting, both in scientific content and in being a great place to meet and network with other researchers. I also got many comments that the banquet (with a dinner speaker and a band) was super worthwhile! We are planning to have another fabulous meeting in New Orleans next May with great scientific sessions and another special banquet (this time with a jazz band).

This year you may notice that the dues for ACA membership are going to be a little higher than in the past, and I want to tell you how important your dues are for making our ACA work and why we needed to increase them.

About half of the effort of the Buffalo ACA office is devoted to running our Annual Meeting, and half is devoted to taking care of the ACA itself. This second portion includes working with and sending notices to members, posting on the ACA web site, working with the ACA Council and its three yearly meetings, and helping all our committees and Scientific Interest Groups with their work and administrative needs.

Our Annual meeting normally costs about as much to run as it brings in in revenue. The other half of the ACA Buffalo office effort is paid for largely from membership dues and from proceeds from advertising in the *RefleXions* newsletter. The cost of this ACA Buffalo office effort is about $160,000 per year, while membership dues have been about $100,000 and net proceeds from *RefleXions* about $30,000. This means that in recent years the ACA has operated at a net loss of about $30,000 per year. We have a sizeable reserve, but it could not sustain such a loss for many years. To address this important need, this year the ACA membership present at the ACA Business Meeting in Denver voted to increase the membership dues for regular members from $110 to $145. The new dues are in line with those of other societies like the ACA (the old dues were much less than average) and are anticipated to bring the ACA budget much closer to break-even. Along with cost-cutting measures by the ACA this should help keep the ACA financially healthy for the coming years.

Why is your membership in the ACA so important? The big reason is that your membership is crucial for keeping the ACA going. Your support of the ACA in turn makes our Annual Meetings that are so successful possible. Your membership in the ACA also is crucial for our outreach efforts including workshops, K-12 education including crystallization competitions, and the ***ACA History*** pages on the ACA web site.

I hope that you will be renewing your membership this fall and that you will encourage your colleagues to do so as well! Looking forward to seeing everyone at the next ACA Annual Meeting in New Orleans May 26-30, 2017! And don't forget to send your best science to our Journal, *Structural Dynamics*!

Tom T
Tom Terwilliger, 2016 ACA President


Michael James

RefleXions from Canada

One of the major topics of discussion in several of the recent ACA Council meetings has been the dramatic drop in membership. In 1995 there were 2400 members; at present there are 1017. Membership in the ACA by Canadian crystallographers is also down substantially. Presently, we have only 62 dues-paying members and nine of those members (14%) are retired crystallographers. On the one hand, it is heartening to see that our retired crystallographers are still supporting the ACA but on the other hand, what are the reasons for this huge overall drop in membership? A year or so ago, Louise Dawe and I put together a survey that was circulated to about 200 Canadian crystallographers. We were hoping to discover the reasons for the lack of enthusiasm in joining the ACA. We were disappointed in the small number of responses that we received (~15%) and it was difficult to come up with substantial reasons for that lack that we could hope to rectify. Perhaps the most common reasons were joining societies and attending meetings that were more directly related to the respondent's lines of research or interest. However, to ignore the opportunity to attend workshops held by those who developed the algorithms or wrote the code to carry out crystallographic procedures seems to me to be a major oversight. To me, personally one of the more important reasons for maintaining my membership in the ACA is the pleasure of renewing friendships that often go back several decades, on an annual basis. It is great to see many of those crystallographers who started when I did, still active scientifically and still doing the research that they love.

I am very disappointed` in the lack of membership in the ACA in our major Canadian Centres of Research. From a scan of the list of the current members from Canada, I count only six from U Toronto and adjoining hospitals, and one of those is retired. There are only two from UBC and other centers in the lower mainland of British Columbia. There are only two Canadian members of the ACA from the Canadian Light Source (CLS) in Saskatoon and only three in the Montreal area one of whom is a senior administrator in McGill U and no longer active in crystallographic research. Even more depressing is looking at ACA members in my own department at U Alberta. There could be eight who are active structural biologists or students, but I am the only one who is a member of the ACA. What is the problem? I will leave this question open for now, but I hope that those who do have a chance to read it will put some serious thought into answering WHY? One of the very best reasons that I can see for being a member in the ACA is the opportunity for our students to present their results to their peers and to learn so much more about crystallography than can be taught in didactic formal courses.

So I should stop this rant and concentrate on some of the good things that are going on in Canada. In the summer issue of *RefleXions* (2016), I wrote about the meeting held in May at the CLS, Saskatoon, on Automation in Macromolecular Crystallography and organized by Pawel Grochulski (CLS) and Tom Caradoc-Davies (Australian Synchrotron). There have been two other meetings held in Canada since then.

The Canadian Chemical Crystallography Workshop for 2016 (CCCW16) is in its 7th year of operation. Each year it is associated (the week prior to or following) with the Canadian Chemical Society meeting. It was held this year in Halifax at Saint Mary's U, from May 30 to June 3. As is typical with these CCCW workshops, the participants worked with the free "OLEX2" software and solved and refined several crystal structures each. Practice data sets were supplied, or participants had their own data sets that could be used for their own research projects. This is a very intensive course and covers topics from crystal growing, space group theory, data collection, and structure solution and refinement methods, to structure finalization. The CCCW16 was organized by Jim Britten (McMaster U) and by Jason Masuda and Katherine Robertson (Saint Mary's U). In addition to these three talented people, there were six other instructors/organizers who contributed to the program.

This year there were 17 students (graduate and undergraduate levels) who attended. They came from universities as far away as Victoria B.C. and Memorial U Newfoundland; most of the students were, quite naturally, from the Atlantic Provinces. I am grateful to Louise Dawe for her summary of the workshop. Information on the program, speakers and their presentations can be obtained by sending an e-mail to Jim Britten at McMaster U (***britten@mcmaster.ca***). In addition, there are several photos taken during the workshop presentations, and one is included here below of two of the speakers, Amy Sarjeant and Louise Dawe, taken during an outing to Peggy's Cove, Nova Scotia.

Amy Sarjeant, at left, and Louise Dawe at Peggy's Point Lighthouse, Peggy's Cove, Nova Scotia, Spring 2016

Other photos of the CCCW sessions can be found at Twitter: ***https://twitter.com/search?F=tweets&vertical=default&q=%23CCCW16***.

Overall the students had a very positive experience that was reflected in the final presentations of their work during the week. Some students went from never having worked with X-ray crystallographic data, to solving and refining structures from data collected from twinned crystals.

The next meeting that I would like to mention in this issue of *RefleXions* is the 4th Protein Structure, Function and Malfunction (PSFaM) meeting held at U Saskatchewan during June 23-24, 2016. I am grateful to Mirek Cygler for providing a summary of the highlights of the meeting. Whereas the attendees of this meeting come mainly from the Western Provinces of Canada – Saskatchewan, Alberta and Manitoba, there were students and faculty from all of North America present. This year there were ~150 participants at the meeting. The aims of the PSFaM meetings are several-fold: to provide a forum for up-and-coming researchers involved in the study of proteins and of protein structure and function, be they graduate students, post-doctoral fellows or faculty, to present recent results, to engage in discussions about their research, and to meet their peers. This year the meeting was opened by Jim Basinger, Associate Vice-President of Research, U Saskatchewan. Four keynote lectures were presented throughout the two days: Susan Lees-Miller, U Calgary, provided insight into the structure and function of the molecular machinery required for repair of DNA double strand breaks by non-homologous end joining; Sergio Grinstein, The Hospital for Sick Children, Toronto, discussed the role of integrins in forming an expanding diffusion barrier that enables activation of Src-family kinases during phagocytosis; Robert Campbell, U Alberta, described the engineering of fluorescent proteins and their applications to visualize and manipulate protein localization and function; Sriram Subramaniam, NCI, Bethesda, MD, described recent advances in electron microscopy, in cell tomography and in high-resolution structure determination of molecular assemblies. There were eight other invited speakers who presented their recent results on a variety of subjects including: the role of iron-sulfur cluster helicases in maintaining genome stability, the structural features of bacterial receptors to host proteins, the importance of ubiquitin-associated motifs in health, proteomic and transcriptomic analysis leading to the discovery of an essential regulator of *Pseudomonas* species biocontrol, and the N-terminal dependent protein degradation as a regulator of programmed cell death. Ten other talks, chosen from the submitted abstracts, were given by the trainees. There were a total of 36 poster presentations in addition to the talks. Titles of the talks and links to the abstracts can be obtained at the following website: ***http://cmcf.lightsource.ca/psfam***.

Apart from my rant that started this article off, there are other good things happening in our Canadian Division that are evidenced by the attendance at the lunchtime meeting of the Canadian Division at the Denver meeting. This meeting was chaired by Paul Boyle (Western U) and was attended by 14 Canadian members of the ACA. This is the largest attendance of a Canadian Division meeting that I have been to in the past several years. Several important decisions were made at the meeting including the announcement of the award of an Etter Student Lecturer Award to Marcia Chaudet (U Waterloo).

Planning for the next ACA meeting, to be held in New Orleans in May 2017 is well underway. The Canadian Division will co-sponsor, with a variety of SIGs, several sessions at this meeting. Some of these will require people to act as co-chairs, so if anyone knows a suitable person for any of the sessions listed below, please contact Paul Boyle at ***pboyle@uwo.ca***.

1. NMR Crystallography
2. Enzymes of Post-translational Modification
3. Thermodynamics of Ligand Binding (co-chair Michael James)
4. Home-Built Software (sponsored by Service SIG)
5. Joint Methods for High Rate Data Processing for XFEL and Synchrotron (sponsored by Light Source SIG)

Turn to p. 4

I would like to point out that the ACA Council has willingly agreed to promote PSFaM and any other of our Canadian meetings, such as the CCCW and the BHT Meeting, on the ACA website. All that is required is a link to the meeting and any photographs for advertisements.

Finally, I am very sorry to bring you the news of the death of Stanley C. Nyburg (1924 – 2016). Stan was a Professor in the Chemistry Department at U Toronto for many years before retiring and moving back to London, England. He is survived by his daughter Anna Nyburg of Imperial College London. Kings College London holds an archive of his work there.

This is my penultimate article in *RefleXions* as the Canadian Representative on the ACA Council. My appointment ends as of December 31, 2016. I would like to thank the Co-Editors, Judy Flippen-Anderson and Tom Koetzle for their patience and superb editing of my articles. There are two top-notch candidates ready to take my place in the upcoming elections. Their platforms and backgrounds have been published in the Summer, 2016 issue of *RefleXions*. Have a read of their qualifications and please vote in the upcoming elections. Of course you have to be a member of the ACA in order to have a ballot! This is another excellent reason for you to renew your membership!!!

Thank you for the opportunity to have served as the Canadian Representative on the ACA Council for the past three years.

Michael James

Editor's Note: Election results have just come in! **Tomislav Friščić** will be the next Canadian Representative on ACA Council.

From the Editor's Desk

This issue features reports from the ACA's Annual Meeting in Denver, held in late July. Connie Rajnak has put together the cover and ***What's on the Cover*** (see p. 8) featuring our 2016 Etter Early Career Award winner, Jason Benedict, as well as the photo collages on pp. 17-18.

Our coverage of the Annual Meeting depends upon the efforts of many people. These include the session organizers and poster prize judges, who have drafted reports. We owe a special thank you to our *ACA RefleXions* Photographer Peter Müller and to Richard Bromund for their fabulous photos, along with our student volunteers responsible for the session group shots coordinated by George Lountos with assistance from Kristina Vitale.

Our gold open-access journal, *Structural Dynamics*, published jointly by ACA with AIP Publishing, continues to grow and thrive. For additional information on *Structural Dynamics*, see pp. 6-7. We are particularly encouraged to be able to report that Thomson-Reuters has assigned *Structural Dynamics* an impressive initial impact factor of 3.667. ACA members can take advantage of a special discounted rate when publishing their work in *Structural Dynamics*!

This issue of *RefleXions* is quite full and so we've decided to hold the workshop reports from Denver for our winter issue, along with those from our travel award winners. Stay tuned!

Tom Koetzle

News from ACA History Online

Recently we added a new section to the ***ACA History*** pages, *Impact of Structural Science*. Here we will post articles that describe the historic advances in structural science during the 20th century, with special emphasis upon how the discoveries impact our economy, healthcare, and our understanding of the natural world. The first article in this category is "History of NSLS – First Light to Shutdown" by Alison Sundermier and Vivian Stojanoff (reprinted from *ACA RefleXions*, 2015:2, 47-52). If you would like to contribute an article to this section, please contact Virginia Pett (***pett@wooster.edu***).

If you haven't already done so, check out the 20 movies already posted at the ACA YouTube channel: ***http://www.youtube.com/c/AmericanCrystallographicAssociationHistory***. Are you an expert at movie-making, or would you like to learn how to do it? We have video files from several previous ACA meetings and would welcome assistance with turning them into movies that we can add to the channel.

Webmaster Vanessa Reitz has updated the History banner (see above) and added a "donate" button to the Home page. If you enjoy the content of ***ACA History***, please test the new button!

Virginia Pett

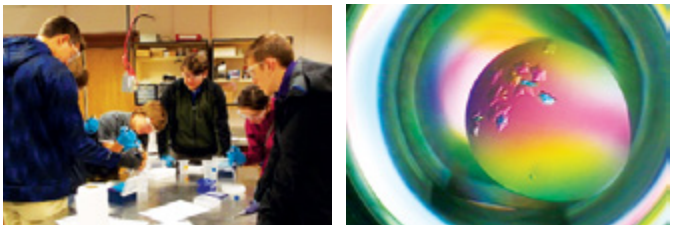
High-School Crystallography Outreach (Sponsored by YSSIG)

We at YSSIG appreciate the importance of getting students interested in crystallography early in their careers, and for the past few years we have organized crystallography events for high-school students from the surrounding area of the coinciding ACA meeting. We find that this encourages younger students to attend the ACA meetings, and many years' previous events have become self-sustaining programs that do not require an annual ACA meeting to be held nearby.

This year a class of 12 students from Liberty Commons High School, of Fort Collins Colorado, took a day trip to Colorado State U in mid-May to learn more about protein crystallography. The event was hosted by Professor Shing Ho of the Department of Biochemistry and Molecular Biology, with assistance from several other professors, post-docs, and graduate students at CSU.

Shing Ho (right) presents to students of Liberty Commons High School. The use of 3D glasses makes for an exciting introduction to crystallography!

Lessons were broken into several modules and included a 3D presentation on protein structure and an interactive computational portion on the visualization of electron-density maps. The students also received further information dependent on their background; physics students were taught about X-ray diffraction theory, while the chemistry students had a module on protein purification.



Left: Students crystallize lysozyme through vapor diffusion. Right: Some of the beautiful lysozyme crystals grown by the students. The crystallization kits were generously donated by Hampton Research.

Students examine an electron-density map and molecular model for lysozyme, using the Coot visualization software.

The students were also given a tour of CSU's X-ray facilities and were able to crystallize the model protein lysozyme, as well as visualize their crystals under a microscope. Supplies for the protein crystallization were generously donated by Hampton Research. We would like to thank Hampton, as well as everyone involved for making this year's outreach a success!

The event was well received by both the students and teachers, and the participants are planning on holding it again in the future. We also plan on organizing a similar event in the New Orleans area next year. If anyone would be interested in participating, either from the high-school or university level, please let us know!

Kimberly Stanek and Martin Donakowski

Ultrafast Technology in Switzerland

Fundamental and practical challenges facing our society can be addressed with new methods and thus approached from a new perspective. Examples of present day challenges are energy

conversion, information technology, new materials and biology and medicine. Over the last decade, ultrafast science and technology have made enormous progress, opening a large variety of new research fields and applications. Examples include table-top high-harmonic generation that allows new forms of spectroscopy and diffraction, lab-based sources of ultrashort electron pulses and sources of terahertz radiation that open new directions in materials science, chemistry and biology, and new sources of ultrashort X-ray pulses such as X-ray free electron lasers.

The Lausanne Centre for Ultrafast Science (LACUS) brings together teams working in Ultrafast Science and Technology with experimental and theoretical methods as well as those using ultrafast technology in different applications. Research areas are very diverse, spanning from fundamental to applied research, and they present a very high degree of complementarity. Several groups that are pioneers in ultrafast science and technology will pool their expertise in the development and the use of advanced ultrafast laser technology, X-ray and electron technology and associated methods, along with theory. The Centre also aims at complementing and strengthening existing Swiss scientific infrastructures, e.g. the Swiss Light Source and the SwissFEL.

Majed Chergui, Editor-in-Chief of *Structural Dynamics*, is the Founder and first Director of the Centre.

Remembering Ahmed Zewail

On August 2, 2016, Caltech Professor and Nobel Laureate Ahmed Zewail passed away at the age of 70. He was a member of the Advisory Board of *Structural Dynamics*. One can say that the entire field of ultrafast structural dynamics was born from his achievements. Back in the mid-1980s, he was the first to use femtosecond laser technology to solve problems in chemistry and biology. In this respect, he implemented the so-called pump-probe method in the femtosecond time domain, which he applied systematically to problems of growing complexity. This culminated in his earning the Nobel Prize in Chemistry in 1999. Parallel to these achievements, throughout the 1990s, he also pioneered ultrafast electron diffraction and microscopy, demonstrating their power at solving problems in chemistry, biology and materials science.

Ahmed Zewail had an amazing ability at communicating the power of the methods he developed and the significance of his findings, by identifying the system that would best explain a phenomenon. He was a real genius, the kind of person for whom no matter how complex a question was, he would find the answer. As a matter of fact, femtochemistry and ultrafast electron-based science developed into dynamic fields in less than 10 years thanks to the spectacular, yet deep, breakthroughs he achieved.

Being from Egypt, he always felt he had a duty to help and lift the level of education in his country in particular, but also in southern countries in general, what he used to call the "have nots". His dream for decades was to create a first class scientific university in Egypt, and this dream became reality in the past few years.

The scientific community is not only mourning the death of a leader and a pioneer in science, but also a personality with a vast culture, a contagious enthusiasm and uplifting spirit and most of all, with a never failing humbleness, respect and kindness in his relation to anyone.

He was a staunch support of *Structural Dynamics* having contributed two exciting papers since its launch in 2014:

Ultrafast electron crystallography of the cooperative reaction path in vanadium by Ding-Shyue Yang, Peter Baum, Ahmed H. Zewail *Struct. Dyn.* 3, 034304 (2016); *Ultrafast core-loss spectroscopy in four-dimensional electron microscopy* by Renske M. van der Veen, Thomas J. Penfold, Ahmed H. Zewail *Struct. Dyn. 2,* 024302 (2015)

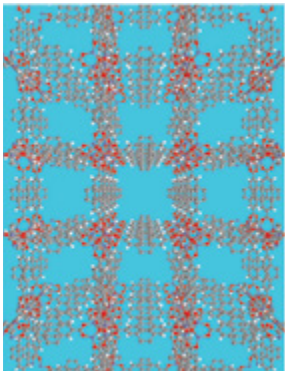
Majed Chergui

Structural Dynamics Prizes

ACA Poster Prize: Ayaka Harada (School of High Energy Accelerator Science, Tsukuba, Japan) was awarded the prize for her poster titled *Substructure determination for native-SAD phasing* (Co-authors Yusuke Yamada (KEK); Dorothee Libschner (LBNL); Naohiro Matsugaki and Toshiya Senda (KEK)). For more information on Ayaka's prize, turn to p. 10.

ACA Raffle: Meeting attendees who visited the *Structural Dynamics* booth were entered into a drawing for a waiver of 'author charges' for a submission of a paper to the journal. ACA member Qiu-Xing Jiang (U Florida – Gainesville) won the raffle. His research reflected in the paper he submitted to the meeting, titled *Chemically functionalized carbon films for cryoEM imaging* (Co-authors Marc Liaguno (Yale U) and Gaya Yadav (U Florida)) will be a perfect fit for *Structural Dynamics*.

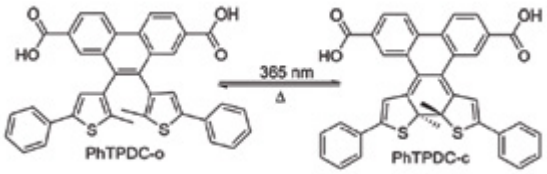
ECM Poster Prize: The selection committee (John Helliwell, Chair, Christine Beavers, Semën Gorfman, and Bob von Dreele) selected Ioana Sovago (U Copenhagen, Denmark) for her poster titled *What happens when thermal motion is frozen? A case study of polymorph stabilities for gallic acid monohydrate*.



Jason Benedict, University at Buffalo Chemistry Department, received the **2016 Margaret C. Etter Early Career Award** and presented a lecture preceding the Etter Symposium at the annual meeting of the ACA in Denver.

Jason's research ranges from light-based computing and communication to the environmentally-friendly and cost-effective conversion of light from the sun into fuels and/or electrical energy. Understanding and controlling the interaction of light and matter remains one of the great scientific challenges of the 21st century. With emphasis on studying light-matter interactions in crystalline materials, research in the Benedict lab involves the synthesis of novel materials and the development of new characterization techniques important to many areas of chemistry and physics. His group develops novel stimuli-responsive crystalline nanoporous materials; fabricates new devices for *in situ* X-ray diffraction experiments including guest exchange and photocrystallography; designs and constructs versatile microscopes for time-resolved spectroscopy and imaging and improved pumping in time-resolved XRD experiments; and explores the effect of the local chemical environment on the nucleation and growth of photoproducts in solid-state chemical reactions and phase transitions.

Jason's group has synthesized and characterized a new diarylethene-based ditopic linker 9,10-bis(2-methyl-3-phenylthiophen-3-yl)-phenanthrene-2,7-dicarboxylate, PhTPDC and prepared a photo-responsive MOF UBMOF-2, see at right.



Ring-opened and -closed structures of the photochromic MOF linker PhTPDC.

In 2014 Jason founded the United States Crystal Growing Competition ***www.uscrystalgrowingcompetition.org***, an important scientific outreach activity designed to provide K-12 grade students and teachers a fun, hands-on STEM experience as well as an exciting competition. In the 2015 contest, more than 90 participating schools and households sent in almost 70 crystals from 27 different states!

The cover image with the UBMOF-2 crystal lattice was kindly supplied by Jason Benedict. A related image appeared in the background on the cover of *New Journal of Chemistry* in January 2016.

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1. I.M. Walton, J.M. Cox, C.A. Benson, D.G. Patel, Y-S. Chen, J.B. Benedict, *New J. Chem.*, 2016, **40**, 101.
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4. I.M. Walton, J.M. Cox, J.A. Coppin, C.M. Linderman, D.G. Patel, J.B. Benedict, *Chem. Commun.*, 2013, **49**, 8012.
5. J.M. Cox, I.M. Walton, J.B. Benedict, *J. Mat. Chem. C*, 2016, **4**, 4028.

How to Make an Impactful Scientific Poster

- Do you plan to present a poster at a conference?
- Are you interested in effective ways to organize your poster content?
- Care to learn what graphics programs poster prize winners use?
- Would you like to become an expert in effective delivery of your project to the visitors of your poster?

If you answered yes to any of these questions, the new valuable resource at the ACA home page, ***Impactful scientific poster***, is for you: ***http://www.amercrystalassn.org—>Meetings—>Poster Preparation***. In all, 24 co-authors put their heads together to generate this web article. Past ACA poster prize laureates shared their posters, seasoned poster judges provided indispensable insights into effective poster organization, and everyone shared ideas on how to make poster session experiences advantageous to both the presenters and attendees.

This is awesome wrapped in awesome: from choosing font sizes to available graphics programs to the design and content organization to oral poster delivery… look no further: here you will find comprehensive advice on impactful poster preparation along with links to additional resources. The web article also offers warnings on poster mistakes and pitfalls. The last section is dedicated to poster evaluation: what poster judges take into consideration, what questions they ask, and what tools are available to them. All co-authors are listed on the web, but we particularly thank David Rose for sharing a ***Poster Presentation primer*** linked to the site.

The ***Impactful scientific poster*** web page is a live document. You are invited to share your advice and insights with the webmaster in order to further improve this practical compilation.

Ilia Guzei
ACA Denver Poster Chair

Dynamics of a poster session viewed from overhead

Pauling Poster Prizes

The **Pauling Poster Prize** was established by the ACA and is supported by member contributions to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was a very supportive member of the ACA for many years. At each annual meeting the seven best *postdoctoral, graduate or undergraduate* poster presentations receive Pauling awards. Some of the awards consist of $250, a complimentary banquet ticket, and a copy of a Linus Pauling book. The three **ACA Pauling Poster Prizes** honor Linus Pauling's contributions to science and U.S. crystallography; the **Herman R. Branson Pauling Poster Prize** recognizes the contributions of Herman Russell Branson, one of the first African American physicists to make crystallography the focus of his research; the **Muttaiya Sundaralingam Pauling Poster Prize** recognizes the groundbreaking crystallographic research on the stereochemistry of nucleotides and nucleic acids done by Muttaiya Sundaralingam and his colleagues; the **Louis Delbaere Pauling Poster Prize** in honor of Louis Delbaere, former ACA President from Canada, and sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, is given to the highest ranked *graduate or undergraduate* poster from a Canadian laboratory; and the **IUCr Pauling Poster Prize** sponsored by the International Union of Crystallography, is given to a *graduate or undergraduate* poster selected by the committee. The winner of the IUCr Pauling Prize receives complimentary online access to all IUCr journals for one year or a complimentary volume of *International Tables* or other IUCr publications.

At Denver, eligible posters were evaluated for the Pauling Poster Prize by a panel of 15 judges. Students were judged both on the work presented on their posters and on their general knowledge of the subject and crystallography. The posters and their presenters were all found to be excellent, making the task of determining the best posters very difficult. Below are the seven winners of the 2016 Pauling Poster Prizes. Photos are shown of winners who were able to be attend the conference banquet and accept their awards in person from Poster Chair Ilia Guzei. For additional information on two of the ACA Pauling prize-winning posters, 34-SU and 159-SU, turn to the **General Interest Posters** section, p. 39.

ACA Pauling Poster Prizes:

Darpandeep Aulakh, Clarkson U, poster **12-SU**: *Metal-Organic Frameworks as Platforms for the Controlled Nanostructuring of Single Molecule Magnets*.

Carrie Lomelino, U Florida, poster **34-SU**: *Non-classical, Diol-based Inhibition of Carbonic Anhydrase IX as a Potential Breast Cancer Therapy.*

Carrie Lomelino, at left, with Ilia Guzei

Lauren Stevens, U Maryland, poster **159-SU**: *Synthesis and Characterization of Novel Low Valent Aluminum Clusters*.

Lauren Stevens, at left, with Ilia Guzei

Herman R. Branson Pauling Poster Prize:

Jens Lübben, Heinrich Heine U, Düsseldorf, Germany, poster **63-SU**: *Automated Rigid Body Segmentation*.

Jens Lübben, at left, with Ilia Guzei

Muttaiya Sundaralingam Pauling Poster Prize:

Ryan Jackson, Montana State U, poster **103-SU**: *CRISPR RNA-guided DNA interference in Escherichia coli*.

Ryan Jackson, at left, with Ilia Guzei

IUCr Pauling Poster Prize:

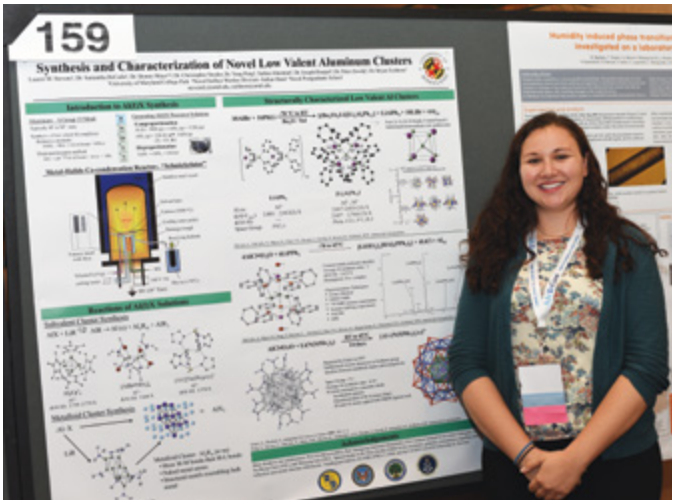
Alina Morales, undergraduate, Grand Valley State U, poster **52-SU**: *Novel Boronic Acid Inhibitors for the Class D β-Lactamase OXA-1*.

Alina Morales, at left, with Ilia Guzei

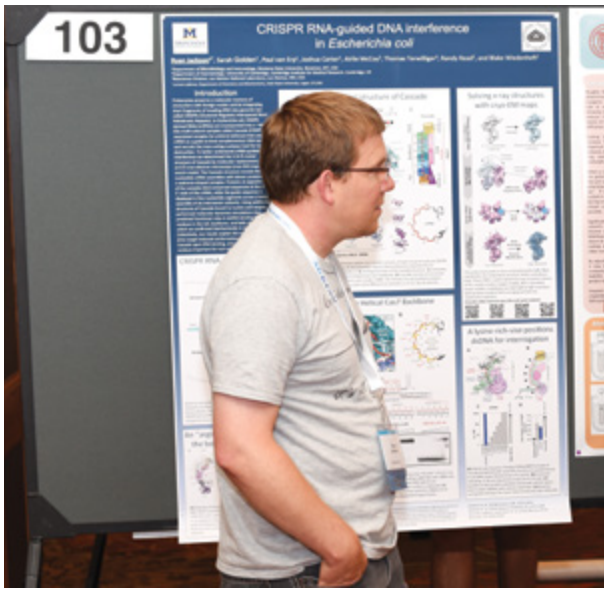
Louis Delbaere Pauling Poster Prize:

Jinhong Hu, U Calgary, Canada, poster **52-SU**: *Identification of the Inhibition Mechanism of Hydroxycitrate on Human ATP Citrate Lyase through X-ray Crystallography*.

Pauling Poster Prize judges for 2016 were: **John Bacsa**, **Jim Britten**, **Maksymilian Chruszcz**, **Marijana Dakovic**, **Michelle Dolgos**, **Martin Donakowski**, **Qiu-Xing Jiang**, **Eric Montemayor**, **Marilyn Olmstead**, **Rachel Powers**, **David Rose**, **Balasubramanian Venkatakrishnan**, **Carrie Wilmot**, **Andrey Yakovenko** and committee chair **Andrew Howard**.



Lauren Stevens with her winning poster



Ryan Jackson with his winning poster

Structural Dynamics Poster Prize

The **Structural Dynamics Poster Prize** is sponsored by ACA's gold open-access journal, *Structural Dynamics*, published jointly with AIP Publishing. The Structural Dynamics Prize is awarded for excellence in research on structural determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies.

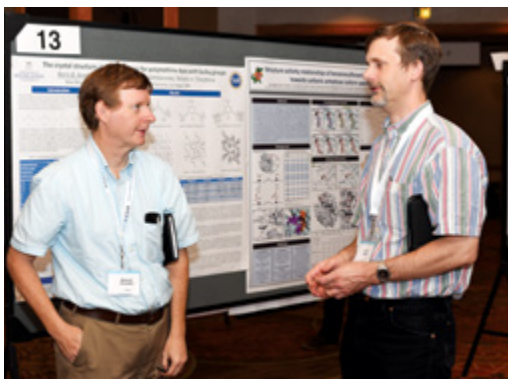
This year's prize was awarded to **Ayaka Harada**, School of High Energy Accelerator Science, Tsukuba, Japan, for her poster **3-SA**: *Sub-Structure Determination for Native-SAD phasing*.

Ayaka Harada, at left, with Ilia Guzei

Ayaka and her colleagues (co-authors Yusuke Yamada, Dorothee Libschner, Naohiro Matsugaki, and Toshiya Senda) solved the crystal structure of vanillate/3-O-methylgallate O-demethylase (LigM) by native sulfur SAD phasing resulting from a thorough evaluation of merging and scaling methodologies and parameters in order to optimize the anomalous sulfur signal. The protein, LigM, has 14 methionines in a total of 471 residues and crystallizes with symmetry $P2_12_12_1$ and four molecules in the asymmetric unit. In all, 30 data sets were collected at the Photon Factory. Each data set was processed with three different merging and scaling approaches. Then each subset of merged and scaled data was analyzed for both strength of the native sulfur anomalous signal and quality of the sulfur-substructure solution. The results of this study demonstrate the influence and sensitivity that resolution range for merging and scaling has on the sulfur anomalous signal and the subsequent success of native sulfur SAD phasing.

The judges for this year's Structural Dynamics Poster Prize were **Stephan Ginell**, **Blaine Mooers**, and committee chair **Lisa Keefe**.

Lisa Keefe



Richard Alexander, at left, and Kevin Battaile at a Denver poster session

RCSB Protein Data Bank Poster Prize

The **RCSB (Research Collaboratory for Structural Bioinformatics) Protein Data Bank Poster Prize** recognizes a poster presentation involving macromolecular crystallography by a student (*graduate or undergraduate*). The award consists of two educational books and an announcement on the RCSB PDB website (***www.rcsb.org***) and newsletter. The judges for 2016 were **Marie Fraser**, **Janet Newman**, **Jessica Vey**, and committee chair **Alexander Kintzer**.

This year the prize went to **Miguel Torres** for his poster **90-SA**: *Crystal Structures of Plant N-Methyltransferase Complexes Reveal New Insights into Substrate Recognition and Catalytic Mechanism*, poster #90 in the category Hot Structures I. Miguel is a graduate student working at U Calgary, Canada.

Alexander Kintzer

Journal of Chemical Crystallography Poster Prize

The **Journal of Chemical Crystallography Poster Prize** recognizes the best student, *graduate* or *undergraduate*, poster presentation in the area of chemical crystallography or small molecule structure determination and analysis. Springer's *Journal of Chemical Crystallography* sponsors the prize.

The winner this year was **Juby Varghese**, Clarkson U, for her poster **127-SA**: *SCXRD Meets PXRD to Investigate Temperature Induced Polymorphism in a Metal-Organic Framework*. Juby will receive a book of her choice from Springer.

An honorable mention was awarded to **José A. Carmona-Negrón**, U Puerto Rico, for his poster **66-SA**: *Synthesis, Characterization, and Application of Ferrocene Complexes as Estrogen's Pendant Groups for Breast Cancer Treatment: an Approach to Design Novel Metal-Based Therapeutic Drugs*. For more on José's work, see the **General Interest Posters** section, p. 39.

The judges for this year's Journal of Chemical Crystallography Poster Prize were **Lauren DePue**, **Frank Fronczek**, and committee chair **Graciela Díaz de Delgado**.

Graciela Díaz de Delgado

CrystEngComm Poster Prize

CrystEngComm (published by the Royal Society of Chemistry) is pleased to sponsor a prize to be awarded to the best student, *graduate or undergraduate*, poster presentation in the area of crystal engineering/supramolecular chemistry. The winner receives an RSC book voucher, and an announcement is posted on the *CrystEngComm* website (***www.rsc.org/Publishing/Journals/CE/about.asp***).

Serena Seshadri, an undergraduate from Georgetown U, was recognized for her winning poster **117-SA**: *Patterned Crystallization on Unpatterned Substrates*.

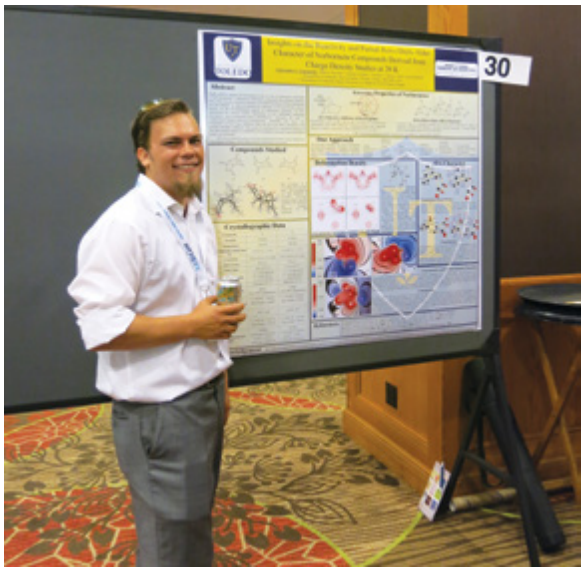
In addition, **Nara Guimaraes**, U Sao Paolo USP, Brazil, received honorable mention for poster **95-SA**: *X-ray Analysis for the Ternary ZrO_2-Y_2O_3-Nb_2O_5 Used as Thermal Barrier Coating*.

CrystEngComm Poster Prize judges for 2016 were **David Grossie**, **Alexander Filatov**, and committee chair **Christine Beavers**.

Oxford Cryosystems Low Temperature Poster Prize

The **Oxford Cryosystems Low Temperature Poster Prize** is *open to all participants* and is awarded to the best poster describing work in low-temperature crystallography. The winner receives a cash prize donated by Oxford Cryosystems, Inc.

This year's winner of the Oxford Prize was **Christopher Gianopoulos**, U Toledo, for his poster **30-SA**: *Insights on the Reactivity and Partial Retro-Diels-Alder Character of Norbornene Compounds Derived from Charge-Density Studies at 20 K*, shown below. In a study of two norbornenes combining



Christopher Gianopoulos. Photo by Milan Gembicky.

low temperature (20 K) X-ray diffraction measurements and DFT calculations with periodic boundary conditions, Christopher and his co-authors (Alan Pinkerton, Bartos Zarychta, Simone Cenedesa, Vladimir Zhurov) have shown that topological analyses of the total charge density provide additional support for the presence of retro-Diels-Alder character in norbornenes, independent of bond distances, on the basis of the electron density and its curvature.

In addition, **Zhijie Chua**, U Toledo, received honorable mention for poster **164-SA**: *Charge Density Analysis of 2,5-Dichloro-1,4-benzoquinone (DCBQ) at 20 K*.

Judges for the 2016 Oxford Cryosystems Low Temperature Poster Prize were **Marcus Bond**, **Marian Szebenyi**, and committee chair **Milan Gembicky**.

Philip Coppens discussing poster 164-SA with poster session attendees including Yang Chen, facing Philip, and to his left Krishnayan Basuroy.

MiTeGen - Society of Physics Students Undergraduate Poster Prize

The **Undergraduate Poster Prize**, established in 2014 to encourage participation of younger scientists in crystallographic research, is co-sponsored by the AIP Society of Physics Students and MiTeGen and recognizes the best *undergraduate* poster presentation. The recipient of this award receives a $250 cash prize, generously donated by MiTeGen and SPS, along with a $250 gift card for crystallographic supplies though MiTeGen.

This year's undergraduate prize was awarded to **Sofia Antal**, from the Chemistry Department at New Mexico Highlands U.

Sofia Antal, at left, with Ilia Guzei

Sofia was recognized for her work on crystalline capture of post-combustion carbon dioxide molecules, presented on poster **124-MO**: *Crystalline Products of CO_2 Capture by Piperazine Aqueous Solutions*.

The judges for the 2016 Undergraduate Poster Prize were **Aaron Celestian**, **Brad Conrad**, and committee chair **Kimberly Stanek**.

Kimberly Stanek

Editor's note: Photos in the **Poster Prizes in Denver** section by Peter Müller, except where otherwise noted.

Taylor & Francis Biomolecular Crystallography Poster Prize

The **Taylor & Francis Biomolecular Crystallography Poster Prize** is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The winner receives a copy of Bernhard Rupp's book *Biomolecular Crystallography* donated by the Taylor & Francis Group.

The 2016 winner was **Massimo Sammito**, U Göttingen, Germany, for his poster **89-SA**: *Solving Protein Structures Without a Model or Experimental Phases*. Massimo described the *ab initio* structure determination of a 150 amino acid, all-β viral protein called N-Terminal A46, using data to 1.55 Å.

Massimo Sammito, at left, with Ilia Guzei

Massimo utilized BORGES_MATRIX to extract from the PDB a library of small fragments containing three antiparallel β-strands. This fragment library was then used as input to the ARCIMBOLDO_BORGES pipeline utilizing Phaser and SHELXE to phase the structure.

The judges for 2016 were **Annette Langkilde**, **Surajit Banerjee**, and committee chair **Robyn Stanfield**.

Robyn Stanfield

Contributors to this Issue

Heba Abourahma, Paul Adams, Oluwatoyin Asojo, Christine Beavers, David Belnap, Jason Benedict, Jim Britten, Richard Bromund, Branton Campbell, Chelsy Chesterman, Louise Dawe, Graciela Díaz de Delgado, Vicky Doan Ngyen, Libby Dowdall, Martin Donakowski, Larry Falvello, Joseph Ferrara, Barry Finzel, Bruce Foxman, Frank Fronczek, Milan Gembicky, Stefan Ginell, Elizabeth Goldsmith, Ana Gonzalez, Danielle Gray, Kushol Gupta, Ilia Guzei, Katarzyna Handing, Christina Hoffmann, Ashfia Huq, Jan Ilavsky, Michael James, Lisa Keefe, Alexander Kinzer, Paul Langan, Anna Llobet, George Lountos, Maria Miller, Eric Montemayor, Peter Müller, Sean McSweeney, Allen Oliver, Katie Page, Arwen Pearson, Virginia Pett, Rachel Powers, Daniel Rabinovich, Connie Rajnak, Joe Reibenspies, Aaron Robart, David Rose, Carl Schwalbe, Yulia Sevryugina, Sangita Sinha, Carla Slebodnik, Stacey Smith, Kimberly Stanek, Robyn Stanfield, Charlotte Stern, Robert Sweet, Marian Szebenyi, Joe Tanski, Tom Terwilliger, Brian Toby, Anastasiya Vinokur, Mark Whitener, Kraig Wheeler, Carrie Wilmot, Peter Wood, Kevin Yager, Andrey Yakovenko

The ACA's **66th Annual Meeting** kicked off in Denver on Friday, July 22, 2016 with five workshops – on **The CSD Python API: A Foundation for Innovation**; **Computational Approaches to the Structural Modeling of Biological Macromolecules using Small-Angle Scattering**; **Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials**; **Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques**; and a **SHELX Workshop**. A **First Time Attendee and Student Meeting Orientation** was held Friday evening, followed by the **Opening Reception Exhibit Show** generously hosted by the exhibitors. Reports from the **Workshops** and from this year's **Travel Award Winners** will be featured in our winter issue of *ACA RefleXions*.

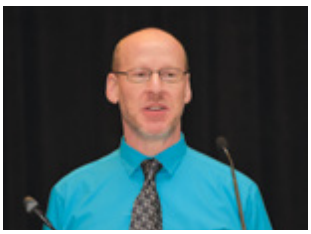
The **K. Trueblood Award** for 2016 was presented to **Axel Brunger**. **Elspeth Garman** received the **I. Fankuchen Award**, **Benno Schoenborn** was honored with the **Robert Bau Award**, and **Jason Benedict** received the **Margaret C. Etter Early Career Award**. Jason's work is featured on our cover (see also ***What's on the Cover*** on p. 8). The **ACA Transactions Symposium**, *Structural Dynamics*, was chaired by **Jason Benedict** and **Arwen Pearson**.

The meeting wrapped up on Tuesday evening with ACA's annual **Awards Banquet**. The evening's program chaired by ACA President, **Tom Terwilliger**, included the presentation of the **ACA Fellows – Class of 2016**: **Gerard Bricogne**, **David Brown**, **Charles Campana**, **Bryan Chakoumakos**, **Yu-Sheng Chen**, **Frank Fronczek**, **Michael James**, **Brian Matthews**, and **Arnie Rheingold**. The ACA honored this year's 14 **Poster Award Winners** along with three students selected to receive an honorable mention from among the exceptional array of posters presented at the meeting (see pp. 9-12 for news on the Poster Awards). This year's program also featured a fascinating talk by **Phil Plait**, a/k/a the Bad Astronomer, emphasizing critical aspects of communicating our science to a broad audience in the age of Snapchat and Twitter. To cap off the evening, our Past President, **Chris Cahill**, arranged for an ACA meeting first – attendees were treated to dancing with a live band, joined by Chris himself on drums. For an upbeat take from Christine Beavers on the banquet and the Bad Astronomer's talk, turn over to pp. 14-15.

Amy Sarjeant and **Edward Snell** were **Program Chairs** for the meeting; **Ilia Guzei** was **Posters Chair**; **George Lountos** 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. AIP Publishing's **Robert Finnegan** did his usual great job with the **Exhibit Show**.

ACA RefleXions Co-Editor Judy Flippen-Anderson, at left, and Winnie Wong-Ng

Jobichen Chacko, at left, and Irimpan Mathews discussing a point in the meeting exhibition hall



Phil Plait, the Bad Astronomer, delivering his talk at the Awards Banquet

L-R: Arthur Schultz, Larry Falvello and Tom Emge taking a break from a poster session

ACA President Tom Terwilliger, at left, with Past President Chris Cahill

L-R: Structural Dynamics Assoc. Editor George Phillips with Anthony Solis and Jessica Hoy of AIP Publishing

Photos by Richard Bromund or Peter Müller. Denver Meeting Logo Design: John Aspinall.

An Evening with Phil Plait, the Bad Astronomer

We were very fortunate this year at the banquet to have a guest speaker, **Phil Plait**. To put my excitement in context, we will take a little trip to his and my favorite social medium: Twitter.

Twitter is a different type of social media format for one main reason: brevity. You need to squeeze your thoughts down to a scant 140 characters. This can be extremely challenging, and if you exceeded this limit, the site's mascot used to admonish you to be more clever! Cleverness is what keeps bringing me back to Twitter – that and an abundance of wonderful scientists who are active on the site. Phil Plait, who goes by ***@BadAstronomer*** on Twitter, is one of many prominent scientists whom you can follow, and then hear their every tweet. I enjoy hearing about everything from astrophysics to politics from Phil, Katie Mack(***@AstroKatie***) and Neil deGrasse Tyson(***@Neiltyson***), among many others. They use a combination of humor and science to reach out to a diverse audience. In a feeble imitation of some of my Twitter science heroes, I attempt similar outreach, mixed in with a gratuitous amount of horse selfies.

One of the challenges of being on Twitter as a scientist is deciding how to present your public persona. Twitter is an international platform, and one tweet can easily go around

Twitter exchange where I learned about our guest speaker. (OMFG= oh my freaking gosh (some explicit variants possible)).

the world if its message resonates widely. Many scientists and academics on Twitter are very conservative in their tweeted views, in order to not incite the wrath of an ideological mob, or the ire of funding organizations. Unfortunately, this approach limits their appeal to the general population, which limits the propagation of their message. It's a very difficult balance to manage.

With this in mind, let's talk about our most excellent guest speaker. Phil Plait has a background in astronomy, with his Ph.D. studies focused on supernova SN 1987A (***https://en.wikipedia.org/wiki/SN_1987A***). He now runs a blog for *Slate* magazine, where he features lots of epic astronomy stories, but also more diverse topics, such as climate change. He is not afraid to be humorous, provocative or direct, if it gets his message out to the wider public. I was ecstatic when I heard he was going to be speaking at our closing banquet.

Despite not being a crystallographer, Phil came equipped with enough crystallography knowledge to get our attention. On Tuesday, one day before the banquet, he tweeted a link to his new blog post, which featured lots of talk about symmetry

Phil's tweet on extraterrestrial quasicrystals. Inset: a QR code that links to the article.

and atomic bonding, in order to make a challenging topic, like quasicrystals found in a meteorite, accessible. It was a wonderful read and a great outreach piece for crystallography in general.

The final day of the meeting arrived, and I was lucky enough to be part of the vanguard of crystallographers who met Phil in the Sheraton lobby. He was excited, and possibly a bit surprised by our level of excitement. His talk lived up to our hype. Entitled "Science Communication in the Age of Snapchat," he told us that he had really wanted to call it "Crystal Blue Persuasion." "Better get ready to see the light," he said, speaking a couple of lines of the popular 1969 song. He dove into a short description of his science outreach methods, with making videos and sharing fun images prominent among them. He showed some favorites, referenced the internet's general love of cats, but questioned if cats were nearly as cute as his goats. He implored us all to

consider ourselves science communicators, because "the public loves science," but that "science doesn't speak for itself, it needs an advocate." He also wanted to remind us that science communication needs to be done by scientists who aren't afraid to be human. Being human on social media reminds the public that science isn't a monolithic thing – it is something that is done by humans. He mentioned an unidentified ACA member who was active on Twitter, and this person was outspoken, passionate, and often explicit, but these characteristics humanized their tweets and made them more accessible to the general public.

After his enthusiastic presentation, Phil was treated to the best banquet entertainment in recent history – Past President Chris Cahill playing drums with a band, complete with dancing crystallographers! Many of us, having live-tweeted along to his talk, felt newly invigorated about science outreach over social media, but we put that feeling aside temporarily, so it wouldn't detract from the socializing and cavorting. Now that we have all gone our separate ways, it's time to get excited again. To help, I have collected all the tweets that contained ***#ACADenver*** into a Storify post, which is a convenient way of looking at social

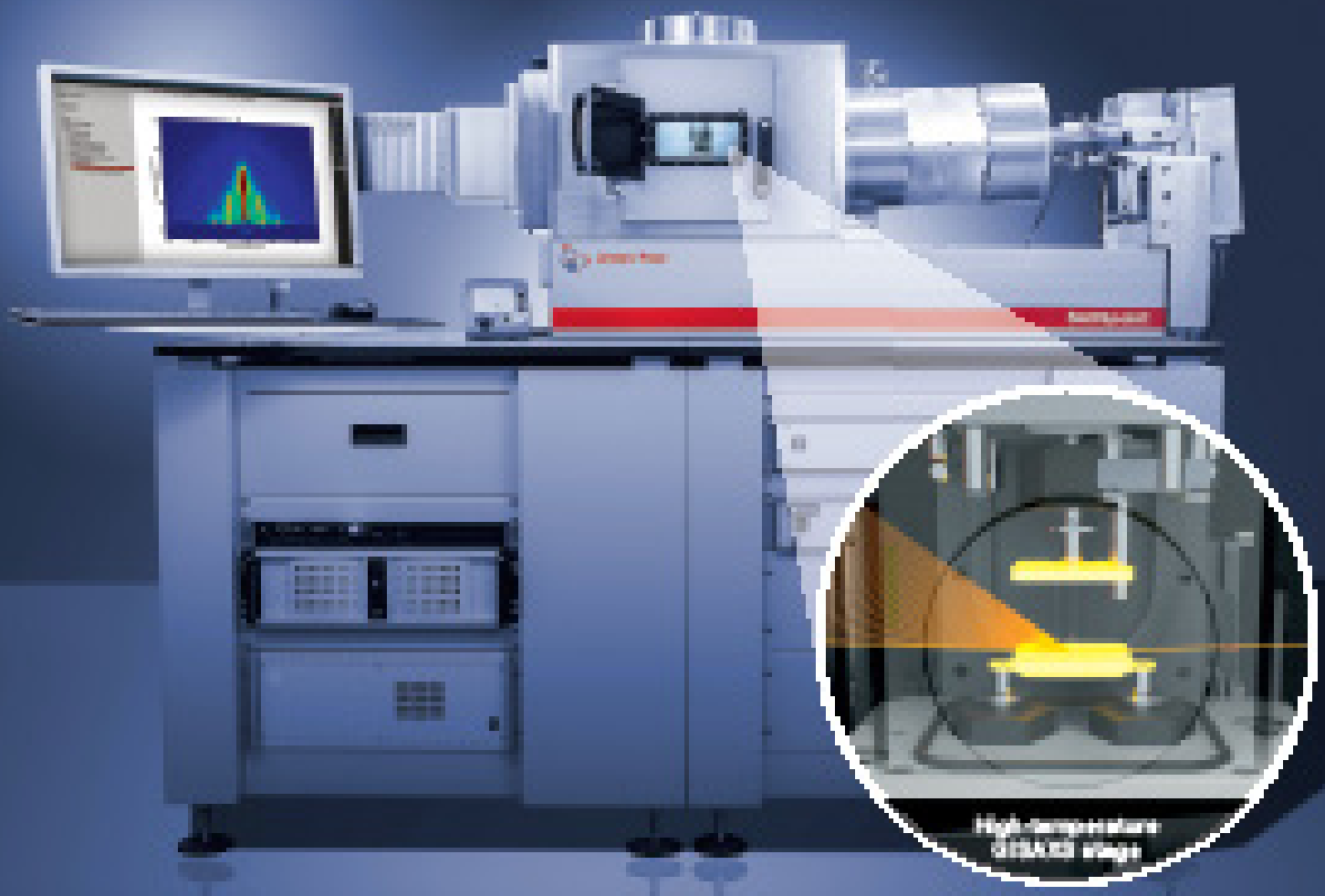
A screenshot of the #ACADenver Storify page, with a QR code for the link inset.

media without needing to log into an account. This will let you reminisce over the meeting, see who among your crystallographic peers is on Twitter, and perhaps entice the non-Twitterers among us to dip that proverbial toe in the water. I encourage everyone to take the Bad Astronomer's words to heart, and see what social media science outreach has to offer. Our science has so much to offer the world, and we are the people who must speak for it. I hope to see you all on Twitter!

Christine Beavers

The world's brightest footprint

Anton Paar



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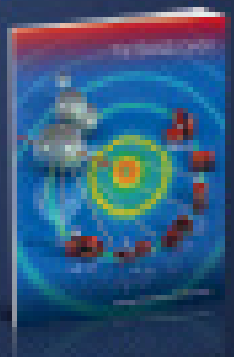

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Top, L-R: Kristina Vitali with Marcia Colquhoun in back making horns; Anthony Solis, Charles Campana, Ilia Guzei. 2nd row: Liz Carter, S. N. Rao, George Phillips.

3rd row: Louise Dawe, Tom Terwilliger, Tom Koetzle, Amy Sarjeant. Across the bottom: Joe Tanski, Lauren DePue, Sue Byram, Elspeth Garman.

Photos by Richard Bromund or Peter Müller

Top: Audience Overview. 2nd row, L-R: Andrey Yakovenko with his baby; Elspeth Garman after her Fankuchen Award lecture; Benno Schoenborn talking with Tom Terwilliger and Virginia Pett after his Bau Award lecture. 3rd row: Amy Katz and Jenny Glusker talking with Carol Brock; Noriko Inoguchi and Michael James. Bottom row: Samatar Jirde and Marvin Hackert; David Rae and Simon Coles.

Photos by Richard Bromund or Peter Müller

AW.01: Axel Brunger is Honored with the Trueblood Award

ACA President Tom Terwilliger, at right, presents Axel Brunger with the 5th Trueblood Award. Photo by Peter Müller.

*The 2016 recipient of the **K. Trueblood Award** is **Axel Brunger**, Professor of Molecular and Cellular Physiology at Stanford University and a Howard Hughes Medical Institute Investigator, for his work on crystallographic methods and the study of challenging biological systems. Axel received the award at the July ACA meeting in Denver, where he delivered a fascinating lecture focused on an important biological problem (synaptic vesicle fusion), which he has been studying for many years, and how this work has benefitted from the development of new technologies (free-electron lasers).*

The award, which was established in 2001, recognizes "exceptional achievements in computational or chemical crystallography" and honors Ken Trueblood's role in the early use of computers and the development of crystallographic computer programs. Axel himself has had a huge impact on the field of structural biology and X-ray crystallography, with many vital contributions over the past three decades in the area of computational methods. His development of simulated annealing methods for structure refinement, and assessing over-fitting with the free-R factor have become standards in X-ray crystallography. The more recent development of the deformable elastic network (DEN) method in collaboration with Gunnar Schroeder and Michael Levitt has enabled the refinement of challenging structures at low resolution. The X-PLOR and CNS software systems changed the way researchers approached solving and refining macromolecular structures, by X-ray crystallography and NMR spectroscopy.

Axel's passion for tackling computational problems was evident from his award presentation, where he talked about how new computational methods are making it possible to extract high-quality crystallographic data from experiments at X-ray free electron laser (XFEL) sources. These developments have been driven in part by Axel's decision 20 years ago to take the leap into the field of experimental structural biology, determined to understand the molecular basis of synaptic vesicle fusion – central to the transmission of signals between neurons. He has studied the large collection of proteins that assemble to regulate and drive membrane fusion, recently arriving at crystals of large complexes presenting technical challenges in the form of weak diffraction, radiation damage and limited crystal availability. Axel showed how serial XFEL diffraction experiments have led to significantly better data resolution, structure solution, and ultimately new biological insight. However, to do this he emphasized that it was necessary to develop new methods for indexing, integrating and optimizing the experimental diffraction images.

I'm sure many in the audience left Axel's talk with a renewed urge to tackle a challenging biological problem. I suspect that some left eager to write new computer programs. I hope that everyone left with an appreciation of Axel's huge contribution to the field of X-ray crystallographic methods development, and a realization that even in such a mature field many challenges remain that need to be solved.

Paul Adams

AW.02: Jason Benedict Receives the Etter Early Career Award

Jason Benedict, at left, accepting the Etter Early Career Award from ACA President Tom Terwilliger. Photo by Peter Müller.

*The **Etter Early Career Award** for 2016 was presented to **Jason Benedict**, Assistant Professor, Department of Chemistry, University at Buffalo. The Etter Award, established to honor the memory of Professor Margaret C. Etter (1943-1992), recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career.*

Jason was honored for his innovative research exploring light-matter interactions in crystalline materials, work featured on our cover. For more information on Jason and research from his group, see ***What's on the Cover*** on p. 8.

The **Etter Early Career Session**, **01.04**, immediately followed Jason's award lecture on Sunday morning, see p. 21 for more.

AW.03: The Bau Award to Benno Schoenborn

Benno Schoenborn, at left, receiving the 2nd Bau Neutron Diffraction Award from ACA President Tom Terwilliger. Photo by Peter Müller.

*The **Bau Neutron Diffraction Award** for 2016 was presented to **Benno Schoenborn**, a retired Senior Fellow at Los Alamos National Laboratory, for his pioneering research in macromolecular neutron crystallography and the design and development of the neutron crystallography beamline (Protein Crystallography Station, PCS) at the Los Alamos Neutron Scattering Center (LANSCE). This award is given in memory of Professor Robert Bau from the University of Southern California (1969-2008), a past President of the ACA (2006). Professor Bau made major contributions to the development of the technique of single-crystal neutron diffraction and to its applications in chemical and biomacromolecular crystallography. Benno Schoenborn, born in Basel, Switzerland, is the second recipient of this triennial award.*

Turn to p. 20

For many American structural biologists, Benno Schoenborn is known as the father of macromolecular neutron crystallography, because of his leading role in pioneering development and application of the technique over almost a half century. New ground was first broken at the High Flux Beam Reactor (HFBR) at Brookhaven National Laboratory in the 1960s. Using a monochromatic beam and a single-bin detector, it took Benno several months to collect sufficient data on Walter Hamilton's single-crystal diffractometer to determine the neutron structure of the transport protein myoglobin. Benno's goal was to identify the location of hydrogen atoms involved in bonding the anesthetic xenon. Although many at the time considered it to be a wild-goose chase, the experiment was a success, establishing beyond doubt that neutron crystallography is a powerful technique for directly visualizing hydrogen atoms in biological macromolecules. For the next three decades the number of studies remained small because of the limited number of available neutron beamlines, and their relatively weak flux compared to X-ray facilities thereby requiring large crystals that are often difficult to grow. However, those studies were of great importance because of the vital and unique information that they provided on the role of hydrogen in enzyme mechanisms, hydrogen bonding, and water structure.

Over the past two decades several further technical developments at neutron sources in the United States, Europe, and Asia have continued to push sample size requirements down below 0.1 mm^3 and data collection times down to a few days, rather than months. I had the privilege of working with Benno on one of those developments. After moving from Brookhaven National Laboratory to Los Alamos National Laboratory in 1993, Benno began work on designing the first neutron protein crystallography station (PCS) for a spallation neutron source. At spallation sources, neutrons are produced in pulses and time-stamped, they then travel as a function of their energy so that they are detected at different times-of-flight (TOF). The TOF Laue technique has all of the advantages of conventional and Laue methods, but does not suffer from reflection overlap and the build-up of background over wavelength range. Benno saw that this characteristic could have major advantages for neutron protein crystallography.

When Benno received funding from the U.S. Department of Energy to build PCS, I moved from the Institut Laue Langevin in France to join him in this ambitious project. With colleagues Eric Pitcher, Phil Ferguson, and myself, Benno designed every component of PCS to maximize the neutron intensity and reduce background scattering. The PCS beam line turned out to be a big success, allowing larger proteins, for which large crystals are nearly impossible to grow, to become amenable to neutron crystallography. In addition to providing important scientific insights into enzyme mechanism, PCS was a proof-of-principle for the technique of TOF Laue macromolecular neutron crystallography. TOF Laue macromolecular crystallography beam lines with game changing new capabilities are now being designed, constructed and operated at powerful next-generation spallation neutron sources across the world, including the Spallation Neutron Source (SNS) and the Second Target Station (STS) at Oak Ridge National Laboratory, the European Spallation Source (ESS) and the Japan Proton Accelerator Research Complex (J-PARC). These powerful new tools have their origin in a heroic experiment conducted by a visionary scientist, Benno Schoenborn.

Paul Langan

AW.04: Elspeth Garman Receives the Fankuchen Award

ACA President Tom Terwilliger, at right, presenting the Fankuchen Award to Elspeth Garman. Photo by Peter Müller.

The **I. Fankuchen Award** *was established in 1971, "to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography." It would be hard to think of anyone more deserving of that accolade than the 2016 awardee,* ***Elspeth Garman****, Professor of Molecular Biophysics at Oxford University, U.K. Elspeth accepted the award at the Denver meeting with an entertaining, wide-ranging talk that aptly demonstrated her skills as a speaker/educator as well as a highly impactful scientist.*

Elspeth's passion for education began early when, characteristically, at the age of 18, she spent 10 months teaching in Swaziland. That experience led to her lifelong association with Africa, including her role as a foster parent. Astonishingly, Elspeth returned after 40 years to the very classroom in which she had taught, finding it essentially unchanged.

Elspeth's scientific background began in nuclear physics. During her training, she developed her skills in instrumentation and coding, and recognized the importance in believing in your data, even if they clash with accepted dogma. After several years as a postdoc and Research Officer in Nuclear Physics at Oxford where she learned, among many other things, about the care and handling of liquid nitrogen dewars, Elspeth was recruited to the Laboratory of Molecular Biophysics by Louise Johnson and David Phillips in 1987. At LMB, Elspeth oversaw the diffraction facilities with such care that, eventually, the instrumentation received a longevity award from Rigaku, before finally earning a well-deserved (working) retirement in Mexico. As part of her job, Elspeth trained countless budding crystallographers in data collection, including a session with Dame Margaret Thatcher who, indeed, never made it as a chemist.

At LMB, Elspeth developed many of the early techniques for cryo-crystallography of macromolecules including, among many other developments, the manufacture of loops (using her baby daughter's hair), and refinement of the magnetic pin holders and other cryo-tools that are now essential implements in macromolecular crystallography laboratories. Beginning in 1987, she became a "synchrotron junkie." This led to her seminal contributions in understanding and controlling radiation damage in protein crystals, including her group's development of the RADDOSE program.

In keeping with the spirit of the Fankuchen Award, Elspeth

described her communications activities, starting with some experiences with the press, her extensive training workshops all around the world, and her public presentations. In his introduction, ACA President Tom Terwilliger gave a famous quote concerning Fankuchen that he, "treated members of his group as his family." The same can definitely be said of Garman. Her list of undergraduate project students and junior interns filled almost an entire slide, and she was obviously personally engaged with each and every one (several of whom eventually joined her research group as graduate students). Elspeth Garman surely represents the embodiment of the talents and dedication that the Fankuchen Award was established to recognize.

David Rose

01.04:Etter Early Career Session

L-R: Vicky Doan-Nguyen, Kimberly Maize (at rear), Madushami Dharmarwardana, Martin Donakowski (at rear), Anastasiya Vinokur, Arshad Mehmood, Gavin Mitchson (at rear), Bradley Hintze. Katarzyna Handing and Jose Olmos are not shown. Photo by student volunteer.

The **Etter Early Career Session** chaired by Anastasiya Vinokur, U Wisconsin – Madison, and Martin Donakowski, Naval Research Laboratory, featured rising stars of the ACA and showcased the diversity of the crystallographic sciences with speakers from backgrounds ranging from small molecule to macromolecule studies. The session served to highlight exceptional submitted abstracts of graduate students and postdoctoral scientists. The first speaker of the session was **Madushani Dharmawardana**, U Texas Dallas. She demonstrated how thermochromic crystals of butoxyphenyl N-substituted naphthalene diimide exhibited color change as a function of temperature due to local changes in the individual molecular configurations and intramolecular distances, which in turn affected the charge-transfer dynamics. A further examination of local structural order was presented in the entirely inorganic system of $La_2Zr_2O_7$ thin films: **Gavin Mitchson**, U Oregon, spoke about his findings made via X-ray electron microscopy of increased cation (La/Zr) ratios at the thin film interfaces. **Vicky Doan-Nguyen**, U California Santa Barbara, continued with an examination of the local-to-mid-range structure of transition-metal sulfide systems via pair distribution function (PDF) studies, a technique that allows crystallographers to understand semi-crystalline (and even non-crystalline) materials: a real demonstration of the strength of crystallographic sciences! Diving even further into local-structure study, **Arshad Mehmood**, Texas Christian U, presented a talk examining ultra-high resolution ($d \approx 0.5$ Å) study of 1-(2,3-dichlorophenyl)piperazine. This high resolution allowed visualization of electron-density distributions for valence shell and bond characterization, going beyond the determination of atomistic structure and into electron localization!

Bradley Hintze, Duke U, began the bio / macromolecular portion of the Etter Early Career Session with an examination of "local structure" DNA base pair mismatching. Specifically, his talk examined non-Watson-Crick base pairs – known as Topal-Fresco base pairs – such as A-C, G-T, A-A, G-G, and G-A and presented an analysis of such mispairs found in the Protein Data Bank (PDB). Moving on to the structure-function relationships, **Kimberly Maize**, U Minnesota, presented examinations of an enzyme for nucleotide monophosphate prodrugs with a discussion of three key complexes that rationalize the biochemically observed substrate selectivity. With a continuation of the build up from small-molecule to macromolecular crystallography, **Katarzyna Handing**, U Virginia, then presented a talk on cetirizine (trade name Zyrtec) with the first crystal structure of a mammalian serum albumin at a resolution of 2.1 Å; the researchers found cetirizine was bound to two sites that differed from previously proposed binding sites for mammalian albumins. The session culminated with a presentation by **Jose Olmos**, Rice U – the YSSIG Etter Student Award winner – on findings from an X-ray Free Electron Laser (XFEL) study of β-lactamase – the causal agent of tuberculosis, *Mycobacterium tuberculosis*. In his talk, Jose described captured enzyme dynamics via time-resolved crystallography and notably accomplished this within samples that were uniformly initiated to obtain structural intermediates. The presented work stressed both the importance of high-quality crystal growth in methods for jet stream techniques as well as the burgeoning field of XFEL studies.

Overall the Etter Early Career Session both presented premier talks and showcased the excellent work being done by a diverse group of young scientists.

Martin Donakowski
Anastasiya Vinokur

Jose Olmos receiving the Etter Student Lecturer Award from Session Chair Martin Donakowski. The Young Scientist SIG selected Olmos as recipient for this Early Career Session. Photo by student volunteer.

TR.01: The Transactions Symposium: Structural Dynamics

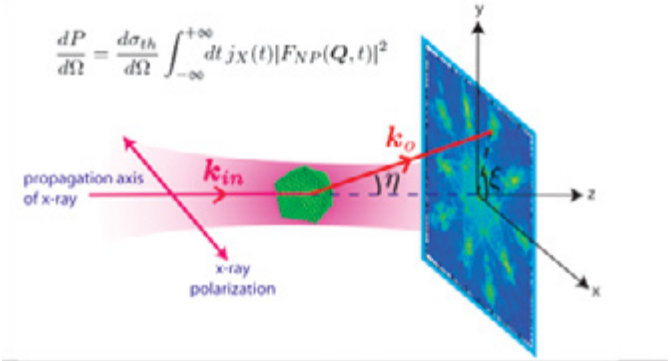
L-R: Arwen Pearson, Charles Carter, Adrian Goldman, Niranj Chandrasekaran, Linda Young, Wilfred Fullagar, Lin Chen, Jason Benedict, Jacqueline Cole, Sarah Perry. Photo by Peter Müller.

This year's **ACA Transactions Symposium** was focused on the growing area of structural dynamics and featured speakers talking on a diverse range of topics, from small to macromolecules and from femtoseconds to seconds. **Philip Coppens**, U Buffalo, a pioneer in the field of time-resolved crystallography, kicked off the symposium presenting a selection of key results from his many years of research on photoisomerizations, dimerizations, polymerizations, linkage isomers, ring openings and short-lived excited states. Philip's key message was that crystallography is not restricted to just giving information on static ground-state structures, but that the developments over the last decades in instrumentation, sources and analysis tools mean it is also able to provide detailed insights into dynamic behavior.

With the stage well set we then moved on to much larger and slower things with a presentation from **Adrian Goldman**, U Leeds, U.K., about the use of crystallography to probe the mechanisms of two pyrophosphatase enzymes, one soluble and one membrane bound. By hydrolyzing pyrophosphate, these enzymes provide a thermodynamic driver for many biological processes. Using a combination of mechanistic trapping, with mutants and different substrates, in parallel with complementary biochemical studies Adrian has been able to catch the pyrophosphatases in action with a series of crystallographic snapshots, like frames of a movie. These have enabled him to propose a detailed structural mechanism for both the pyrophosphate hydrolysis and, for the membrane bound system, how this is then coupled to the pumping of H^+ and Na^+ across the cell membrane.

The next talk took us back into the small molecule realm as **Jacqueline Cole**, U Cambridge, U.K., presented dynamic crystallographic studies on a series of ruthenium compounds that function as photoswitches or phototransducers and have exciting possibilities for the development of light-driven nanomaterials. Jacqui showed that understanding how the molecular properties of these materials are coupled to their response to light excitation is an absolute requirement for their rational engineering into devices.

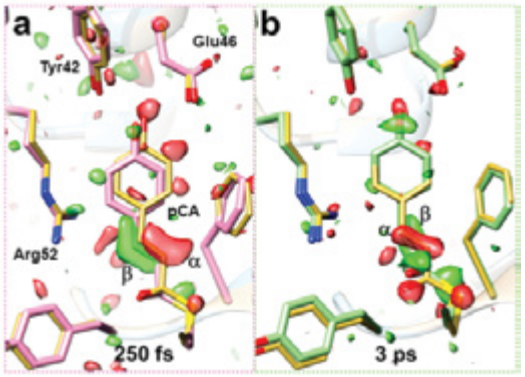
We then moved on to an extremely dynamic talk by **Linda Young**, Argonne National Laboratory, on the use of free electron X-ray lasers (FELs) to study atomic and molecular structure. Linda's talk took us on a journey from the very, very small, looking at the response of atoms to an ultrashort, ultra bright FEL pulse to the use of such pulses to move beyond crystallography to coherent diffractive imaging of single molecules, even of single proteins (see image below). She made it clear that the properties of the FELs give us an unprecedented window into the ultrafast structural dynamics of molecules.



We closed the morning session with a talk by **Niranj Chandrasekaran**, U North Carolina at Chapel Hill, selected from among the submitted abstracts. Niranj presented his work on the development of a new, computationally cheap algorithm, PATH, for the prediction of transition-state conformations in enzyme reactions where the chemical step is accompanied by a protein structural rearrangement.

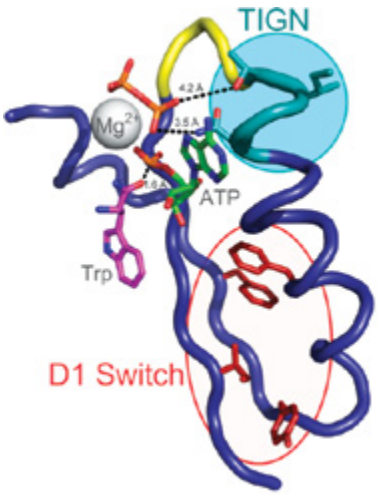
After lunch we reconvened for the afternoon session. This began with a great talk from **Marius Schmidt**, U Wisconsin – Milwaukee, about the use of time-resolved serial femtosecond crystallography to study photoactive yellow protein (PYP), a prototypical light sensor in bacteria (see illustration on the next page facing). Although PYP has been extensively studied over

the years by ultrafast spectroscopy and Laue crystallography, direct visualization of the very early steps of its photocycle have been hampered by the lack of high-brilliance, sub-picosecond X-ray pulses. The advent of FELs has finally allowed structural biologists to begin to peek at these very fast structural changes. Marius presented his recent work examining the excited-state dynamics from 100 femtoseconds to 3 picoseconds. This has enabled him to structurally characterize the transition through the conical intersection from excited to ground state.

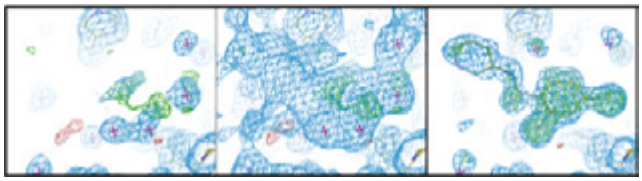


We stuck with FELs for the next talk by **Lin Chen**, Argonne National Laboratory, but this time looked at the use of complementary X-ray spectroscopic methods to characterize structural changes on ultrafast time-scales. Lin presented her work on the relaxation processes in excited transition-metal complexes, which can initiate a variety of photochemical processes on picosecond and subpicosecond time-scales. As in the previous talk, the ability of FELs to access the subpicosecond regime has had a massive impact on what we can learn about electronic and nuclear dynamics in these systems.

The next talk, by **Charles Carter**, U North Carolina at Chapel Hill, was our second selection from the submitted abstracts. Charlie presented a fascinating set of experiments aimed at elucidating the role of different protein domains in facilitating catalysis (see image below). By systematically removing the N- and C- terminal domains that bracket the core catalytic domain of Tryptophanyl-tRNA synthetase and carrying out detailed kinetic analyses, he was able to elucidate the contribution of each domain to the catalytic rate enhancement and show that the dynamics of these two flanking domains are coupled to the catalytic step.

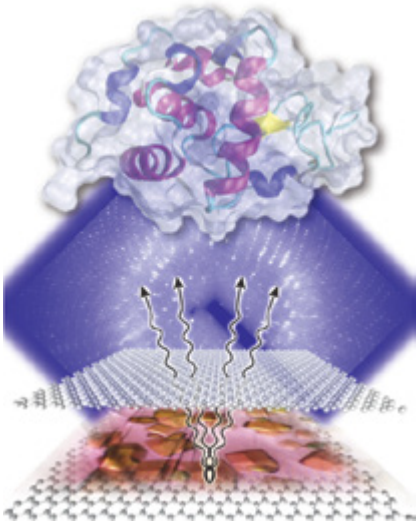


After coffee the final portion of the symposium began with a talk from **Nick Pearce**, U Oxford, U.K. Nick presented his work on the interpretation of the very weak electron-density signals in macromolecular crystallography associated with either low-occupancy ligands or disordered loops/side-chains. Nick's work has taken advantage of the rapid development of both beamline automation and detector speeds over the last 10 years, which mean we now routinely collect hundreds of datasets for a macromolecular target. By combining all these data an extremely well-defined "ground-state" electron-density map can be obtained. Datasets that differ from this "ground-state," for example with a ligand bound or a displaced loop, can be readily identified. In addition the ensemble "ground-state" provides very clear electron density for the crystallographically-ordered solvent molecules that often occupy a binding site in the absence of ligand. Nick presented a new electron-density analysis tool, PanDDA, that corrects for this "back-ground" noise in ligand complex structures, or structures where a protein loop has rearranged and reveals clear electron density for modeling (see image below).



Our penultimate talk, by **Wilfred Fullagar**, Australian National U, described recent advances in ultrafast X-ray experiments that are being performed in conventional laboratories as opposed to large synchrotron or XFEL facilities. By combining sub-picosecond hard X-ray pulses generated using femtosecond laser systems with cryogenic microcalorimeter arrays, Wilfred showed several examples of measurements that highlighted a few of the specific advantages of this lab-based technique, including the ability to perform experiments with polychromic X-ray pulses. Ultimately it is hoped that this table-top approach will be able to complete with more expensive synchrotron techniques.

We closed the symposium with a talk from **Sarah Perry**, U Massachusetts Amherst, on the use of microfluidic devices for sample delivery in time-resolved serial crystallographic experiments (see image below). Whilst FELs have brought



Turn to p. 24

us unprecedented time-resolution, they have also brought new challenges in sample consumption and delivery. Sarah presented work that addresses both of these challenges. Her chips are designed to allow both the controlled, reproducible growth of the hundreds or thousands of crystals needed for a serial crystallographic experiment, as well as to be mounted directly in the FEL beam thus removing the need for crystal "harvesting" before the diffraction experiment. Sarah presented advances in the chip design that enable her to provide ultra-low X-ray absorption and scattering by the chip itself, important to reduce background in the diffraction experiment.

In summary, the symposium provided a broad tour of the topic of structural dynamics, ranging from trapped states to real-time femtosecond experiments. It also highlighted the importance of new sources, sample handling tools, and software for the analysis of the often small structural changes associated with function, especially at fast time-scales.

Arwen Pearson
Jason Benedict

01.02: Using Standard Tools & Methods in Non-standard Ways

This half-day session, co-chaired by Louise Dawe, Wilfrid Laurier U)and Andrey Yakovenko, Argonne National Laboratory, brought together scientists who provided an opportunity for the audience to learn about extending the functionality of their home X-ray scattering devices and techniques in innovative ways. Invited speakers, **Bob He**, Bruker AXS, and **Jim Britten**, McMaster U, Canada, gave complementary lectures that both educated the audience on basic diffraction theory, and then the practical ways that home devices, like a single crystal diffractometer, can have increased functionality for those with different research objectives. Building on this theme, speakers **Milan Gembicky**, U California San Diego, and **Stacey Smith**, Brigham Young U, both demonstrated how in-house engineering can extend the possible applications of diffractometers and increase interdisciplinary research. **Paul Sanschagrin**, Cambridge Crystallographic Data Centre, also contributed a perspective on how to customize and optimize search functionality for the Cambridge Structural Database. Finally, **Marc Giulianotti**, CASIS, provided the audience with information on how to access the International Space Station – United States National Laboratory, for a truly unique research experience.

Louise Dawe
Andrey Yakovenko

01.03: Diversity and Inclusion Evening Session

L-R: Benny Chan, Bradley Hintze, Ana Gonzalez, Tim Herman, Oluwatoyin Asojo. Photo courtesy of Oluwatoyin Asojo.

This session included four talks on successful strategies for approaching diversity issues (e.g. inclusion, retention, and stereotype threat), through training, mentoring or research, and for engaging diverse populations through outreach using crystallography. The session was co-chaired by Ana Gonzalez, SSRL, and Oluwatoyin Asojo, Baylor College of Medicine.

The first talk was by **Tim Herman**, Milwaukee School of Engineering Center of Biomolecular Modeling, who introduced his 15-year efforts to introduce protein structure and function to high-school students. Tim and his colleagues use hands-on, physical models of proteins to educate high-school students and to communicate biological principles. He spoke about two programs that are used to engage students and educators. In the Science Olympiad Protein Modeling Event high-school student teams model protein structures using foam-covered wires called mini-toobers. SMART Teams (Students Modeling A Research Topic) consisting of students and teachers explore structure-function relationships guided by a scientist expert and using the PDB and 3-D printing. These programs have reached over 3000 students. During his interactive talk, Tim modeled building of a zinc finger motif and other protein structures using mini-toobers and gave the audience insights into the lessons that the students could gain from such interactive programs. Teacher training is an integral part of the program. Contributions from industry and local volunteers are very helpful to support this program. The Program is supported by the NIH SEPA (Science Education Partnership Award) program and the HHMI.

The second speaker, **Benny Chan**, The College of New Jersey, spoke about outreach activities to improve the retention and graduation rate of minorities in STEM fields. Benny educated the audience about the leaky pipeline in STEM for underrepresented groups, members of lower socioeconomic status, and a hidden minority group LGBTQ+. He emphasized topics such as implicit bias, identity, intersectionality, and the need to create safe spaces to close the leaky STEM pipeline. He described the experience of LGTBQ+ students, who are more likely to experience harassment and fear of physical aggression. The problem persists for faculty, who consider leaving their field at higher rates than non- LGTBQ+ faculty. Benny described how institutions and professional organizations (such as the American Chemical Society) are taking steps to increase awareness among the staff and acknowledged that the ACA community can implement similar efforts to make a difference.

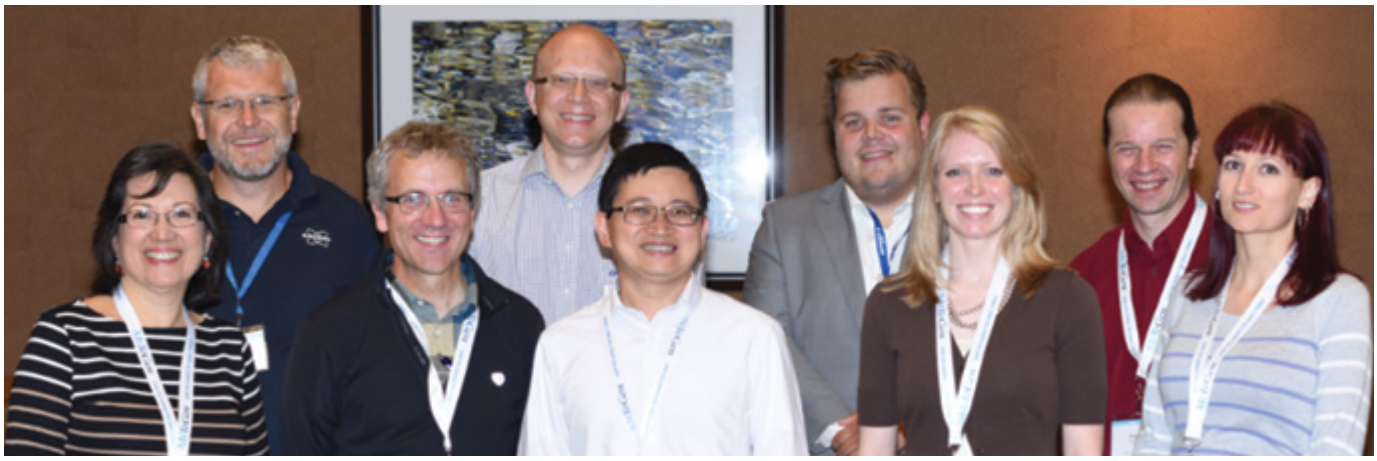
Bradley Hintze, Duke U, was the third speaker. He gave a personal account of how he decided to pursue a career in macromolecular crystallography despite having a disability that prevents him from writing or carrying out tasks that require

fine coordination. While work in a wet lab was not a viable option, the computing component of modern biochemistry offered him a way to contribute to the field. He was encouraged to do a postgraduate degree in the Richardson group, whose main focus is modeling of protein structures, and where he is pursuing a fruitful career. As a final reflection, he mentioned that, in his experience, lack of confidence can be more of a setback than a physical disability.

Oluwatoyin Asojo gave the final talk about her experiences mentoring diverse high school and undergraduate students using crystallography research since 2001. As a black immigrant female professional, minority and female students seeking mentoring have gravitated towards Oluwatoyin at all points in her career. She stressed how rewarding mentoring can be and mentioned that motivated and enthusiastic students can do very good work and if given the opportunity make important contributions to research. Often these students did not even know about STEM careers, and it is exciting to introduce them to these careers. Obstacles towards outreach efforts include lack of funding. Oluwatoyin identified possible sources of funding (NIH supplements and R25, ACS Project SEED, etc.). She finished by encouraging everyone to make conscious efforts to include diverse groups in their research and also partner with existing programs to increase the participation of socioeconomically underserved and underrepresented minorities in STEM.

Oluwatoyin Asojo
Ana Gonzalez

01.05.01: General Interest I



L-R: Graciela Díaz de Delgado, Michael Ruf (at rear), Douglas Juers, Marcus Müller (at rear), Shao-Liang Zheng, Emil Espes (at rear), Stacey Smith, Simon Coles (at rear), Erin Davis. Photo by Peter Müller.

The session began with a focus on education. **Douglas Juers**, Whitman College, opened with his experiences successfully teaching undergraduates about protein structure by guiding them through a SAD experiment in his biophysics laboratory course. **Shao-Liang Zheng**, Harvard U, described his use of case studies as a means of teaching his undergraduate and graduate students not only how to do refinements but also how to evaluate structural models generated by themselves and others. **Simon Coles**, U Southampton, outlined the new Chemistry M.S. program he has designed in which he uses role play and targeted group projects utilizing the XRD, NMR, and MS facilities to teach not only analytical laboratory skills but also business and 'soft' skills such as teamwork, ethics and writing. Role-play projects include writing a popular science article, writing a standard operating procedure, auditing a lab to determine its sustainability, and acting as a facility manager to organize data and finance the facility. Scenarios for laboratory group projects include evaluating a pharmaceutical mixture for patent infringement and analyzing material from a 'drug bust' with the final assessment being a mock hearing before a court or board of directors, as appropriate. All three speakers employ active learning techniques and echoed Simon's theme that learning by doing makes for more effective learning and more employable students.

After the break, the session turned to talks involving the tools used in structural science. **Erin Davis**, Cambridge Crystallographic Data Centre, spoke about tailoring the CSD search tools through the API (Application Programming Interface); with basic Python programming skills, anyone can now build the tools they need to search for the answers they want from the CSD. **Carolyn Brock**, U Kentucky, illustrated how data mining can reveal interesting information; her careful analyses of high Z' materials in the CSD revealed that layers are common in these structures, and the approximate symmetry of the layers can help us make sense of the structure. It may even lead to new insights about nucleation and growth of crystals. **Emil Espes**, Excillum AB, updated us on liquid metal jet X-ray source technology and uses. Stability tests show that their advanced electron beam technology produces a precise and stable Gaussian-shaped spot on the In-Ga metal jet. Some of the metal is inevitably splattered as it is bombarded by electrons from the SEM-like LaB_6 cathode, but the cone-shaped chamber funnels these droplets back into the stream, and the use of heated windows prevents a buildup of the alloy from blocking the exiting X-ray beam. **Marcus Müller**, DECTRIS, described the new PILATUS line of detectors in which each sensor pixel can convert up to 1 million X-ray photons per second directly to current

Turn to p. 26

without the use of an intermediate scintillator. This hybrid photon counting technology minimizes point spread, eliminates dark current and readout noise, and expands the dynamic range of the detector. **Michael Ruf**, Bruker, then described the new CPAD line of detectors that uses an adaptive oversampling algorithm to increase dynamic range and prevent streaking of pixels. The algorithm records data in two modes; the destructive readout mode prevents pixel overload and gives the detector a high dynamic range by reading the signal quickly. The non-destructive readout mode allows the signal to build before the readout, which limits the dynamic range but greatly improves the signal-to-noise ratio.

Stacey Smith

01.05.02: General Interest II

L-R: Thayumanasamy Somasundaram, Zheng-Qing (Albert) Fu, Jürgen Graf (at rear), Graciela Díaz De Delgado, William Duax (at rear), Bi-Cheng Wang, Thomas Peat (at rear), Herbert Bernstein, Arshad Mehmood (at rear), Anna Lübben. Photo by student volunteer.

The **General Interest II** session emphasized macromolecular crystallography and featured a lively mix of talks on methods development as well as on experimental results. Subjects discussed ranged from recent developments in sources and detectors to new software tools. In addition, several speakers highlighted user programs at synchrotron facilities.

02.03: Would You Publish This?

Co-chaired by **Louise Dawe**, Wilfrid Laurier U, Canada, and **Danielle Gray**, U Illinois – Urbana Champaign, the extremely popular session, **Would You Publish This?** continued this year with generous support from Crystallographic Resources, Inc. This fun and collegial evening emphasized open discussions on problem structures presented by the evening's speakers. **Aaron Finke**, Paul Scherrer Institute, Switzerland, **Danielle Gray**, and **Louise Dawe** each presented single-crystal structures that made for excellent pictures, but with data collection or preservation issues that tore the audience on their publication merits. **Christine Beavers**, Advanced Light Source, spoke on issues related to powder data, and the importance of supporting characterizations when working on problem structures. Finally, **Paul Sanschagrin**, Cambridge Crystallographic Data Centre, offered a new tool to the community for data validation.

Louise Dawe
Danielle Gray

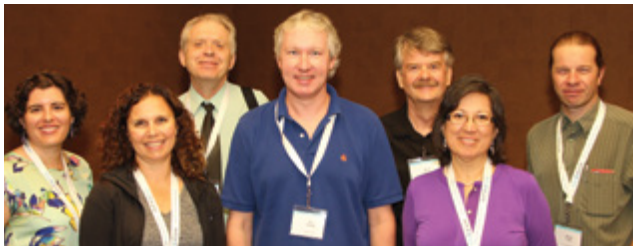
01.08: Career Development

This year the Young Scientist Scientific Interest Group (YSSIG) held a **Career Development** session in place of the traditional Career Odyssey session to examine an active approach to engage young scientists with professional advisement. The session began with a dynamic talk by **Brad Conrad**, Director of the Society of Physics Students (American Institute of Physics) and Sigma Pi Sigma on how to apply one's skills learned in school to one's future career (for industry, governmental, academic, or other paths). Brad's talk included résumé organization, the importance of an elevator speech (including the helpful analogy that 500 business cards means 500 handshakes), the necessity of networking, and the sobering fact that 50+ résumés – custom tailored to each job – might only result in 1-2 interviews and (hopefully) a job offer! The talk was very well received, and further discussions with Brad in the hallway were greatly appreciated by the attendees. Following the presentation, breakout sessions were held for one-on-one advice with attendees and volunteers from the Industrial Scientific Interest Group (ISIG) and senior scientists. The one-on-one sessions provided résumé critiques and general advice of experienced professionals to early career scientists. Such advisement is an indispensable component of the ACA and the reason many return to the ACA conference: the hospitable environment generated by all attendees to assist the community in their careers and science. We are extremely grateful to the volunteers who took time out from their busy conference schedules to assist with the Career Development session: **Richard Staples**, **Andrew Brunskill**, **Louise Dawe**, **Christine Beavers**, **Bruce Noll**, **Michael Ruf**, and **Pete Wood**. We particularly thank **Richard Staples** and **Eugene Cheung** for assisting with volunteer coordination of ISIG and other ACA members.

Brad Conrad from SPS addressing attendees at the session. Photo courtesy of Martin Donakowski and George Lountos.

George Lountos
Martin Donakowski

01.09: Engaging Undergraduates with Crystallographic Research



L-R: Lauren DePue, Rachel Powers, Alexander Nazarenko (at rear), Joe Tanski, Karl Hagen (at rear), Graciela Díaz de Delgado, Simon Coles. Photo by Richard Bromund.

In a half-day session, speakers focused on how to successfully manage a research program incorporating chemical crystallography at a primarily undergraduate institution. The talks featured a mixture of powder diffraction, small-molecule and protein crystallography. **Rachel Powers**, Grand Valley State U, discussed in detail her experience of addressing the challenges of setting up a macromolecular crystallography research program at a predominantly undergraduate institution. **Graciela Díaz de Delgado**, Universidad de Los Andes, Venezuela, offered insight into single-crystal and powder diffraction studies carried out by students at her university, especially studies on materials that can be commonly found at the market. **Alexander Nazarenko**, Buffalo State U, described how to use crystals of sweeteners from everyday products to engage non-chemistry major students with short demonstrations aimed at exposing them to the molecular structure information that may be obtained through X-ray crystallography. **Richard Staples**, Michigan State U, described how he collaborates with faculty at primarily undergraduate institutions so that they can obtain crystal structures without having their own diffractometer. **Joe Tanski**, Vassar College, spoke about strategies for obtaining diffraction instrumentation via grant writing and about success in research involving X-ray crystallography with undergraduates. **Simon Coles**, U Southampton, U. K., described an undergraduate practical involving polymorphism. **Lauren DePue**, U Texas, Austin, discussed engagement of first- and second-year students in hands-on, discovery-based research with the crystallography of lanthanide coordination compounds. **Karl Hagen**, Emory U, wrapped up the session by describing laboratory modules designed to expose students to the synthesis of inorganic materials and powder diffraction.

Joe Tanski
Rachel Powers

L-R: Christine Beavers, Brandon Mercado, Marilyn Olmstead, Marian Szebenyi (facing away from the camera), and Ed Stevens taking in a poster session. Photo by Richard Bromund.

01.10: High Impact Crystallographic Education

L-R: Bruce Foxman, Peter Hoare, Larry Falvello, Paul Cook (at rear), Amy Sarjeant, Dean Johnston (at rear), Louise Dawe, Kraig Wheeler (at rear), Gervais Chapuis. Photo by Richard Bromund.

The speakers in our half-day session offered an extremely broad range of perspectives and techniques for promoting crystallographic education. The talks featured a mixture of topics including novel classroom modules, virtual resources, and innovative active-learning exercises. **Gervais Chapuis**, École Polytechnique Fédérale de Lausanne, Switzerland, described an assortment of topics related to teaching crystallography with innovative tools that featured current trends in crystallographic education, with special emphasis on the effective use of crystallographic applets and online MOOCs. **Louise Dawe**, Wilfrid Laurier U, Canada, recounted her experiences with developing residence-learning communities and the critical use of crystallography in the active learning process, as well as offering several examples of using crystallographic data to support introductory chemistry concepts. **Paul Cook**, Grand Valley State U, described his successes with engaging undergraduate biochemistry students via crystallographic data and interactive graphics programs. **Larry Falvello**'s. U Zaragoza, Spain, descriptive approach to crystallographic lattice types offered insight into the instruction of this important fundamental crystallographic area, and provided several relevant examples that outlined the training process. **Dean Johnston**, Otterbein U, gave an account of the recent developments in his web-based resource, ***Symmetry@Otterbein***, and added several examples of modules that guide users through symmetry operations and other crystal structure features. **Bruce Foxman**, Brandeis U, discussed online resources that provide a unique look at the historical aspects of crystallography and lead readily to guided inquiry into crystallographic symmetry, space groups, and crystal twinning. **Peter Hoare**, Newcastle U, U.K., showed the utility of the WebCSD platform for engaging pre-baccalaureate students and gave several practical examples, including his online 'Bite-sized Learning and Teaching Resources'. To complete the session, **Amy Sarjeant**, Cambridge Crystallographic Data Centre, gave an insightful perspective on the state of crystallographic education in the U.S. and continued the theme of data mining of crystal structures by showing the importance of well-placed CSD-derived instructional modules for education in science.

Bruce Foxman
Kraig Wheeler

01.11.01 & 01.11.02: Standard Practices in Crystallography II: Structure Refinement and Validation

Group Photo I of the Standard Practices in Crystallography session; L-R: Peter Müller, Tom Terwilliger, Diana Tomchick, David Rae, Claudia Wandtke, Paul Adams. Photo by Peter Müller.

This very well attended full-day session was organized by Peter Müller, MIT, and was the second of a series of educational sessions sponsored by the Standing Committees "Continuing Education," and "Data Standards and Computing." The session was co-sponsored by the Scientific Interest Groups, "General Interest," "Service Crystallography," "Small Molecules," and "Bio Mac."

The opening presentation by **William Ratcliff**, NIST, introduced

a *Bayesian Library for the Analysis of Neutron Diffraction Data* that proposes an algorithm to sample parameter space instead of traditional least squares fitting. **David Rae**, Australian National U, pointed out that *When Alternative Layer Stackings Cause Commensurate Structures to Co-Exist the Interpretation of the Diffraction Data May Not Be Unique*, and **Claudia Wandtke**, Georg August Universität, Göttingen, Germany, discussed an aspherical modeling as a method for *Identification of Unknown Metal Atoms in Coordination Compounds*.

Following the coffee break, the focus of the session turned to macromolecular structures. **Tom Terwilliger**, Los Alamos National Laboratory and current ACA President, spoke about *Model-Building Using Cryo-EM and Crystallographic Maps* and how those two methods can and should be used in combination. **Diana Tomchick**, U Texas Southwestern Medical Center, gave a report about *Strategies to Address Challenging Macromolecular Structural Projects in the Context of an Academic Service Laboratory*, and **Paul Adams**, Lawrence Berkeley Laboratory, gave an update of the current status of *Validation of Macromolecular Structures*.

Group Photo II of the Standard Practices in Crystallography session; L-R: George Sheldrick, Carl Schwalbe, Jens Lübben, Ton Spek, Daniel Kratzert, Peter Müller, Tom Emge. Photo by Peter Müller.

The afternoon part of the session dealt entirely with small-molecule structures: **Peter Müller**, MIT, talked about *Use (and Abuse) of Restraints in Structure Refinement*, and **Jens Lübben**, Heinrich-Heine-Universität, Düsseldorf, Germany, introduced *An Enhanced Hirshfeld Test – Validating Atomic Vibrations in Crystal Structures*. Under the title *DSR – Modelling of Disorder with new GUIs for ShelXle and Olex2*, **Daniel Kratzert**, Albert-Ludwigs-Universität, Freiburg, Germany, introduced his software plugin and fragment database, and **Tom Emge**, Rutgers U, gave an example of *Patterns of Residual Electron Density that Persist in Well-Determined Crystal Structures of Iridium Compounds*.

The following two presentations were more general in nature and sparked interesting discussions about structure validation: **Carl Schwalbe**, Cambridge Crystallographic Data Centre, U.K., reported on a number of *OH···HO Clashes in Recently Published Structures* and **Ton Spek**, Utrecht U, The Netherlands, summarized *What is Needed for Proper Structure Validation and How to Interpret and Act upon Validation ALERTS*. In discussing some intricacies of *Crystallographic Algorithms for Multiple-CPU Computers*, the final presentation by **George Sheldrick**, Georg August Universität, Göttingen, Germany, addressed the recent trend to parallel processing in crystallographic computing and revealed a number of interesting tricks to enhance software efficiency.

The session was videotaped, and when all permissions have been obtained the video will be made available on the ACA home page together with the slides of all presentations. As mentioned above, this was the second in a hopefully long series of **Standard Practices in Crystallography** sessions. Next year, at the annual ACA meeting in New Orleans, the third **Standard Practices** session will be about *Communicating Crystallographic Results*.

Finally, it should be mentioned that two of this session's speakers were recipients of **Margaret C. Etter Student Lecturer Awards**: Claudia Wandtke received the Etter award from the Service Crystallography Scientific Interest Group and Jens Lübben was the Small Molecule Etter awardee.

Peter Müller

Editor's Note: See below for the complete list of Etter Awards for 2016.

2016 Margaret C. Etter Student Lecturer Awards

Biomac	**Stefan Imseng, U Basel**	**Materials Science**	**Daniel Mast, U Nevada Las Vegas**
Canadian	**Marcia Chaudet, U Waterloo**	**Neutron Scattering**	**Amber Larson, U Maryland**
Fiber Diffraction	**Brendan Sullivan, Purdue U**	**Powder Diffraction**	**Dan Taylor, U Maryland**
General Interest	**Jens Lübben, Heinrich Heine U**	**Service Crystallography**	**Claudia Wandtke, U Göttingen**
Industrial	**Mikaela Pyrch, George Washington U**	**Small Molecule**	**Victoria Hall, Georgetown U**
Light Sources	**Charles Bury, U Oxford**	**Young Scientist**	**Jose Olmos, Rice U**

01.12: Things We No Longer Need to Know

L-R: Robert Von Dreele, Amy Sarjeant (at rear), Paul Boyle, William Clegg, John Rose (at rear), Larry Falvello, Mathias Meyer (at rear), Carla Slebodnick, Charlotte Stern, Xiaoping Wang. Photo by Richard Bromund.

Things We No Longer Need to Know was originally proposed as a session topic with an ironic twist, to focus on the rapid pace at which our functions as diffractionists and structural chemists and biologists are being transferred to hardware and software. So do we really still need to know how to examine systematic absences to determine a space group? Should our students really still study the point group table? Or perhaps we ought to seek out new, higher-level skills now that our advanced machinery can handle matters that in the past required long training and experience. Even an unswerving crystallographic Luddite would agree that the write-permit ring (one of which appeared at the session) is an object of the past.

In the actual event, the session attracted a mix of talks that reflected the whole spectrum of perspectives that its title suggests – instructive procedures from the past, tools for the future and present practice that can be instructed by past practices.

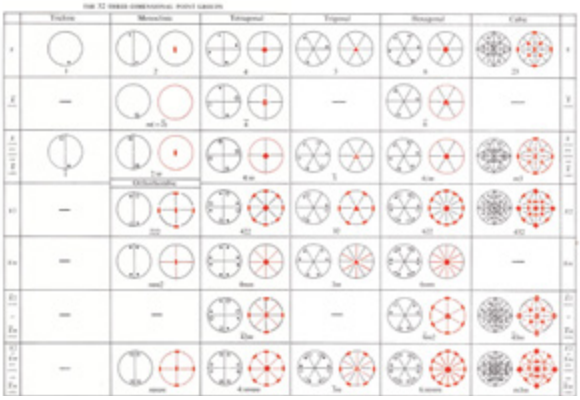
A past item that is instructive today is data collection using a CAD4 diffractometer, described in detail by **Paul Boyle**, U Western Ontario, Canada. One of the functions of this diffractometer, which would still be useful today if it were available, is the measurement of as full as possible a psi-scan on a general reflection. The main function of this procedure, for absorption correction, is now done differently; but the use of psi-scans to identify multiple reflection would still be useful.

The future of data collection was also reflected at the session, in talks by **Mathias Meyer**, Rigaku Oxford Diffraction, on *The Art of Good Diffraction Experiments* – which included a 37-second start-to-finish structure analysis – and by **Xiaoping Wang**, Oak Ridge National Laboratory, on 3D single crystal neutron diffraction at sub-atomic resolution, and how it is done at SNS.

John Rose, U Georgia, shared a view of the future of structural biologists, *Button Pushers or Crystallographers*? with a detailed exploration of the various parts of a structural biology study and what the practitioner will have to know. John's talk left the clear impression that the day of the button-pusher is still pretty far into the future.

The question of what we no longer need to know is a hot-button issue in crystallographic education. Knowledge of crystallographic symmetry would seem to be of lasting importance, yet the increased capability of programs to identify and manipulate symmetry has produced the impression that detailed knowledge of the subject is of less immediate importance than once may have been the case. **Bill Clegg**, Newcastle U, U.K., (*Some Reflections on Symmetry*) used concrete examples to demonstrate the need for expertise, and the relative facility with which errors can arise in structure analyses in the absence of careful examination by an expert operator.

Carla Slebodnick, Virginia Tech, gave a presentation on the crystallographic point groups and on their arrangement in the well-known point group table. This table (see graphic shown at right), which Carla called the "periodic table of crystallography," is a concise grouping of the crystallographic point symmetries into sets with common properties. The columns represent principal symmetries and thus crystal systems, and the seven rows group symmetries with common properties – including two rows of pure rotational groups, two rows with only polar groups (with one exception), and two rows of centric point groups. **Larry Falvello**, U Zaragoza, Spain, rounded out the topic of crystallographic education with a presentation on the use of modern software features to help students visualize the concept of the reciprocal lattice.



The large audience got a glimpse of a few items that, in the future, it may not be necessary to know as a result of new developments in the software offered by the Cambridge Crystallographic Data Centre. **Amy Sarjeant** of the Centre described several new tools, including an easily managed system for transformations, which as of this writing will be included in a forthcoming release of the program Mercury.

In a session replete with interesting talks, a distinct high point was a scholarly presentation by **Bob Von Dreele**, Argonne National Laboratory, titled simply *FORTRAN?* Bob placed Fortran in its historical perspective with a description of the principal advances that have taken place in its capabilities since its introduction in 1954. Arriving at the present, he placed Python alongside its venerable elder, with an effective comparison of capabilities and efficiency – the latter in terms of programming effort and also in terms of

the computations themselves. While Bob left it to the listener to draw conclusions about the utility of each of these two languages, he suggested that both Fortran and Python have places in the current crystallographic programming landscape.

Things We No Longer Need to Know enjoyed a capacity audience from start to finish. All of the talks were well received, and the breadth of topics covered made for a well-rounded program.

This session received generous support from Crystallographic Resources, Inc., from Rigaku Oxford Diffraction, and from the ACA.

Carla Slebodnick
Charlotte Stern
Larry Falvello

02.02: Structure-Property Relationships

L-R: Karah Knope, Christine Beavers (at rear), Paul Forster, Lauren Hatcher, Mikaela Pyrch, Carl Schwalbe (at rear), László Fábián, Victoria Soghomonian, Daniel Fredrickson, Peter Wood. Photo by student volunteer.

This session highlighted some of the most exciting science going on around the world in the area of structure-property relationships with presentations focused on a range of properties including photo-reactivity, gas adsorption, conductivity, vibrational modes, solvation, solubility, melting points and luminescence.

We began the first half of this session with **Lauren Hatcher**, U Bath, U.K., giving an excellent overview of her recent research into photo-switching in nitrite linkage isomers. Using a specially designed LED ring, Lauren's group have managed to achieve photo-switchable materials with high conversion rates at near-ambient conditions. Their Pd(II)-nitrite system shows 100% conversion in pseudo-steady-state experiments at 240K, which is approaching the region of viable operating temperatures for practical applications (see also: *CrystEngComm* **2016**, *18*, 4180).

Paul Forster, U Nevada, Las Vegas, next introduced us to the world of combined simulation and experimentation to study gas adsorption in porous materials. Paul uses grand canonical Monte Carlo (GCMC) methods to study framework-guest systems and finds these approaches particularly useful to help predict and explain adsorption behavior, but warns that care should be taken to use appropriate experimental structures at the basis of simulations. Even apparently rigid frameworks can have enough flexibility to affect the simulated adsorption properties for a given guest (see also: *Phys. Chem. Chem. Phys.* **2015**, *17*, 18904).

Karah Knope, Georgetown U, shared with us her group's work on bismuth frameworks designed to encompass lanthanides, and provoke favorable interactions between the ligands and the lanthanides to produce light emission. She also encouraged us to champion the U.S. Crystal Growing Competition contest in our communities, and encourage participation in our local schools (see also ***www.uscrystalgrowingcompetition.org***).

In one of the most characterful talks of the whole meeting, **Carl Schwalbe**, Cambridge Crystallographic Data Centre, U.K., opened up by comparing his presentation to a selection of Tchaikovsky's movements in the theme of doleful despair! He then went on to talk about the relationships (or surprising lack of) between the crystal packing arrangements and the physico-chemical properties such as melting point and solubility in a series of gemfibrozil salts. To fully ensure that viewers went away with a strong memory, Carl also described these salts by comparing the common salt arrangement in the series to "a mother holding her baby in her arms"!

The second half of the session started with **László Fábián**, U East Anglia, U.K., who premised his talk on the question, "Can we know which compounds are at risk for solvate formation?" To the general crystallographer, solvates are commonly merely a nuisance, but in the pharma community, a solvate can make a safe compound toxic and unstable. To tackle this issue, László utilized the Cambridge Structural Database and extracted a data set of over 19,000 molecules with reported solvent of crystallization that either did or did not form a solvate. Large molecules and molecules with a large degree of branching were strongly correlated with solvate formation; future work is aimed at intramolecular interactions that may also be involved (see also: *Cryst. Growth Des.* **2016**, *16*, 70).

Mikaela Pyrch, George Washington U, was awarded the Industrial SIG Etter Student Lecturer Award for her talk on uranyl hydrolysis products, which form dramatically different structures depending on the reaction conditions. Mikaela noted that as the reaction pH increased, so did the nuclearity of the produced compounds.

Daniel Fredrickson, U Wisconsin-Madison, described the idea of chemical pressure as a simulation tool. Chemical pressure can be thought of as the push/pull relationship between atoms, i.e., atoms that are strongly attractive and are trying to pull towards each other can be considered to have negative chemical pressure, whereas repulsive atoms would have positive chemical pressure. This concept, combined with information about electron density and ionicity, was shown to be helpful in understanding band structures in intermetallic compounds (see also: *Chem. Mater.* **2016**, *28*, 3171).

Our last speaker of the day, **Victoria Soghomonian**, Virginia Tech, told us about a strontium manganese vanadate system with complex electrical and structural properties under pressure. Victoria was able to measure the conductivity and single-crystal structures under pressure, and noticed that conductivity step-changes didn't always equate to structural changes in this system, but that structural changes did entail conductivity changes. Her talk nicely captured the essence of this session – that structural knowledge can be immensely helpful in understanding physical properties.

Peter Wood
Christine Beavers

02.04.01 & 02.04.02: Advances in Supramolecular Chemistry

L-R: Heba Abourahma, Jennifer Swift, Raul Castaneda, Marijana Đaković, Christer Aakeroy, Susan Reutzel-Edens, Kraig Wheeler, Gracia El-Ayle, Graeme Day and Balasubramanian Venkatakrishnan. Photo by Mark Whitener.

The **Advances in Supramolecular Chemistry** session revolved around three general themes: small molecule, organic cocrystals; metal-organic container molecules and extended structures; and computational methods in pharmaceutical solids.

The morning session started with a talk by **Christer Aakeröy**, Kansas State U, who showcased practical applications of supramolecular chemistry. Christer demonstrated the use of the principles of supramolecular chemistry in the solid state to prepare cocrystals. He explained that by selecting the proper cocrystal former, one is able to modulate the properties of the resulting cocrystal and consequently its application. Christer presented examples that employed the hydrogen and the halogen bond in their design for application in the pharmaceutical, agrochemical and energetics industries.

Session chair Heba Abourahma, at left, and Victoria Hall, the Small Molecule SIG choice to receive the Etter Student Lecturer Award. Photo by Mark Whitener.

Victoria Hall, Georgetown U, recipient of a 2016 **Etter Student Lecturer Award**, described a tactic for interfering with uric acid crystallization. Uric acid crystallization in humans is associated with the formation of kidney stones and gout deposits. Victoria presented an approach to making stable cocrystals with uric acid using bi- and tridentate hydrogen bonding cocrystal formers. Solubility studies of the cocrystals indicate that they are up to 60% more soluble in model urine than pure uric acid.

The second half of the morning session shifted to presentations in the general area of metal-organic structures. **Zhenqiang (Rick) Wang**, U South Dakota, illustrated how supramolecular interactions are utilized to construct a new class of metal-organic supercontainers (MOSCs) that mimic enzymes in their reactivity. These containers are based on sulfonylcalix[4]arene-type building blocks along with divalent metal ions and carboxylate linkers and feature multiple binding cavities and tunable chemical functionalities. Rick demonstrated how the structural features of MOSCs allow them to serve as protein mimics with tunable catalytic efficacy. **Korey Carter**, George Washington U, presented recent results of supramolecular hybrid materials based on uranyl oxo atoms. Using organic ligands capable of hydrogen and halogen bonding, Korey presented a series of uranyl molecular complexes, coordination polymers, and heterometallic hybrid materials sustained by halogen-oxo and cation-cation interactions. **Balasubramanian Venkatakrishnan**, Indiana U, described a new strategy that uses macromolecule methods for the structure determination of small molecules and their assemblies. Using the pentagonal macrocycle cyanostar as a model compound, he showed that the of use of dynamics flexible fitting algorithm for X-ray crystallography (xMDFF), along with tools from the macromolecular structure determination suite PHENIX, shows excellent agreement with the small-molecule methods. **Gracia El-Ayle**, Georgetown U, concluded the morning session talking about confining gases inside lipophilic cage molecules based on cryptophane. Gracia presented recent results on the synthesis and single-crystal X-ray data of a derivative of a cryptophane host, trisbromocryptophane-111. She also presented the crystal structures of a series of complexes of the cryptophane derivative with N_2, Ar, Kr, and Xe guests that were studied to better understand gas confinement in the host molecule.

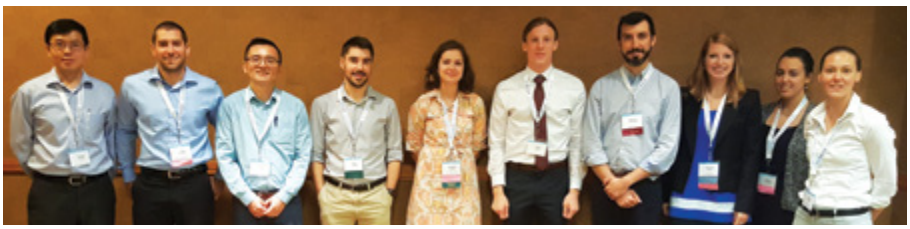
Jennifer Swift, Georgetown U, reported on the synthesis and characterization of a new anhydrous polymorph of thymine that matches a structure previously predicted by energy landscape calculations. Jennifer further detailed the kinetic, mechanistic and structural transformation, in the solid state, of thymine and its hydrated and dehydrated forms. **Kraig Wheeler**, Eastern Illinois U, spoke about quasiracemic materials. Kraig presented new quasiracemates of succinic acid derivatives (chloro- and bromo-) crystallized with tailor-made additives that contain complementary features to the succinic acid reagents, and recent studies that probe the structural boundaries of molecular recognition via quasiracemates. Continuing with the theme of cocrystals, **Marijana Đaković**, Zagreb U, Croatia, talked about exploring reliable methods for transferring specific supramolecular motifs from organic to metal-organic systems. Using acac-based metal(II) complexes with pyridine-type ligands decorated with the oxime moiety as model compounds, Marijana demonstrated that obtaining the targeted supramolecular assembly is achievable by tuning the strength of competing hydrogen-bond donors and acceptors. She further supported the findings with thorough theoretical analysis of molecular electrostatic potential surfaces

and interaction energies. **Raul Castaneda**, New Mexico Highlands U, discussed the different packing patterns in mixed donor-acceptor cocrystals of trimeric perfluoro-o-phenylene mercury (TPPM) and benzo[1,2-b:6,5-b']dithiophene-4,5-dione (BDDO). Through a series of seven cocrystals, Raul showed that depending on the nature of the BDDO substituent, different types of contacts (e.g., Hal···Hal, Hg···O, Hal···O, π···π) are observed, which ultimately lead to different packing patterns in the cocrystals.

The late afternoon portion of the session emphasized computational and design methods of pharmaceutical solids. **Susan Reutzel-Edens**, Eli Lilly & Company, showcased two molecules that demonstrate the use of computational crystal structure prediction as a first step towards the digital design of a drug and as a complement to experimental solid form screening. **Graeme Day**, U Southampton, U.K., presented recent results of computational studies aimed at informing the development and application of crystal structure prediction methods. The results from a large-scale study of polymorph lattice energy and dynamics indicate that there is very small difference in the energy between polymorphic pairs. Graeme also presented recent applications of crystal structure prediction in the design of porous organic crystals.

Heba Abourahma
Kraig Wheeler

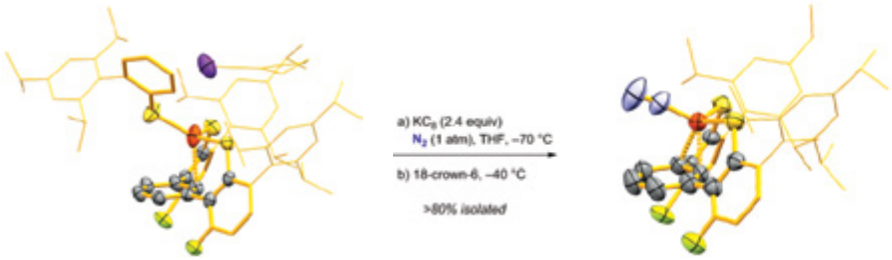
02.05: Cool Structures



L-R: Xiaoping Wang, Gian Surbella, Chunhua Hu, Pete Wood, Anastasiya Vinokur, Keith Taddei, Brandon Mercado, Elizabeth Koch, Marina Solomos, Karah Knope. Photo courtesy of Xiaoping Wang.

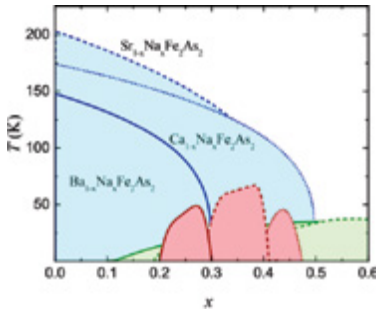
The **Cool Structures** session featured a wide selection of talks on topics ranging from phase transitions and polymorphism to magnetic ordering. As examples of the content of the lively program, summaries of two presentations are presented below.

Like many of the participants in the session, **Brandon Mercado**, Yale U, employed the session title as both a metaphorical and literal vantage from which to discuss his results. He reviewed several metaphorically "cool" small molecule mimics of the iron–molybdenum cofactor (FeMoco) found in nitrogenases (enzymes used by certain microorganisms convert atmospheric dinitrogen to ammonia, thereby providing essential nitrogen atoms for higher organisms). The central iron sites that are coordinated to sulfur and carbon atoms in FeMoco have been proposed to be the substrate binding sites. Addition of electrons to the resting state causes the FeMoco to react with N_2, but the geometry and bonding environment of N_2-bound species remain unknown. The iron-sulfur-carbon small molecule mimics of FeMoco provided evidence for a pathway where an Fe-S bond is cleaved in FeMoco, which leaves an open site to coordinate dinitrogen to iron. These molecules were unstable at ambient conditions and required that material be kept cool, in the literal sense, from the time they were synthesized through crystallization and diffraction.

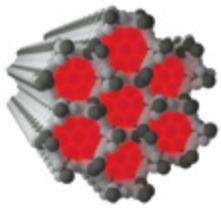


A full report of the work that Brandon presented in Denver may be found in I. Čorić, B.Q. Mercado, E. Bill, D J. Vinyard, P. L. Holland, *Nature* **2015**, *526*, 96-99.

Keith Taddei, Oak Ridge National Laboratory, established the universality of the Double-**Q** magnetic structure in the hole-doped 122 iron-pnictide superconductors. The Double-**Q** phase – a novel magnetic structure born of the superposition of two spin-density-waves – strongly indicates the importance of spin-fluctuations in the dynamics of these materials and their role in stabilizing superconductivity. Magnetic and nuclear structural ternary phase diagrams of $(Ba_{1-x}Sr_x)_{1-y}Na_yFe_2As_2$ and $(Sr_{1-x}Ca_x)_{1-y}Na_yFe_2As_2$ were reported, see image below, showing a continuous and smoothly evolving Double-**Q** phase; revealing it to be a fundamental feature of these systems.



Editor's Note: To close out the **Cool Structures** session, **Pete Wood**, Cambridge Crystallographic Data Centre (CCDC), reported the first structures showing neon captured within an organic or metal-organic framework. *In situ* high pressure gas flow experiments performed at APS using the X-ray powder diffraction technique at low temperatures managed to elucidate the structure of two different metal-organic frameworks with neon gas captured within the materials. The structure of neon encapsulated within the framework known as NiMOF-74, a porous framework built from nickel metal centers and organic linkers, is pictured below. According to Pete, "The structures reported here show the first observation of a genuine interaction between neon and a transition metal, suggesting the potential for future design of selective neon capture frameworks."



Neon observed experimentally within the pores of NiMOF-74 at 100 K and 100 bar of neon gas pressure. Figure courtesy of CCDC.

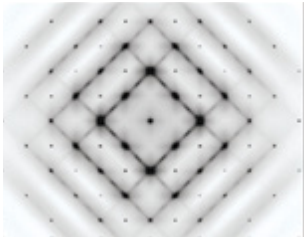
02.06: Making Sense of Diffuse Scattering

Evidence is mounting that the overall structure derived from the Bragg lattice represents the governing framework in which function-defining interatomic and intermolecular interactions take shape. The true key to functionality, however, is often determined by structure fragments of higher mobility or less perfect ordering. This deviation from 3D periodicity, whatever its origin, is manifested in the diffraction pattern as oriented diffuse scattering. This session gave us a snapshot of current capabilities in data collection and interpretation.

Yaohua Liu, Oak Ridge National Laboratory, described the CORELLI neutron spectrometer at the SNS, which is capable of collecting data from samples at 300mK to 1500K, at high pressure or in a magnetic or electric field. Data, such as diffuse scattering from correlated local disorder in crystalline materials, can be monitored remotely using the Mantid software package. **James Neilson**, Colorado State U, presented a stacking-fault analysis of the diffuse scattering from amorphous iron-oxide materials, pushing the study beyond the capabilities of standard PDF analysis. **Martin Donakowski**, U.S. Naval Research Laboratory, showed us the power of differential PDF analysis in the study of a 3D porous composite of nanoscale MnO coated carbon nanofoam paper, isolating the scattering of the oxide phases from the carbon scattering.

Matthew Krogstad, Northern Illinois U, was an ACA rookie who gave an excellent presentation on the comparison and analysis of low-temperature neutron (CORELLI) and X-ray (CHESS) elastic diffuse scattering from a single crystal of the relaxor ferroelectric PMN-xPT. The remaining speakers presented two different approaches for the determination of the real-space origins of diffuse scattering in single crystals. **Thomas Welberry**, Australian National U, presented a thorough analysis of the diffuse scattering patterns obtained from a single crystal of $HgBa_2CuO_{4+\delta}$, as published by Izquierdo *et al*. (2011), *Journal of Physics and Chemistry of Solids*, 72: 545–548. Richard gave us a detailed model that accounted for every feature in the diffuse pattern, along with a very educational, visual explanation for each step in the process. If you would like to learn more about this process, have a look at his textbook *Diffuse X-ray Scattering and Models of Disorder* (Oxford University Press, 2010).

An alternate method to determine a model for the short-range order was presented by **Arkadiy Simonov**, Oxford U, U.K., using a 3D pair-distribution function. The diffuse scattering of $Cd(CN)_2$ (see Figure opposite) was analyzed using Arkadiy's program YELL. After accounting for the main Bragg spots using the average long-range structure, a model for the static and dynamic short-range behavior of the cyano groups was determined.



An extensive survey (one participant, Carolyn Brock) determined that this was the best session of the meeting. The organizers wish to thank William Ratcliff for going above and beyond (redefining?) the duties of a SIG Chair to help recruit excellent speakers to ensure the success of this session.

Christina Hoffmann
Jim Britten

03.01.01 & 03.01.02: Structure-based Drug Design

Participants in session 03.01.02; L-R: Erin Davis, Lance Westerhoff, Helen Blanchard, Jim Kiefer, Barry Finzel, Akilah Murray, Chelsy Chesterman, Matthew Calabrese, Jing Wang. Photo by student volunteer. Unfortunately no photo was available for session 03.01.01.

The Biological Macromolecules SIG, Industrial SIG, and YSSIG jointly sponsored two half-day sessions titled, **Structure-based Drug Design**, organized by Barry Finzel, U Minnesota,and Chelsy Chesterman, Rutgers U. The sessions included 13 excellent presentations with content ranging from over-arching reviews of mature drug discovery efforts driven by iterative structure-driven design (e.g., Bcl-2 antagonists; BACE inhibitors; HIV integrase inhibitors) to more preliminary fragment-based crystallographic screening. Common themes included improvement of ligand affinity and achieving selective binding. Two talks stood out for their novelty and breadth. **Matthew Calabrese**, Pfizer, provided an excellent summary of a wide-ranging effort to understand the mechanism of AMP-Kinase activators of interest in diabetic neuropathy applications. The large multi-chain oligomer complexes studied explain allosteric activation by small molecules. **Jim Kiefer**, Genentech, gave a fantastic talk describing the first structures of histone demethylase KDM5 that is important in the epigenetics of cancer progression. The structure was obtained only after overcoming a number of technical challenges in protein expression and crystallography.

Barry Finzel
Chelsy Chesterman

Pamela Schoenborn, at left, with Paul Langan. Photo by Richard Bromund.

Bob Finnegan of AIP Publishing, hard at work on arrangements for the Exhibit Show. Photo by Richard Bromund.

03.04: Molecular Machines

L-R: Jai Wei, Emmanuel Skordalakes, Melanie Ohi, Stefan Imseng, Fred Dyda, Evan Worden, Aaron Robart, Eric Montemayor. Photo by student volunteer.

The molecular machines session focused on the structure, dynamics, and mechanisms that protein and protein nucleic acid complexes employ to perform essential tasks in biology.

Stephan Imseng, of the Meyer group at U Basel, Switzerland, was awarded this year's Biological Macromolecules SIG **Etter Award** and presented a tour de force story on the architecture of human mTOR complex 1. Stephan's work integrated X-ray crystallographic techniques solving the structure of the human Raptor protein, with cryo-EM to illustrate how Raptor communicates with the active site in the ~1 MDa holoenzyme complex. Congratulations Stephan!

Melanie Ohi, Vanderbilt U, presented her group's work on capturing high-resolution cryo-EM snapshots of the *S. pombe* spliceosome. The spliceosome is a highly dynamic complex, and Melanie's work highlighted the use of temperature-sensitive mutations to capture and purify unique spliceosome assemblies. She also presented a versatile DID tagging tool that provides easily visualized beacons in cryo-EM to identify the location of individual proteins in complex assemblies.

Evan Worden, of the Martin group at U California Berkeley, showed us how the 26S proteasome is constructed to deconstruct. Evan's work provided structural information on the Rpn8/11 heterodimer, and how conserved insertion loops rearrange around the active site to perform highly specific deubiquitination of protein substrates targeted for destruction.

Jai Wei, of the Tong group at Columbia U, told us an interdisciplinary story of the yeast Acetyl-CoA carboxylase enzyme. Jai solved the structure of the 0.5 MDa ACA complex both by crystallography and cryo-EM, pinpointing the structural basis for Soraphen A inhibition and enzyme control by phosphorylation. Jai's story included an intriguing example of divergence between crystal and cryo-EM structures, and through meticulous experimentation he identified a component of the crystallization solution causing a large-scale conformational change in the ACA complex.

Fred Dyda, NIH, presented his group's work on the mechanism of cut-and-paste DNA transposition, and how individual active sites within a transposase dimer perform DNA strand acrobatics to form dsDNA breaks. Fred's talk provided a structural rationalization for the conservation of A and T positions in the Hermes transposon insertion site, and an elegant mechanism of how these sites are important to ensure transposons can mobilize themselves out from new insertions within a genome.

Emmanuel Skordalakes, Wistar Institute, concluded the session with a talk focused on the structure of the POT1/TPP1 heterodimer. These proteins are core components of the shelterin complex, and serve as guardians of the genome by stabilizing telomeric DNA repeats found at chromosome ends. In his POT1/TPP1 structure Emmanuel showed that a previously unresolved portion of TPP1 adopts a holiday junction resolvase fold, hinting at important functions in modulating higher order D-loop structures formed by telomeres. Finally, Emmanuel's group analyzed human mutations in POT1/TPP1 linked to cancer, showing that disruption of the dimer interface leads to genomic instability through telomere loss resulting in chromosome fusions.

Eric Montemayor
Aaron Robart

03.06: Cryo Electron Microscopy and Electron Diffraction

This session focused on new developments in cryogenic electron microscopy (Cryo-EM) and electron diffraction, as well as on the structure of large molecules or assemblies partially or completely determined by employing these methods.

David Belnap, U of Utah, who co-chaired the session, led off by providing a broad, historical overview of developments in Cryo-EM culminating in the on-going revolution in three-dimensional, transmission Cryo-EM that has enabled the determination of structures at near-atomic resolution and the resolution of structural heterogeneity. David concluded his presentation with a description of the limitations of Cryo-EM, and how it complements or competes with X-ray crystallography and nuclear magnetic resonance as the principal method for determining high-resolution structures.

Next, **Robert McKenna**, U Florida, presented translational studies that show great promise in clinical trials, wherein adeno-associated viruses (AAVs) are being developed as vectors for corrective human gene delivery. The location of epitopes on AAV1, 2, 5, 6, 8 and 9 to which monoclonal fragments (Fabs) bind was identified by medium (10-5 Å) resolution CryoEM

Turn to p. 36

studies. This allowed selection of an appropriate AAV variant for treatment. Additionally, high (4-3.5 Å) resolution Cryo-EM studies showed that significant main- and side-chain movement is induced within the AAV2 capsid by pH changes encountered in the endo/lysosomal pathways at 6.0, 5.5 and 4.0, compared to pH 7.4. Together these results show that AAV-Fab interactions involve a common set of footprints that overlap some receptor binding sites and transduction determinants, suggesting potential mechanisms of antibody virus neutralization. These structural insights will guide the future design of AAV capsids for effective gene delivery.

In the third talk, **Ryan Jackson**, formerly at Montana State U and currently at Utah State U, described the determination of the structure of the *E. coli* CRISPR RNA-guided surveillance complex, called Cascade (CRISPR associated complex for antiviral defense), by molecular replacement using a Cryo-EM map as the search ensemble, combined with phase extension into high-resolution diffraction data via iterative rounds of averaging non-crystallographic symmetry related density, followed by density modification. This was a technically challenging process, and Ryan also presented the streamlined protocol developed with his coauthors for solving X-ray structures with EM maps. This protocol uses freely available software tools (Chimera, CCP4, Coot, and Phenix) and is supplemented with online tutorials and videos.

The plenary speaker, **Tamir Gonen**, HHMI Janelia Research Campus, described MicroED, a method developed by his group to use electron diffraction from microscopic crystals to determine high-resolution protein structures by using an electron cryo-microscope (CryoEM) in diffraction mode. The crystals used can be a billion times smaller in volume than those normally used for X-ray crystallography. Tamir described the basics of the MicroED method, from concept to data collection, analysis and structure determination, illustrating how samples that were not analyzable by other methods could be studied by MicroED. Tamir's group uses a medium-cost microscope and yet has achieved 1.0-Å resolution for some structures. The proteins his group investigates using this method are membrane proteins important in maintaining homeostasis in the brain. Tamir concluded his talk by highlighting how this new method is providing information to understand major brain diseases like Parkinson's disease.

Next, **Sulochanadevi Baskaran**, U California Berkeley, presented Cryo-EM reconstructions of the 360 kDa class III phosphatidylinositol 3-kinase (PI3K) complex that includes PI3K, the regulatory subunit Vps15 and the coiled coil heterodimers of Beclin 1 and Atg14. This complex phosphorylates phosphatidylinositol to produce phosphatidylinositol 3-phosphate and is critical for autophagy, an essential vesicular degradation pathway conserved in eukaryotic cells. Sulochanadevi described the process of purifying recombinant PI3K complex, generating 3D reconstructions of the PI3K complex by negative stain electron microscopy and determining the location of individual protein domains by tagging different protein termini with maltose binding protein. These studies showed that the quaternary complex is a V-shaped structure, and current studies are focusing on understanding the mechanism and regulation of the complex.

The session ended with a talk by **Qiu-Xing Jiang**, U Florida, who described a chemical engineering procedure recently developed by his group that enables the linkage of bioactive ligands such as Ni-NTA, DNA/RNA oligos, protein G, antibody fragments, lipid molecules, and sugars to the surface of nanometer-thick carbon films, which they call the ChemiC films. The ChemiC films enable the use of (sub)nanogram quantities of biological complexes and of difficult specimens that do not concentrate adequately in solution or distribute well on the surfaces of conventional glow-discharged carbon films for making CryoEM grids for imaging. The traditional method also wastes 99% or more of the sample. This method can also be used for micro-crystals suitable for electron diffraction, as the vitrified ice layer can be made as thin as 20-30 nm in order to significantly decrease background noise from ice scattering. Qiu-Xing's group used RNA-ligands on ChemiC films to study the interaction between short RNA-ligands and the C3PO, a ribonuclease enzyme that functions to activate the RISC complex in the RNAi pathway. Their CryoEM studies suggest a mechanism of RNA-dependent assembly of the active complex and catalysis dependent turn-off of the enzyme, explaining how the RNA substrates are enclosed within the protein enzyme, as was shown by previous crystallographic studies.

David Belnap
Sangita Sinha

03.07.01: Hot Structures I

The **Hot Structures I** morning session featured three papers on pathogen function, as well as several other highly newsworthy reports. **Jobichen Chako**, National U Singapore, **John Jimah**, a graduate student at Washington U School of Medicine and a Beryllium travel award recipient, and **Diana Tomchick**, U Texas Southwestern Medical Center, spoke on pathogens. Respectively, they provided insights into the chaperoning and construction of the Type III secretion system tip, the structure of a malarial protein involved in parasite cell exit, and a very intriguing dimeric sensor of human bile salts. **Toshiya Senda**, KEK, Japan, presented data indicating that a lipid kinase, PI5P4Kβ, may be the cellular sensor of GTP, in an interesting combination of biochemical detective work and structural biology. **Titus Boggon**, Yale U, presented the first structure of a new kinase recognition mechanism exhibited by Lim kinases. In addition to those mentioned above, two more noteworthy proteins were discussed. **Ralf Ficner**, U Göttingen, Germany, presented the first structure of a nuclear pore FG motif interaction with an exportin, and **Alex Kintzer**, U California San Francisco, presented the structure of a voltage-gated pore, which, together with other structures, suggests details of the voltage gating mechanism. In all, it was an eye-opening session!

Elizabeth Goldsmith
Kimberly Stanek

03.07.02: Hot Structures II

L-R: Qiujia Chen, Yalemi Morales, Bruce Bowler, Kimberly Stanek, Blaine Mooers, Eric Montemayor, George Lountos, Christopher Jones. Photo by Maria Miller.

The **Hot Structures II** afternoon session featured talks centered on the general theme of structural analysis of nucleic acids and/or protein:nucleic acid complexes. **Qiujia Chen**, Indiana U School of Medicine, started the session by describing his recent research that focuses on understanding the role for SETMAR in gene regulation from crystal structures of the DNA-binding domain of SETMAR bound to terminal inverted repeat DNA. **Kimberly Stanek**, U Virginia, then described the first structural analysis of two potential Hfq homologs from the genome of the deep-branching thermophile *Aquifex aeolicus*. The next speaker in the session, **Yalemi Morales**, Utah State U, received a graduate student travel award funded by Beryllium for presenting her work on the structural and biochemical characterization of the frequency-interacting RNA helicase from *Neurospora crassa*. **Christopher Jones**, NIH, rounded out the first half of the afternoon and described his recent work on the structural analysis of the ZTP riboswitch from *Fusobacterium ulcerans*.

Following the break, **Blaine Mooers**, U Oklahoma Health Sciences Center, presented work from his group in which they analyzed the structures of double-stranded RNAs with open major grooves from trypanosome RNA editing. **Eric Montemayor**, U Wisconsin–Madison, presented the structure of U6 small nuclear RNA with a wild-type internal stem loop. **Martin Horvath**, U of Utah, described the structure of MutY complexed to DNA with a transition state mimic that provided insights into the mechanism of BER glycosylases. To close the session, **Bruce Bowler**, U Montana, presented his recent structure that revealed how cytochrome c binds detergent hydrocarbons in a well-defined pocket.

George Lountos

03.08: Structural Enzymology

The **Structural Enzymology** session was aimed at connecting with scientists who work on innovative methodologies that are related to enzyme kinetics, and attempt to explain an enzyme's mode-of-action by examining the intermediates of catalytic reactions using X-ray crystallography and related structural biology methods. The session started with a presentation by **Maksymilian Chruszcz**, U South Carolina, who focused on antimicrobial resistance and the need for the development of novel therapeutics. He presented on several proteins from the lysine biosynthesis pathway (absent in mammals) that could be viable as drug targets. In particular, blocking the activity of DapB seems to be very promising and would induce defects in the bacterial cell wall that are similar to those caused by β-lactam antibiotics. Following Maks, **Ghader Bashiri**, U Auckland, New Zealand, discussed the catalytic cycle of MenD from *Mycobacterium tuberculosis*, which catalyzes the first step in the menaquinone biosynthesis. Menaquinone is an essential component of the respiratory chain. Both the electron transport system and ATP synthesis are viable anti-TB drug targets. The next speaker, **Andrey Kovalevsky**, Oak Ridge National Laboratory, presented X-ray structures of the catalytic subunit of the cAMP-dependent protein kinase (PKAc) in complex with various substrates, nucleotides and cofactors. Andrey used time-lapse to capture the PKAc active site before the reaction initiation and metal ions are bound, and in this way completed all the gaps in our knowledge of the phosphoryl transfer reaction by PKAc. Rounding out the first half of the session, **Oleg Borbulevych**, QuantumBio Inc., talked about XModeScore, a method for the determination of hydrogen atom locations and protonation states. He showed that the program can be applied to structural enzymology to explore the protonation patterns within the active site of enzymes.

Following coffee, **Elwood Mullins**, Vanderbilt U, described the first example of a non-base flipping DNA glycosylase structural mechanism employed by the bacterial AlkD enzyme during DNA repair. The new paradigm also employed CH-π interactions to stabilize the transition state. In a combined X-ray and neutron crystallography study, **Brad O'Dell**, North Carolina State U, described oxygen species bound to a Cu-dependent polysaccharide monoxygenase (PMO), a fungal enzyme that can act on crystalline cellulose. Brad proposed a mechanism in which dioxygen pre-binds to the enzyme before moving to the equatorial ligand binding site on the copper, ultimately being reduced to hydrogen peroxide. The 2016 Canadian **Margaret C. Etter Student Lecturer Award** went to **Marcia Chaudet**, U Waterloo, who described both the structure of a maize chitinase (ChiA) that attacks fungal pathogen cell walls, and the fungal protease that hydrolyzes ChiA to a truncated form. The protease targets a linker in ChiA, and using an active site mutant Marcia was able to crystallize the protease with both full-length ChiA and just the linker peptide. Finally, **Bernhard Lechtenberg**, Sanford Burnham Prebys Medical Discovery Institute, described his structure of the E3 ubiquitin ligase HOIP in complex with an E2-ubiquitin conjugate, which represents the first step in the reaction of a RING/HECT-hybrid catalytic mechanism. In addition, the binding of an allosteric ubiquitin to the complex was observed in the crystal structure as well, and this leads to the straightening of a kinked helix that is required to activate NF-κB in a cellular assay.

Carrie Wilmot
Katarzyna Handing

Jim Britten, at center, engaged in a lively discussion at the CCDC booth in the Exhibit Show. Photo by Peter Müller.

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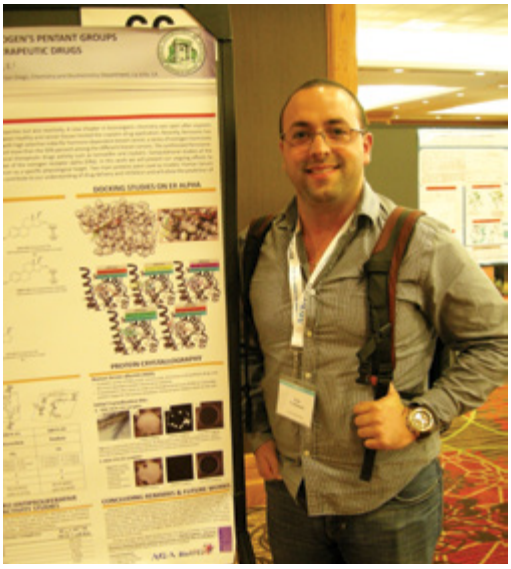
General Interest Posters

Once again I have made a selection based on my interests and idiosyncrasies, from the wealth of informative and clearly presented posters on offer in Denver. Thus I was looking particularly for examples of drug design and new insights into chemical bonding. You will note that in a number of cases my personal choice was matched by carefully considered evaluation from the poster prize judges, who awarded prizes or honorable mentions to these posters. The complete roster of 2016 poster prize winners may be found on pp. 9-12.

Poster **66-SA**: *Synthesis, Characterization, and Application of Ferrocene Complexes as Estrogen's Pendant Groups for Breast Cancer Treatment: an Approach to Design Novel Metal-Based Therapeutic Drugs*, presented by **José Carmona-Negrón**, Puerto Rico. This poster was awarded Honorable Mention for the **Journal of Chemical Crystallography Prize**, see p. 11.



José began by mentioning the discovery, very surprising at the time, that an inorganic complex could have anti-cancer activity. Cisplatin [(SP-4-2)-diamminedichloroplatinum(II)] was found to be a particularly powerful antineoplastic drug. It binds to DNA, creating cross-links that eventually lead to programmed cell death. Unfortunately, although it kills the fastest proliferating cells first, it damages not only cancer cells but also normal cells, causing severe side effects. More recently, ferrocene was found to have antineoplastic activity. Again, though, anxiety arose that lack of specificity would cause side effects. José and his colleagues pursued the objective of attaching ferrocene to estrogen so that it would specifically target estrogen receptor positive breast cancer cells. The project began with successful attachment of ferrocene to estrogen by a short linker group, either on the A ring or on the D ring. The position and stereochemistry of attachment was verified by crystal structure determination of five products. These new drugs were tested against hormone dependent MCF-7 breast cancer cell lines and showed comparable antiproliferative activity *in vitro* to that for conventional therapeutic drugs such as tamoxifen and cisplatin. Next, it was necessary to show that these derivatized estrogen molecules were still capable of binding to the estrogen receptor protein. Feasibility was demonstrated by docking studies with estrogen receptor alpha. Finally, protein crystallographic studies were initiated on complexes with human serum albumin, which could act as a carrier for the drugs.

Poster **159-SU**: *Synthesis and Characterization of Novel Low Valent Aluminum Clusters*, presented by **Lauren Stevens**, U Maryland, recipient of an **ACA Pauling Poster Prize**. See pp. 9-10 for photos of Lauren receiving her prize from ACA's Poster Chair, Ilia Guzei, and showing off her prize-winning poster.

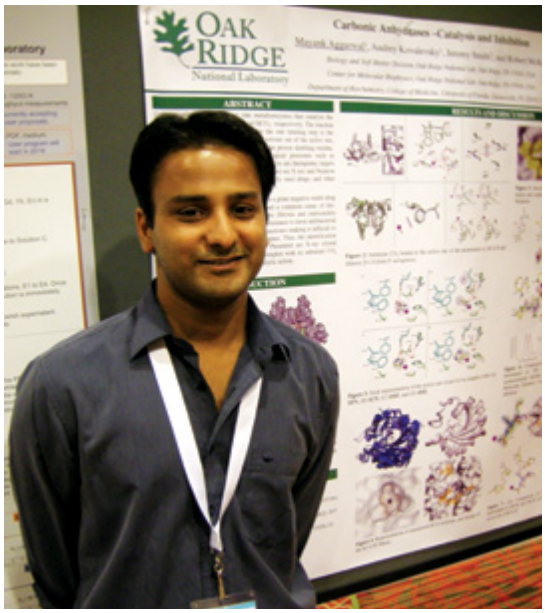
Years ago I had thought that aluminum chemistry could be summed up by saying that Al (and Ga, too) existed as the neutral metal or the formally tripositive ion, and not much else of interest could occur. Lauren showed quite convincingly that this idea was much too simple. With suitable apparatus Al can be persuaded to exist as low-valent ions in remarkably complicated clusters. The apparatus was initially designed by Hansgeorg Schnöckel of U Karlsruhe, Germany, and has been nicknamed the "Schnöckelator" by the Maryland group. Because the products are air- and moisture-sensitive, the system must be leak-proof; and the products are collected at dry ice temperature. A solution of AlX (X = Cl or Br) is first prepared. Reaction of AlX with an organolithium compound LiR removes LiX and forms AlR, which disproportionates into Al metal, AlR_3, and a subvalent Al cluster compound such as $Al_4Cp^*_4$ ($Cp^* = C_5Me_5$). Only X-ray crystallography could determine the structures of these complicated and diverse materials, which are sometimes built around polyhedra of Al atoms. The Al-Al distances, which can be as short as 2.644 Å or as long as 2.779 Å, provide information about bonding. Particularly noteworthy is the novel mixed-valent species $[Li_4Al_5Ph_{12}]^-$, in which a substituted hetercubane type core is formed from Al and Li atoms. A central Al^{1-} is bound to four apical Al^{2+} ions, which alternate with Li^+ ions at vertices.

They say that you can't teach an old dog new tricks (although our 9½ -year-old border collie would disagree). Carbonic anhydrase (CA) is a very old dog indeed. As the PDB101 Molecule of the Month in January 2004 it was described with the customary clarity. This article cited entry 1CA2, dating from 1989, as the definitive refined structure at 2.0 Å resolution; but a 2.0 Å structure was already published in 1972 [A. Liljas et al., *Nature New Biology*, **235**, 131-137]. That study was carried out so early, partly because it was technically feasible, but mainly because of the great biological importance of CA. It has a very high turnover rate, and it is responsible for clearing CO_2 from our tissues in the form of HCO_3^- and then regenerating CO_2 in the lungs so that it can be exhaled. Isoforms of CA are useful in making gastric secretions acidic and pancreatic secretions basic. Because carbonic anhydrase II, the structure of which was reported in PDB entry 1CA2, is found in a wide variety of tissues, its inhibition can cause undesirable side effects. However, isoform IX is upregulated in many aggressive cancers, and therefore its inhibition has become a hot research topic. Poster **34-SU** by **Carrie Lomelino** describing her research into a new class of diol-based inhibitors of CA IX won an **ACA Pauling Poster Prize**, as noted on p. 9. Two other posters provided additional insight into this topic and will be summarized here.

Turn to p. 40

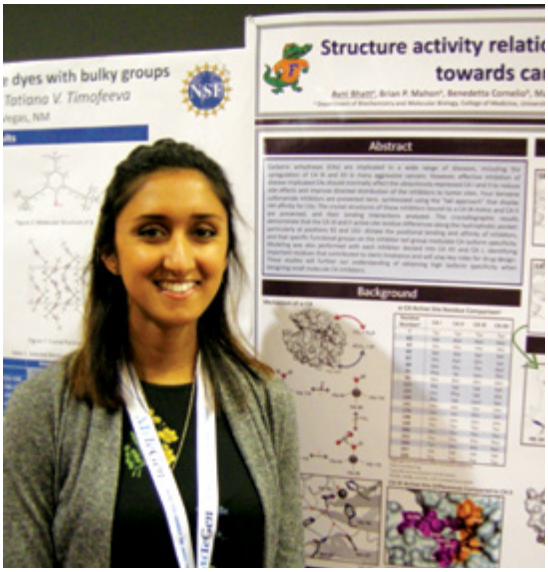
General Interest Posters, ctd.

Poster **2-SU**: *Understanding Carbonic Anhydrase Inhibition using X-rays, Neutrons, and Molecular Dynamics*, presented by **Mayank Aggarwal**, Oak Ridge National Laboratory



Using a combination of X-ray diffraction, neutron diffraction, and molecular dynamics, Mayank obtained a more complete picture than ever before of the interaction of human CA II with commonly used drugs. The sulfonamide drugs acetazolamide, methazolamide, and brinzolamide are potent inhibitors of CA and have particular value in the treatment of glaucoma. Comparison of neutron and X-ray data for complexes of these inhibitors bound in the active site of CA II enabled the hydrogen bonds to be clearly seen, not just inferred. Molecular dynamics provided a comparison of binding affinities. The opportunistic pathogen *Pseudomonas aeruginosa* also has a form of CA. If a selective inhibitor of this type of CA can be found, it might provide a therapeutic alternative to antibiotics that are of limited effectiveness against this bacterium. Mayank presented the structure of CA from this organism in complex with its substrate and with small-molecule inhibitors.

Poster **14-SU**: presented by **Avni Bhatt**, U Florida



With CA isoforms IX and XII being associated with cancer cells, but CA II being ubiquitous, Avni designed four derivatives of benzenesulfonamide with a "tail" attached at the *para* position that was intended to probe the binding sites of the enzymes. The eventual goal is selective inhibition of the former isoforms but not the latter. While CA IX does not form suitable crystals, the sequence of CA II can be modified to resemble that of CA IX in the active site region; and this CA IX-mimic is amenable to crystal structure determination. Avni presented the structures of the four inhibitors bound to CA IX-mimic and CA II. Residue 131 is important, being Val in CA IX-mimic but Phe in CA II. Val allows more room than Phe for a large hydrophobic tail, and indeed the candidate with the largest tail (3-quinolinyl) has a Ki of 0.2 nM for IX but 2.5 nM for II. The compound with a 3-formylphenyl tail has the lowest K_i against CA XII. On the other hand, small hydrophilic tails are expected to be inimical to selectivity since they could interact with the conserved residue Gln 92. Avni also presented the results of *in silico* docking to CA XII with future work intended to study binding to this isoform crystallographically.

Carl Schwalbe

04.01: Opportunities from New and Improved Sources

L-R: Lonnie Berman, David Waterman, Jose Martin Garcia, Paul Langan, Thomas Ursby, Aina Cohen, Simon Morton, James Holton. Photo courtesy of Sean McSweeney.

In a session well attended from first to last, with standing-room-only for the majority of the talks, listeners with a range of scientific challenges heard of opportunities to meet them. The session consisted of a total of eight presentations from mature and early stage X-ray and neutron sources.

Paul Langan, Oak Ridge National Laboratory, presented the opportunities offered by neutron experiments. The instruments available for biological studies at the existing high-flux reactor and spallation sources were explained and a convincing case made for their value. More than 25% of the experiments performed at these instruments are targeted to biology, supporting neutron crystal diffraction, small- and wide-angle scattering, as well as imaging, and other techniques to probe dynamics of biomolecules.

Following on, **Lonny Berman**, Brookhaven National Laboratory, described the history, scope and configuration of the new national light source NSLS-II with a particular emphasis on the NIH-funded beamlines for structural biology. The latest, still very early, results were presented as well as the aim and ambition of the mature stage of the project. Lonny's presentation emphasized the importance of having clear and strenuous technical criteria in place so that difficult science can be addressed and new opportunities can emerge.

The ALS at Berkeley is in the process of building a new suite of high-flux, dual-beam beamlines in a project they call Gemini. **Simon Morton**, Lawrence Berkeley National Laboratory, described the rationale for the design, the collaboration with the ALS accelerator team, and the guiding specifications for the project. The first portion of the project is nearing completion, and when finished Gemini will offer new operation and scheduling opportunities for the structural biology community. The project shows clear prioritization and emphasis on both the workflow of the experiment and the opportunity for future upgrades.

The first of the next generation of synchrotron light sources, MAX-IV, has come into operation, and **Thomas Ursby**, Lund U, brought us up to speed on the progress at the complex in Lund, Sweden. In addition to the new light source, the complex envisaged in Sweden will host the European Spallation Source and the Science and Innovation campus, and has the possibility for extension with a free-electron laser facility. A range of beamlines supporting imaging, spectroscopy, scattering, and diffraction covers the biological program. Thomas touched on all these approaches whilst revealing in most detail the state of the macromolecular crystallography beamlines. The first of these beamlines has undertaken first commissioning experiments and test-structure determination – all within a few months of the X-ray shutters being opened for the first time!

The excitement that serial femotosecond crystallography has aroused in the community using the LCLS is being transferred to a number of light sources, with multiple experiments occurring at sources round the globe. One of the leading groups in the technique was represented by **Jose-Manuel Martin Garcia**, Arizona State U, who described experiments using a viscous injector system that had been undertaken at the APS at the ID23 beamline. The presentation demonstrated both the enormous potential of the approach and the magnitude of the challenge ahead if this is to become a routine part of the beamline portfolio of tools. (The not-obvious opportunity presented by the viscous injector is that the gel-like lipidic cubic phase has become an often-successful medium for growth of membrane-bound proteins.)

How well do we understand the diffraction and scattering processes underlying the experiments we undertake? This was the subject of the thought-provoking presentation by **James Holton**, SLAC, wherein he discussed the importance of being able to simulate diffraction experiments, and how the knowledge gained in this way can be brought to use in the deconvolution of the data created in the most challenging experiments. The impact of these simulations on the development of new sources and experiments was discussed.

James Holton's presentation had raised challenges that were then taken up by **David Waterman**, CCP4, U.K., in describing the current state of the collaboratively produced, open-source data-integration and measurement software DIALS. In addition to describing the philosophy and organization of the DIALS program, David described innovations in the indexing of diffraction patterns from multiple crystals, joint refinement of orientation against all available data, the problems of merging multi-crystal data sets, as well as the remarkably complex issue of obtaining good background subtraction in diffraction experiments.

Bringing the session to a fittingly up-beat conclusion was **Aina Cohen**, Stanford U, who described the synergies between developments at SSRL and at the LCLS, culminating in the construction of a new dedicated macromolecular crystallography facility housed at LCLS. This facility, named MFX, will provide a much needed boost in access to LCLS for structural biology. MFX has recently been brought into life, with the first full experiments to follow closely on the heels of the Denver ACA meeting.

Sean McSweeney
Robert Sweet

04.02: Surfaces and Interfaces

The **Surfaces and Interfaces** session dealt with a variety of materials that can be laid down in thin films with interesting, and often useful, properties. **Detlef Smilgies**, Cornell U, led off with a description of some of the many experiments in soft matter carried out at the D1 station at CHESS, with a particular focus on metal nanoparticles functionalized with organic ligands. Detlef also described the recent use of the SNIPS (Self-assembly plus Non-solvent-induced Phase Separation) technique, using a doctor blading device, to prepare membranes with well-defined pores, for functions such as desalination.

Zhang Jiang, Argonne National Laboratory, continued with the nanoparticle theme and described some experiments, at sector 8-ID of the APS, examining the properties of nanoparticle membranes assembled on the surface of water droplets and then transferred to a substrate (see below). Although the original nanoparticles

Production of 'Janus' membranes. From Z. Jiang et al., Nature Materials 14, 912-917 (2015).

are spherically symmetric, the environment at the surface of a droplet – air on one side and water on the other – breaks the symmetry, and the membranes behave differently depending on whether the air-facing side or the water-facing side faces out from the substrate. In an SEM, these membranes tend to fold up, always bending towards the water-facing side. A combination of GISAXS, Raman spectroscopy, and molecular dynamics simulations was used to study these 'Janus' membranes.

Turn to p. 42

After a break, session co-organizer **Kevin Yager**, Brookhaven National Laboratory, moved on from nanoparticles to block copolymers and described laser zone annealing of thin films of such molecules. By tightly focusing a laser beam into a line directed at a film mounted on a substrate, and translating the sample, a combination of an intense thermal gradient and a shear field is generated, which leads to rapid ordering of the molecules in the film. Different nanoscale lattices can be generated by controlling the annealing parameters, and layering the ordered materials.

Josh Choi, U Virginia, also looked at control of a self-assembly process, but his material was an organic-inorganic perovskite intended for use in solar cells. Such perovskites are an attractive alternative to silicon for solar cells because of their lower cost. Yet there are challenges for these materials: their performance is not yet as good as it could be, and the perovskite films are not very stable under ambient conditions. The size and orientation of grains within a film affect performance, and Josh investigated additives that altered these properties, using GIXS to monitor the growth of films *in situ*. With an appropriate additive, it was possible to create a film with uniform grain orientation.

Our final speaker, **John Smedley**, Brookhaven National Laboratory, moved away from organics and solvents, to talk about the preparation of K_2CsSb films for X-ray emission from photocathodes. The films are prepared by deposition in a vacuum, monitored by *in situ* X-ray scattering. John presented a fascinating story of the complex transitions that occur during the process, and how they are affected by the choice of starting material, the order in which components are added, and the amount of each element used. The best results have been obtained using simultaneous co-evaporation of all three elements in precisely controlled proportions, to produce a very smooth film with high quantum efficiency.

Marian Szebenyi
Kevin Yager

04.03: Multiple Crystal Techniques

The aim of the **Multiple Crystal Techniques** session, chaired by Stephan Ginell and Ana Gonzalez, was to present recent developments in methods for sample handling, data collection and processing in experiments involving large numbers of samples. While the use of multiple samples in macromolecular crystallography is not a new practice, the construction of serial femtosecond crystallography facilities at XFELs has resulted in a boost to the field and spurred the development of new instrumentation and software for experiments at XFEL and synchrotron beamlines.

The synergy between new and conventional light sources was a main topic in the presentation by **Aina Cohen**, Stanford U, who talked about the development of several high-capacity sample holders, suitable for use with automated sample mounters and *in situ* crystal growth, and specialized software written for Blu-Ice/DCSS for automated, fast centering of the samples in the X-ray beam. These tools were devised for fixed-target serial crystallography experiments at LCLS, but can equally be used to facilitate sample handling and experiment throughput for experiments at synchrotron sources. Aina described MFX, the first instrument at LCLS dedicated to femtosecond serial crystallography. **Gwyndaf Evans**, Diamond Light Source, U.K., talked about the development of microfocus facilities at the Diamond beamline VMXm, designed to handle samples between 50 and 0.5 micron in size. The instruments implemented at the beamline include an SEM to visualize dose-sensitive samples using low-energy electrons. Gwyndaf also mentioned ongoing improvements in DIALS and BLEND to provide a semi-automated tool to merge data from multiple crystals. Software developments were also the main focus of the talk by **Artem Lyubimov**, Stanford U. He spoke about the program IOTA, for improved detection of spots in single-shot still diffraction images, and PRIME, used for merging, scaling and postrefinement of serial crystal data. These two programs, implemented within the ***cctbx.xfel*** suite, were critical for the determination of a high-resolution structure for Synaptotagmin/SNARE complex using only 297 diffraction images. In the second part of his presentation, Artem discussed two fixed-target delivery devices optimized for the precise location of crystals: micropatterned silicon nitrate chips consisting of hydrophobic and hydrophilic surface layers, and a microfluidic flow chip with hydrodynamic crystal traps.

In the second part of the session, **Christian Burton**, Aston U, U.K., described a microfluidic-based device engineered at Aston that uses acoustic fields to set up a standing-surface acoustic wave to transport slurries of crystals into the beam without any contact; the instrument is suitable to handle crystals between 1 and 200 microns in size at room temperature, in mother liquor or other environments, and has been tested at the I24 Diamond beamline. **Bob Thorne**, Cornell U, described new *in situ* data collection plates developed by MiTeGen. The construction and materials of the plate make it easy both to inspect the samples with a microscope, and to expose the crystals to the X-rays in different orientations without increasing the background, while providing uniform vapor equilibrium for consistent and reproducible crystallization conditions and to avoid dehydration. Bob also introduced the Hyper quenching cryo-cooler used to improve isomorphism between frozen crystals by eliminating differences caused by the cooling procedure.

The last two presentations in the session focused on the data and experimental results. **Aaron Finke**, Paul Scherrer Institute, Switzerland, spoke about optimizing native phasing experiments. Because these experiments involve anomalous differences of at most approximately 1%, collection of high-multiplicity data is needed while at the same time avoiding radiation damage. He explained how to use the ISa parameter displayed by the program XDS to determine the optimal exposure time. Although collecting multiple sweeps from a crystal without exceeding a dose of 0.5 MGy often results in successful phasing, sometimes data from multiple samples or different parts of the crystal must be merged in order to obtain the needed multiplicity; as an example, Aaron described an experiment in which the structure was solved from 992 micron-sized lysozyme crystals grown *in meso*. Our last speaker, **James Holton**, SLAC, noted that using simulated data with a read-out, noise-free detector, it is possible to obtain similar results either by assembling a complete dataset from small

oscillation wedges from multiple crystals, for a total dose D per crystal, or by spreading the same dose D over a full 360 degree sweep of just one crystal. The latter approach potentially simplifies the data collection strategy for multicrystal data collections. In the second part of his talk, James applied singular value decomposition (SVD) to tetragonal lysozyme structures with a large range of structure factor amplitudes to show that the differences change in a non-random manner and can potentially be used to extract phase information.

Ana Gonzalez
Stephan Ginell

05.01: The Next 100 Years of Powder Diffraction

Powder diffraction crystallography was invented within a few years of the original Laue experiment – independently in both Germany and in the United States – to address needs to complete crystallographic analysis of materials that did not form single crystals. On the centenary, this session was organized to highlight the development of the technique and where the speakers see the technique progressing.

The highlight of the session was a return to the ACA by **David Cox**, who came to the U.S. in 1959 to work at the Westinghouse Company's commercial research reactor, but shortly thereafter moved to Brookhaven National Laboratory where he spent the remainder of his career. It has been quite a few years since Dave's last ACA talk; he commented that his previous talk was delivered from transparencies. Dave was active in neutron powder diffraction crystallography, but saw the importance of synchrotrons for high-resolution instrumentation and developed the perfect-crystal design that is now used across the world. Dave talked about developments in powder diffraction crystallography during his career and inserted recollections of many different people he had the chance to know.

Dave's talk was followed by contributed presentations from **Sanjit Ghose**, Brookhaven, discussing the new synchrotron powder diffraction instrumentation at NSLS-II, and then **Ashfia Huq**, Oak Ridge National Laboratory, who presented results from the leading U.S. neutron diffractometer at the Spallation Neutron Source. Later, **Saul Lapidus**, Argonne National Laboratory, spoke about the 11-BM diffractometer at APS, an instrument designed directly following the original Cox design, but implementing 12 analyzers and detectors allowing 11-BM to significantly exceed the publication rate of every other APS instrument. Saul showed how recent improvements have significantly improved the resolution of 11-BM, which was already the best in North America.

Next, in his invited talk **David Bish**, Indiana U, who also spent many years in government service (at Los Alamos National Laboratory) before joining Indiana, gave us a glimpse of some of the future of powder diffraction with a description of the powder diffractometer currently operating *on the surface of Mars*, in the Curiosity Rover. Powder diffraction is an indispensable tool for understanding the history of that planet's surface through identification of minerals.

Other talks in the session included a presentation from **Angus Wilkinson**, Georgia Tech, who spoke about his crystallographic studies using modern user facility instruments. Also **Thomas Degen**, PANalytical, discussed how laboratory powder instruments have improved – to the level that they can even be used for protein studies. Finally, **Suzanna Ward**, Cambridge Crystallographic Data Centre, U.K., spoke on the contribution of powder diffraction crystallography to the wealth of structural knowledge that crystallography has contributed to science.

Brian Toby
Andrey Yakovenko

05.02: Magnetic Entanglement and Complex Magnetic Materials

New research is beginning to clarify the respective roles of entangled magnetic, orbital, and charge orders in a variety of exotic crystalline phases. Evidence of the coupling of magnetic order to structural or electronic parameters at surfaces, domain walls, and other interfaces now provides exciting opportunities to manipulate and even engineer the properties of multi-functional materials. This session focused on the use of X-ray and neutron scattering methods to characterize subtle magnetic correlations and entanglements.

Sae Hwan Chun, Argonne National Laboratory, opened the session with an invited talk presenting new evidence in the search for quantum spin-liquid (QSL) phenomena of the Kitaev type in the iridate Na_2IrO_3, a material that has been studied intensely during the past five years. Kitaev QSLs, if ultimately realized, will support a variety of fascinating spin-orbit entangled states. Their Argonne group's diffuse magnetic X-ray scattering work reveals that highly anisotropic 'bond directional' interactions dominate the magnetic exchange amongst iridium spins on a bipartite honeycomb lattice, which then secures the magnetic frustration necessary for the QSL ground state at temperatures approaching absolute zero. Invited speaker **Alan Tennant**, and **Huibo Cao**, both from Oak Ridge National Laboratory, presented binary halide α-$RuCl_3$, with its graphene-like honeycomb layers of Ru^{3+} ions, as an alternative route to Kitaev QSL behavior. Huibo described the use of X-ray and neutron single-crystal diffraction to clarify its low-temperature nuclear and magnetic structures, while Alan highlighted the remarkable detection of Majorana fermions in α-$RuCl_3$ via inelastic neutron scattering. Majorana fermions are a special type of fractionalized excitation predicted to occur in the exotic topological states supported by two-dimensional QSLs. Alan further explored the experimental challenges involved in the detection and characterization of other exotic topological states in crystals, such as spin-ice states, topological insulators, and Weyl semi-metals.

Virginie Simonet, Institut Néel, CNRS/UGA, Grenoble, France, presented an invited talk describing the use of magnetic neutron diffraction and inelastic scattering to solve the mystery of unorthodox multiferroicity in the $Ba_3(Nb,Ta)Fe_3Si_2O_{14}$ langasites, which are multi-chiral magnetic systems based on triangular networks of Fe spins. Due to the frustration of colinear configurations, the Fe spins in each layer nominally form the 120-degree structure in plane, but spiral around the c-axis in the out-of-plane direction. Remarkably,

Turn to p. 44

the moments are shown to bunch up rather than stepping uniformly around the spiral. The resulting loss of the 3-fold symmetry axis facilitates a ferroelectric moment. **Javier Campo**, Aragon Materials Science Institute, Zaragoza, Spain, demonstrated that a cycloidal magnetic structure arises in molecular compound $(ND_4)_2[FeCl_5(D_2O)]$ at T_N = 7.25 K, which breaks inversion symmetry and facilitates the formation of ferroelectric order. This surprising structure explains the recently observed multiferroicity and opens the door to a world of multi-functional molecular magnets.

Naveed Zafar Ali, National Centre for Physics, Quaid-i-Azam U, Pakistan, presented a multi-faceted analysis of a series of structural and magnetic phase transitions in $CsCoO_2$, relying on a combination of single-crystal XRD, powder NPD, magnetic susceptibility, and muSR experiments, together with DFT calculations. The tetrahedrally-coordinated high-spin (S = 2) Co^{3+} ions exhibit a long-range 3D antiferromagnetic alignment of chains of ferromagnetically ordered Co-Co spin dimers below 424 K, and a second lower-temperature transition is accompanied by complex relaxation behaviors. **Ovidiu Garlea**, Oak Ridge National Laboratory, employed magnetic neutron diffraction to determine the magnetic structures of two new low-dimensional transition metal vanadates. $K_2Mn_3(VO_4)(CO_3)_2$ notably exhibited alternating layers of edge-sharing MnO_6 octahedra (honeycomb lattice) and CO_3-linked MnO_5 trigonal bipyramids (triangular lattice), giving rise to a sequence of three magnetic phase transitions. Exotic magnetic ground states are then obtained by destabilizing the long-range magnetic order via the application of an external magnetic field. Graduate student **Amber Larson**, U Maryland, won a **Margaret C. Etter Student Lecturer Award** for a brilliant presentation on the structural and magnetic orderings in doped Mn hollandite structures, as determined via joint X-ray/neutron powder diffraction analyses. The ferrimagnetic order induced by substituting cobalt into the $Ba_{1.2}Mn_8O_{16}$, for example, significantly mitigates the antiferromagnetic frustration observed in pure manganese hollandite. And the metal-insulator transition observed in the $Bi_{1.7}V_8O_{16}$, accompanied by an increase in magnetic susceptibility, appears to be driven by commensurate charge order and the formation of V—V dimers and spin doublets.

Anna Llobet
Branton Campbell

05.04: Novel Methods for Emerging Science

L-R: Yu-Sheng Chen, Joseph Ng (at rear), Andrew Martinolich, Joe Reibenspies (at rear), Julien Lhermitte, Xiaobing Zuo (at rear), Bianca Haberl, Irimpan Mathews (at rear), Bob He. Photo by Vicky Doan-Nguyen.

Joseph Ng, U Alabama in Huntsville, led off the session presenting a talk on inorganic pyrophosphatase (IPPase) that was crystallized by counter-diffusion crystallization in the Granada Crystallization Facility (GCF) as a Center for the Advancement of Science in Space (CASIS) payload on board the International Space Station (ISS). **Irimpan Mathews**, Stanford U, presented a talk on the short X-ray pulses produced by X-ray Free Electron Lasers (XFELs). He describe a new sample delivery device for SFX, the Sample Extractor, that may be used to deliver delicate crystals directly from native crystallization solutions. **Yu-Sheng Chen**, U Chicago, presented a talk on ChemMatCARS, which operates an experimental station in the areas of Advanced Small Molecule Crystallography (ASMC), at the Advanced Photon Source (APS) – the premier undulator-based synchrotron source of high-brilliance high-energy X-rays in the U.S. **Bob He**, Bruker AXS, closed the first part of the program with his talk showing us how the availability of two-dimensional X-ray detectors allows acquisition of diffraction patterns covering large solid angle with abundant information about the atomic arrangement, microstructure, deformation and defects of the materials.

Following the break, **Bianca Haberl**, Oak Ridge National Laboratory, presented a talk on high pressure as a unique tool for the synthesis of crystalline phases with tailored functionality. **Xiaobing Zuo**, Argonne National Laboratory, spoke on synchrotron-based X-ray scattering, which can measure structural lengths covering from a few Ångstroms to a few hundred nanometers and has become a very powerful structural tool for supramolecular and nanomaterial study. **Julien Lhermitte**, Brookhaven National Laboratory, gave us a talk on the high degree of coherence and flux of X-rays from next generation synchrotron sources, which permits the measurement of structural information from less-ordered systems over larger ranges of length scales. **Andrew Martinolich**, Colorado State U, spoke on the search for new materials, which is often narrowed by phase equilibria or inhibited by the barriers of reactant diffusion and product nucleation. To round out the session, **Collin Broholm**, Johns Hopkins U, presented information on high magnetic fields that can induce qualitatively new states of matter dominated by quantum effects, for fields beyond 15 Tesla.

Katie Page
Joe Reibenspies

Philip Coppens making last-minute checks ahead of his talk kicking off the Transactions Symposium. Photo by Peter Müller.

05.07: In-situ and In Operando Methods

The topic of this session was using X-ray and neutron scattering to study materials under operational conditions. **Amy Marschilok**, Stony Brook U, opened the session describing her work on characterization of battery systems using energy dispersive X-ray diffraction. **Vicky Doan-Nguyen**, U California Santa Barbara, followed up with work based on local structural analysis to understand the mechanism behind transition metal polysulfide chalcogel conversion electrodes. The energy materials theme continued with the next speaker **Craig Bridges**, Oak Ridge National Laboratory, who spoke about how *in situ* small-angle neutron scattering allows one to understand the porous structure of electrode materials for battery applications. **Hyunjeong Kim**, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, took us back to the use of local structural analysis to understand the structure of thin film, and how one can search for Ti cluster formation in $Mg_{0.7}Ti_{0.3}$ alloy.

After the coffee break, **Daniel Shoemaker**, Arizona State U, discussed the use of *in-situ* diffraction to follow synthesis reactions of inorganic materials. A recently commissioned flow cell that combines neutron pair distribution function studies of catalytic materials simultaneously with *in situ* steady-state isotopic transient kinetic analysis (SSITKA) was the topic of the next presentation, by **James Neilson**, Colorado State U.

Daniel Taylor, at left, receiving his Etter Award from Ashfia Huq. Photo courtesy of Ashfia Huq.

Following James's talk, **Daniel Taylor**, winner of the **Margaret C. Etter Student Lecturer Award** from the Powder Diffraction SIG, discussed how he uses *in situ* X-ray and neutron studies to understand the oxygen conduction mechanisms in oxygen storage materials.

The session ended with two talks highlighting the use of pressure. **Christine Beavers**, Lawrence Berkeley National Laboratory, spoke about work on the recently discovered organic inorganic perovskite structure, and **Dmitry Popov**, Carnegie Institution for Science, summarized the opportunities for single crystal X-ray diffraction under pressure at HPCAT at the APS at Argonne National Laboratory.

Vicky Doan-Nguyen
Ashfiya Huq

05.09: SAS and Integrative Approaches to Complex Structures

The focal points of this small-angle scattering session were complex structures and systems across biology, medicine, chemistry, and material science. The session featured a breadth of expertise across these technical areas and highlighted recent findings that married a number of orthogonal approaches alongside small-angle X-ray and neutron scattering.

The first speaker, **Matt Helgeson**, U California Santa Barbara, presented his laboratory's work on a colloidal system based upon stimuli-responsive, self-assembling nanoemulsions that allow for the creation of structured colloidal gels with hierarchical morphologies. Matt's group brought together neutron scattering, rheology, and statistical mechanical modeling to understand the interactions and assembly mechanisms governing mesoscale processes that give rise to materials with superior mechanical properties.

Sangita Sinha, North Dakota State U, presented her group's research on the structure and function of BECN1 and ATG/KARKOR, key components of the autophagy nucleation complex. This complex is involved in the degradation and recycling of unwanted, damaged, or harmful cytoplasmic components. An integrative approach to the study of this protein was presented, including X-ray crystallography and small-angle scattering to distinguish the BECN1 coiled coil domain homodimer from the ATG14/BECN1 heterodimer. The derived heterodimeric interface was shown to be functionally important for starvation-induced up-regulation of autophagy.

Thomas Weiss, Stanford Synchrotron Radiation Lightsource, highlighted the recent innovations at the small-angle X-ray scattering (SAXS) station at BL4-2: a permanent experimental station at SSRL dedicated to structural biology and biophysics. Thomas discussed key features and technical developments for high-quality data collection, including a software pipeline, beam properties, time-resolved measurements down to the millisecond time-scale, stop-flow apparatus, and size-exclusion chromatography in line with SAXS (SEC-SAXS).

Andrew Allen, NIST, has reviewed recent work on advanced aluminum alloys (Al-Cu-Mg alloys AA2024) using the ultra-small-angle X-ray scattering (USAXS), small-angle X-ray scattering (SAXS) and wide-angle X-ray scattering (WAXS) facility at the Advanced Photon Source. Studies done *in situ* and *in operando* strive to understand the complex kinetics of the cluster-dissolution and S-phase formation processes in these alloys. Using an integrated approach including TEM, thermodynamics modeling, and chemical analysis results contributes to the development of future light alloys for the automotive industry and can also be applied in additive manufacturing. Their results were validated using simulations based on Langer-Schwartz theory and a Kampmann-Wagner numerical method, closing the 'loop' and providing necessary quantitative models for industrial applications.

Pavol Juhas, Brookhaven National Laboratory, discussed the problems with solving the structure of nanoparticles. Some nanoparticles are too small to possess substantial periodic order that gives rise to clear Bragg reflections. In order to correctly characterize such CdSe nanoparticles Pavol, together with the rest of the group of Simon Billinge, combined structure information from X-ray PDF, small-angle scattering, and a minimization of surface area to find the optimum nanoparticle structure. None of these three probes on its own is capable of providing conclusive structure information, but rather each may lead to clearly incorrect minima or produce a large number of degenerate models. Pavol's presentation discussed how to achieve an optimum combination of these information sources while assessing the accuracy and uniqueness of the results.

Kushol Gupta
Jan Ilavsky

ACA Summer Course in Chemical Crystallography 2016

ACA Summer Course 2016, L-R: back row – P. Prabhakar, J. Espinoza, A. Bard, C. Stern, Z. Manning, J. Christopherson, E. Reinheimer, L. Cinninger, C. Malliakas, M. Alaparthi, M. Bosch, I. Valenzuela-Chavira, L. Daniels, A. Sarjeant; middle row – A. Oliver, S. Zhang, B. Althufairi, J. Kaduk, D. Gray, B. Noll, R. Von Dreele, P. Mueller, J. Ridnour, M. Pyrch, M. Burtch, A. Filatov, Q. Wang, D. Bruks, N. Henderson, I. Chakraborty, C. Li, C. Lake, R. Sommers, D. Duchamp; front row – J. Carmona-Negron, S. Martinez, M. Payne, F. Qu, C. Vennari, F. Qin, R. Tang, J. Bertke, S. Carrington, S.-Y. Chien. Absent: R. Papoula.

The ***ACA Summer Course in Chemical Crystallography*** was hosted at the University of Notre Dame from June 12 – 19, 2016. Course organizers were: Allen Oliver (U Notre Dame), Amy Sarjeant (Cambridge Crystallographic Data Centre), Charlotte Stern (Northwestern U) and Christos Malliakas (Northwestern U). Course website: ***http://acasummercourse.net***.

In total 27 attendees were accepted to the course. Participants were predominantly domestic students; however, China, Mexico, Puerto Rico and Uruguay were also represented. On average there were ten faculty in attendance at any one time, and over the span of the week-long course 17 faculty donated their time, energy and enthusiasm. We also thank the ACA, the National Academy of Sciences, Bruker AXS, Rigaku, and Poly Crystallography, Inc. for their generous financial support.

This year we elected to reduce the program from a ten-day course to a seven-day course. Despite this change, the material covered by the course was still similar to previous years. Lectures on the theory of the experiment were presented in the mornings and early afternoons followed by workshop style breakouts and detailed instruction in the various crystallographic techniques.

Participants were grouped into one of six groups based on interests for purposes of the workshops on the first two afternoons/evenings. This also helped to promote networking among the students, especially for international attendees.

Attendees were encouraged to submit samples. There were 20 samples submitted of which 18 yielded data suitable for the participants to analyze. As in past years, we (organizers) encouraged publication of these data with a request that an acknowledgment to the course be included.

We have endeavored to change the focus of the course to better reflect the current status of crystallographic enterprise within the community. In particular, the more practical aspects of crystallography are emphasized. Modern advances in structure solution techniques as well as modern visualization methodology allow for more straightforward instruction to the end-user. We attempt to maintain a balance of modern pedagogy with sufficient fundamental knowledge. We continue to incorporate powder diffraction into the course. This technique is widely applicable, and many of the attendees find the knowledge gained both desirable and useful.

Perhaps one of the most noteworthy points is the level of experience of the attendees. In the last two years we have noticed that there is a larger percentage of attendees who are very familiar with the fundamentals of crystallography. It is clear that even though the course is designed with no prior knowledge in mind (and there are still a significant number of attendees for whom this is the case), many of the attendees are seeking more sophisticated knowledge. We do provide lecture material on more advanced topics, and perhaps more importantly many of the faculty work one-on-one with the students examining and assisting with their problem data. This one-on-one focus helps the students immensely since they can learn directly and at their own pace. More critically, such dedicated efforts develop lasting relationships between established crystallographers and researchers new to our science.

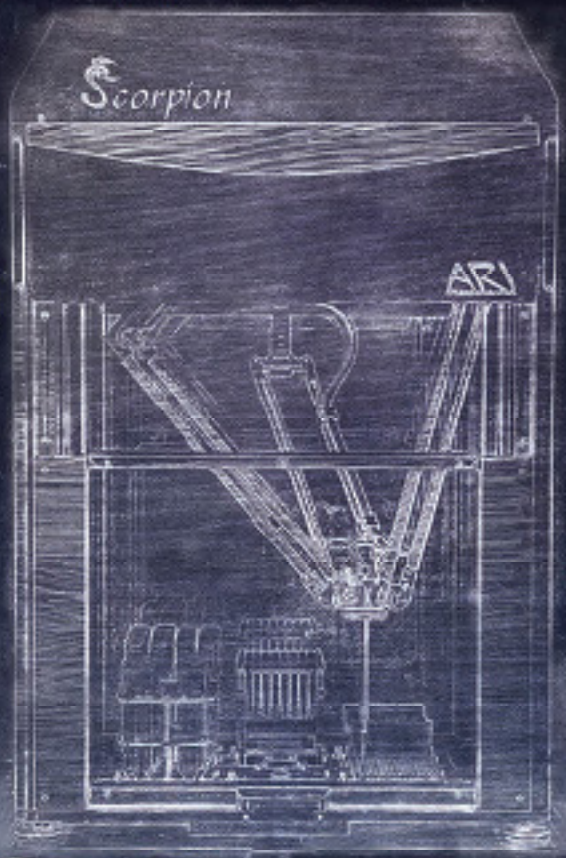
Of note, alumni of the course made six oral presentations at the ACA annual meeting in Denver. Demonstrably, the course has had a positive effect on introducing younger researchers and establishing connections.

The organizers are committed to continuing the legacy of dissemination of crystallographic knowledge to a new generation of crystallographers and researchers that was founded by Ken Trueblood and Bob Sparks. We would like to thank all of our faculty for their generous donation of time, energy and knowledge to this course.

Allen Oliver

TODAY'S LESSON:
WHAT CAN A SCORPION SCREEN BUILDER DO?

- ✓ Build screen blocks
- ✓ Optimize screen conditions
- ✓ Room for 96x 15 ml reagent tubes
- ✓ Access 1.5, 15 and 50 ml tubes
- ✓ Aliquot and normalize salt screens for LCP reactions
- ✓ Aspirate and dispense 1 ul to 1 ml
- ✓ Build multi-dimensional grids, pH, concentrations & titrate additives
- ✓ Set up 24-well plates, protein + screen
- ✓ Anything you can do with a handheld pipettor



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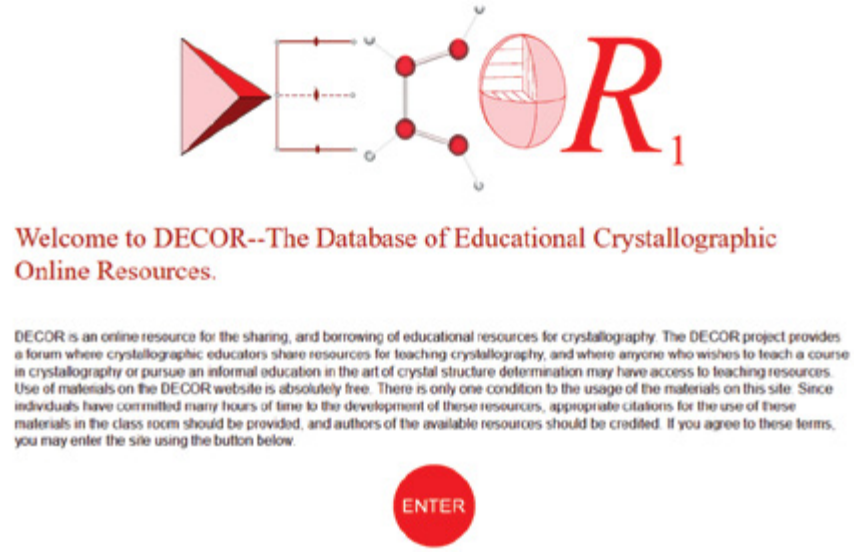
Net RefleXions

Fall is upon us once again. As fun as summer has been, it is finally time for pumpkin spice lattes, corn mazes, and delicious turkey meals. And we can't forget that with arrival of fall, as if by magic, in a blink of an eye college students reappear on campus. Therefore, as we prepare to welcome the new and returning students here in Madison, I wanted to feature in this installment of ***Net Reflexions*** an amazing new teaching tool: The Database of Educational Crystallographic Online Resources or DECOR for short.

In the midst of designing a course, have you, dear reader, ever caught yourself day dreaming? Fantasizing? Wistfully asking yourself: "Wouldn't it be easier to have a single access point to all of the available resources on twinning, instead of googling for hours?" Or maybe with a sigh, you looked out into the distance and wished for a collection of presentations, practice problems, and even laboratory protocols in one place. If that's the case, then I highly recommend you take a look at DECOR, which can be accessed at ***https://decor.cst.temple.edu***.



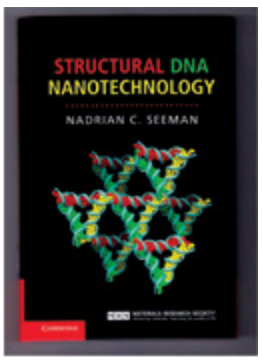
This database was launched earlier this year by Michael Zdilla of Temple U. The inspiration came from Philip Fanwick's article, "Comments on Crystallographic Education," in which he highlights the disparity between how central crystallography is to many fields, and yet how little of it makes it into the undergraduate curriculum. So, Michael set out to develop his own course, but he ran into an issue. "I had to develop almost all my own resources because I didn't really know where to look to find existing resources. By surfing the web I found some great sites, but I wished there were some central location to pool and link out to all these resources." Thus DECOR was born.

DECOR makes finding the right resource amazingly easy. As a guest, you can access the collection according to topic or the type of resource. Topics range from basics such as crystal lattices to more advanced topics such as modulated structures and quasicrystals. Types of resources mainly consist of PowerPoint presentations but also include problem sets and even a crystal growth laboratory. If you decide you would like to use some of the materials you find on DECOR, you are asked to agree to acknowledge the original authors of the resource before you can download it.

Currently, the three main contributors to the database are Michael Zdilla, Philip Fanwick and George Sheldrick. But you too can become a contributor! If you, dear reader, have a fantastic lesson that you would like to "donate" to the crystallographic community, all you need to do is contact Michael Zdilla. Now there is no need to create your own dedicated website.

So, I encourage you to go on and check out DECOR. It might save you some valuable time that you can then spend running a corn maze while drinking your pumpkin spice latte and generally enjoying the fall months to their fullest.

Anastasiya Vinokur



Book Review

Structural DNA Nanotechnology: Nadrian C. Seeman, Cambridge University Press, Cambridge, 2015, 266 pp., ISBN: 978-0521764483

Nadrian C. Seeman has been at NYU since 1988, but wrote most of the book while on sabbatical in 2011 in San Francisco. Seeman is founder of the field of DNA nanotechnology and has received a number of prestigious awards including the Feynman and Kavli Prizes in recognition of his groundbreaking work. Seeman makes a comment that he came up with the idea of making nanoscale structures with DNA in a bar in 1980, but he doesn't elaborate. I would have enjoyed the rest of that story.

The book has 14 chapters. The first four chapters cover the origin of the title topic: DNA nanotechnology. The most important statement in chapter 1 is actually in the caption of Figure 1-8: "the central concept of structural DNA nanotechnology: combining branched junctions into larger constructs." This statement captures the crux of the science Seeman describes throughout the whole book. The next two chapters cover the design of sequences to generate branched junctions and motifs by reciprocal exchange. Here a diagrammatical notation is introduced to display complex structures. This notation is further refined in chapter 4, which covers SS DNA topology starting with knots and nodes, and ending with complicated constructs.

Chapter 5 moves from the theoretical to the practical side and describes how to start building and characterizing structures, mostly through FRET and AFM, but occasionally through X-ray crystallography. Chapter 6 looks at robust motifs, essential for building DNA nanostructures. The next two chapters look at making larger structures and mechanical devices from the basic building junctions and motifs, with the latter chapter ending with a discussion on a (very cool) nanoscale bipedal walker.

Chapter 9 covers the topic of origami, things you can make through folding, and bricks, the building blocks of even larger structures. Chapter 10 picks up where chapter 8 left off and combines the concepts of structure and motion to produce a nano-assembly line. This provides a good segue into the next chapter – a discussion about self-replicating systems.

Chapter 12 covers the concept of computing with DNA. Seeman gives the example of a simple traveling salesman problem and describes how to implement basic logic functionality with DNA. Chapter 13 covers the concepts of triplex DNA, G-tetrads, the I motif and RNA constructs. The final chapter looks at how DNA constructs can be used to organize other objects.

The book uses a copious number of figures to explain the various concepts and is very well referenced.

We probably won't be seeing as many reviews from Jeanette here anymore. She has started publishing articles and reviews on a weekly basis on the NYU site ***scienceline.org***. Her review of *The Gene* by Siddhartha Mukherjee, as well an article on the Zika virus may be found there.

Joseph Ferrara

***Editor's Note**: To read more from Ned Seeman about how he came up with his groundbreaking idea in a bar in 1980, see Ned's memoir on the **ACA History** pages at **http://www.amercrystalassn.org/h-seeman**. (See also ACA RefleXions, 2014:1, 19-23.)*

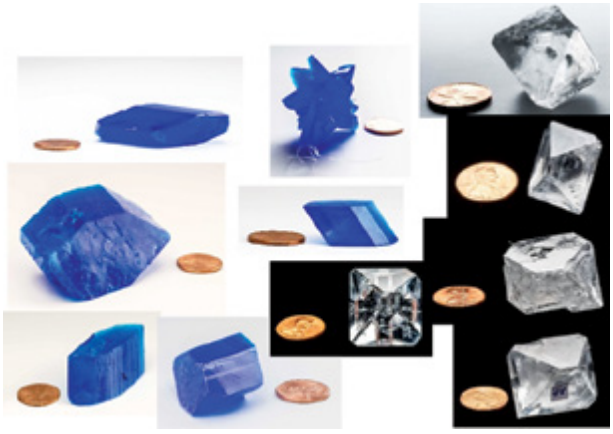
Index of Advertisers

"Sunken treasure," the top contest-inspired artwork among the high-school students. Photo by Ilia Guzei.

2016 Wisconsin Crystal Growing Contest Attracts ~650 Students

The 3rd crystal-growing competition among Wisconsin high-school students ages 15-18, middle-school students ages 11-14, and home-schooled youths was successfully conducted during March through May 2016. The contest, which perfectly aligns with the Wisconsin Idea, inspired participation of over 600 students (272 teams) and teachers from 23 high schools, 12 middle schools, and several home-schooled children from across the state. One of the participants' parents pointed out that contests that promote scientific experimental skills are rare, which makes them very important and gives non-athletes a chance to compete for school prizes.

There were two simultaneous contests, one for middle-school students and teachers, and the other for high-school students and teachers. The main goal of the contests was to grow large, well-formed crystals of two inorganic compounds: middle-school students crystallized colorless alum (potassium aluminum sulfate dodecahydrate, $KAl(SO_4)_2 \cdot 12H_2O$); high-school participants worked with blue vitriol (bluestone, copper (II) sulfate pentahydrate, $CuSO_4 \cdot 5H_2O$). The crystals were evaluated for size and quality by a learned 11-member committee comprised of chemists, crystallographers, a museum manager, and a chemistry graduate student. The crystals are currently on display in the U Wisconsin–Madison Chemistry Department.



The winning crystals of the 2016 Crystal Growing Contest. The middle-school students crystallized colorless alum, whereas high-school participants worked with bluestone. Photo by Ilia Guzei.

In addition to growing crystals, the students were motivated to learn about solution chemistry, compound solubility, purification, crystallization, and optical microscopy. In the process, the students adopted an advanced vocabulary and learned to work in teams, keep detailed records of their progress, communicate with their teammates, and follow good laboratory practices. Students also created artwork inspired by the contest and crystals. Over $1,800 in prizes was awarded to 11 winning teams comprised of 27 students.

Turn to p. 50

At the end of the contest all participants were invited to spend a day on the UW–Madison campus. The visit included guided tours of the Chemistry Department (teaching lab, research labs, X-ray diffraction facility, and glass-blowing shop), and the Geology Museum. The winners were honored at an award ceremony at the Chemistry Department that featured lectures and demonstrations by the faculty, staff and students.

The 2016 WI Crystal Growing Contest winners who were able to attend the award ceremony. Photo by Libby Dowdall.

Judges evaluate crystals and artwork submissions. Photo by Ilia Guzei.

The competition was successful on several levels: the participation has grown since last year, the overall crystal quality has improved, the number of students attending the award ceremony increased, and the number of sponsors has become larger. The latter is important because the contest is organized at no cost to the participants. Additionally, the contest has gained more publicity than in the past – this year it was covered in several on-line news releases, the *Milwaukee Journal Sentinel* and *Oshkosh Northwestern* newspapers, and a number of oral presentations at various venues. Madison Children's Museum featured a three-month long exhibit of crystals and related artwork. The Madison Gem and Mineral Club is interested in collaborating in 2017.

A crystal exhibit at the Madison Children's Museum. Photo courtesy of Madison Children's Museum.

Visitors at the Madison Children's Museum exploring models of sodium chloride and appreciating crystals. Photo courtesy of Madison Children's Museum.

Many teachers and parents wrote testimonials about their contest experiences that are available at ***http://xray.chem.wisc.edu/WICGC_2017.html***. Here is a representative example from ***Kara Klaves***, *JI Case High School, Racine, WI: "We had all of our honors Chemistry students grow crystals in teams. This is the third year we have participated in the crystal competition through UW–Madison. We have loved the experience every year. The competition is well organized and the organizers are definitely enthusiastic about their work. I was also amazed at the discussions that growing crystals stimulated. About a week after the students began growing crystals I heard them arguing about the saturation point of copper (II) sulfate and suddenly they were trying to find solubility curves to prove their point. This type of hands on learning stimulates students interest in Chemistry and they are likely not to forget their experiences."*

The 2016 WI Crystal Growing Contest was sponsored by the American Chemical Society, WI Section; American Crystallographic Association; Bruker AXS; Cambridge Crystallographic Data Centre; Covance; Crystallographic Resources, Inc.; The Evjue Foundation; Hestia Labs; Rigaku Oxford Diffraction; SigmaMillipore; UW–Madison Chemistry Department; and UW–Madison Geology Museum. The organizers are very grateful to the judges and individual contributors.

Ilia Guzei

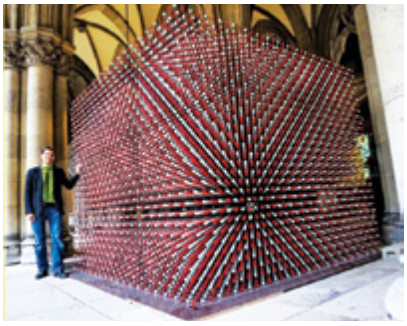
Editor's note: *One of the longest and deepest traditions surrounding the University of Wisconsin, the Wisconsin Idea signifies a general principle: that education should influence people's lives beyond the boundaries of the classroom. Synonymous with Wisconsin for more than a century, this "Idea" has become the guiding philosophy of university outreach efforts in Wisconsin and throughout the world. See:* ***http://www.wisc.edu/wisconsin-idea/***.

Daniel Rabinovich

Spotlight on Stamps – The World's Largest Crystal Structure Model

Some people spend a considerable amount of time and effort building intricate structures, from Star Wars spaceships to life-size model cars, made out of Lego bricks. A few weeks ago, a team of Lego enthusiasts at the Legoland park in Günzburg (Germany) used more than a half-million pieces to assemble a massive tower measuring more than 116 feet tall. Perhaps inspired by such constructive feats, Robert Krickl, a mineralogist, crystallographer, and science communicator living in Austria, set out early in 2014, the International Year of Crystallography, to build the largest model of a crystal structure.

Almost two years later, using 42,875 red and white balls, nearly 12 km of connecting sticks, and some 400 tubes of glue, he completed the assembly of an accurate representation of the crystal structure of sodium chloride (halite). More than 3 meters long in each dimension, the giant cube was certified by the Guinness Book of Records as the largest molecular model ever built. It was on display (see below) from late October 2015 until March 2016 in the courtyard of the Vienna City Hall, where visitors stood in awe looking at Krickl's masterpiece and also learned about crystals and the science of crystallography.



Robert Krikl standing next to his magnum opus

In addition to several public lectures and guided tours, a special Austrian postage stamp with a limited print run of 500 units was issued to celebrate the project. As illustrated below,

the stamp depicts a three-dimensional view of a portion of Krickl's oversized model, a caption in German that declares "The World's Largest Crystal Structure Model," and a specimen of crystalline salt. Whether it is the construction of a Lego sculpture or the generation of a remarkable ball-and-stick model of an ionic compound, such creative endeavors are a source of inspiration for budding scientists and an appealing medium to communicate science to the general public. Keep up the good work, Dr. Krickl!

Daniel Rabinovich

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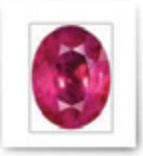

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Frank Fronczek

Puzzle Corner

Crystal Connections #8

What do the answers to these clues have in common?

1) "Small," *auf Deutsch*

2) Detective agency, founded 1850

3) Wetland lacking trees

4) _____ Turks, Ottoman Empire, 1908

5) "Zapatero"," *en Inglés*

6) Washington _____, John Philip Souza march

7) Structural material composed mostly of cellulose, hemicellulose and lignin

Previous Crystal Connections (#7) – They were all crystallographers known for something else:

1) Invented kindergarten – ***Friedrich Froebel*** (Bart Kahr gave a fascinating talk on Froebel at the 2005 Orlando ACA meeting and wrote "Crystal Engineering in Kindergarten," *Cryst. Growth & Design*, **4**, 3-9 (2004), an extremely entertaining and informative read.)

2) British Prime Minister – ***Margaret Thatcher*** (The Iron Lady studied crystallography under Dorothy Hodgkin and wrote her dissertation on the structure of gramicidin.)

3) Nobel Peace Prize winner – ***Linus Pauling*** (in 1962; also Nobel Prize in chemistry, 1954)

4) Discovered radio waves from the sun – ***James Stanley Hey*** (Master's degree in crystallography, U Manchester, 1930. Discovered solar radio interference while operating radar during WW-II.)

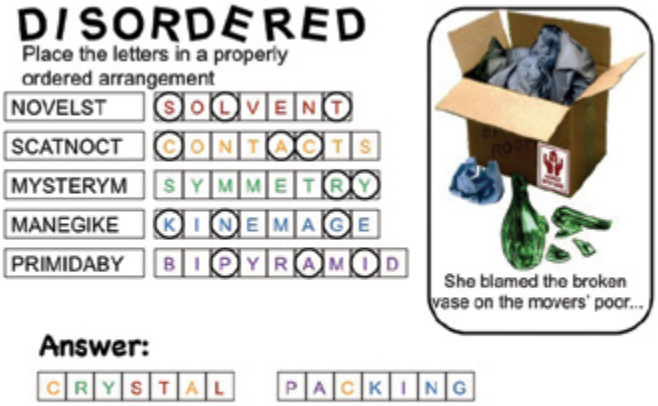
5) Communist who mapped the D-Day landing beaches of Normandy – ***John D. Bernal*** ("Sage" Bernal was instrumental in preparations for Operation Overlord, including suggesting the advantages of an artificial harbor at Normandy. He landed there on D-Day+1. Bernal was a member of the Communist Party of Great Britain.)

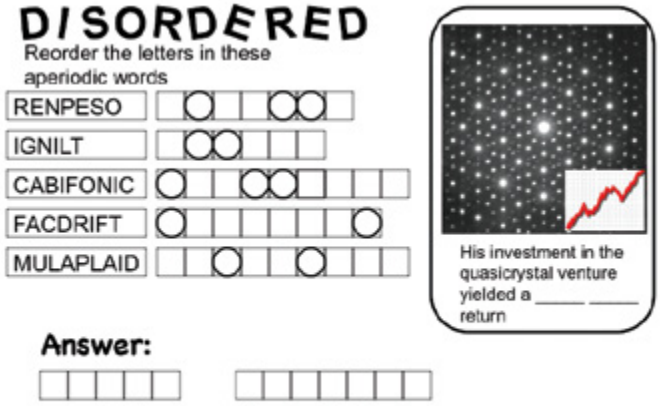
The first to provide the correct solution was **Greg McCandless** (U Texas Dallas).

Ilia Guzei (U Wisconsin–Madison) was the first to send the DISORDERED puzzle solution.

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

Frank Fronczek
ffroncz@lsu.edu





Michael James, at left, with Marcia Colquhoun. Photo by Peter Müller.

Gerard Bricogne, at left foreground, with Martha Teeter. George Sheldrick and George Phillips are visible in the background. Photo by Peter Müller.

ACA NEW ORLEANS

Friday, May 26 - Tuesday, May 30, 2017

Hyatt Regency New Orleans

Travel Grant Application Deadline: February 15, 2017
Abstract Deadline: February 15, 2017
Early Registration Deadline: March 31, 2017
Hotel Reservation Deadline: May 1, 2017

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

www.amercrystalassn.org

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

Program Chair - Yulia Sevryugina
y.sevryugina@tcu.edu

Program Chair - Ilia Guzei
iguzei@chem.wisc.edu

Posters Chair - Bruce Noll
bruce.noll@gmail.com

EDUCATIONAL SESSIONS & YSSIG EVENTS

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Career Development Session
Undergraduate Research Symposium
Engaging Undergraduates with Crystallographic Research
Communicating Science to the Public
Diversity & Inclusion Session
Practicum on Macromolecular Crystallography
Standard Practices in Crystallography
How Do I Get My Data?

ACA AWARDS

Patterson Award honoring Zbigniew Dauter
David Rognlie Award honoring Helen Berman
Elizabeth Wood Science Writing Award honoring James O'Brien
Margaret C. Etter Early Career Award honoring Christine Dunham

SESSIONS

Transactions Symposium – Cryo Electron Microscopy
NMR Crystallography
Integrative Approaches to Structural Biology
Advanced Surface and Interface Scattering & Applications
In situ and Operando Methods
Crystal Structure and Property Prediction
Home-Built Software
Crystal Growth
Mineralogical Crystallography

Transactions Symposium – Cryo Electron Microscopy

Organizer: Stephen Burley (Rutgers University Center for Integrative Proteomics Research; *sburley@proteomics.rutgers.edu*)

The theme of this year's ***Transactions Symposium*** is Cryo Electron Microscopy. Both the symposium and a new session this year on NMR crystallography are dedicated to covering topics of importance to scientists with a wide range of professional backgrounds and designed to emphasize our need for collaboration and cooperation.

Meeting participants working in protein crystallography and practitioners of cryo electron microscopy, tomography, and diffraction will have the opportunity to learn first-hand from internationally recognized experts contributing to the "Resolution Revolution." Recent advances in direct electron detection, automated cryogenic sample handling, phase plate technologies, and correlative cryo fluorescent light/electron microscopy hold considerable promise for protein crystallographers intent on studying larger, more complex, and often heterogeneous (conformational and compositional) assemblies of biological macromolecules that resist crystallization. At the close of the symposium, invited speakers will be asked to contribute to a round table discussion of the important roles that current and would-be cryo-EM/ET/ED practitioners can play in the future of the ACA.

General Meeting Information

Obtaining a VISA: Advanced planning by foreign travelers is critical. We recommend all foreign travelers consider the following when making plans to travel to the U.S.: ***Identify whether a VISA is needed. For those travelers who will require a VISA, applications should be made at least 90 days in advance of the travel date. For further information contact: the U.S. Department of State (http://travel.state.gov/content/visas/en.html) or the International Visitors Office – IVO (http://sites.nationalacademies.org/PGA/biso/visas/index.htm).*** To request a letter of participation from ACA contact the Meeting Registrar at *aca@hwi.buffalo.edu*.

Staying Green: All attendees will receive a hardcopy of the ***Program Book***, but the full set of abstracts will only be available online. We are not planning to have a meeting bag, so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Information: All scientific sessions, workshops, exhibit show, posters and sleeping rooms will be at the Hyatt Regency New Orleans. ***FREE in-room internet*** is included in the sleeping rooms at the Hyatt, so bring your laptops and stay connected to home and office. We are able to offer discounted room rates due to a commitment to contract for a minimum number of sleeping rooms at this hotel. If we do not fill these blocks, financial penalties will be incurred. This ultimately impacts the health of the ACA. Staying at the conference hotel also helps keep future registration fees lower.

A special room rate has been negotiated for students and postdocs. Room sharing can make these rates even more reasonable – use the e-mail ***Room Sharing*** feature under accommodations on the meeting web site at *www.amercrystalassn.org/2017-accommodations*.

Financial Support: Travel support will be available for young scientists. Applications for travel support should be made by February 15, 2017. For additional information see *www.amercrystalassn.org/2017-young-scientists*.

The meeting will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to factors such as ethnic origin, religion, citizenship, language, political stance, gender, or age, in accordance with the statutes of the International Union of Crystallography.

Meeting logo designed by Kandis Elliot

FEBRUARY 2017

11-15 **Biophysical Society. 61st Annual Meeting**. New Orleans, LA
www.biophysics.org/Meetings/AnnualMeeting

APRIL 2017

10-13 **BCA Spring Meeting**. Lancaster University, U.K.
www.bcaspringmeetings.org.uk/home

17-21 **MRS Spring Meeting & Exhibit**. Phoenix, AZ
www.mrs.org/spring2017

MAY 2017

26-30 **ACA 2017 Annual Meeting**. New Orleans, LA
www.AmerCrystalAssn.org

JUNE 2017

2-11 **50th Erice Course: Integrative Structural Biology**. Erice, Italy
www.crystalerice.org/2017/

JULY 2017

24-28 **Borate & Phosphate 2017.** St. Anne's College, Oxford, U.K.
www.borate-phosphate.sgt.org

AUGUST 2017

20-25 **XXVI International Materials Research Congress**. Cancun, Mexico
http://www.mrs.org/imrc-2017

21-28 **24th Congress and General Assembly of the IUCr**. Hyderabad, India
www.iucr2017.org

JULY 2018

20-24 **ACA 2018 Annual Meeting**. Toronto, ON, Canada
www.AmerCrystalAssn.org

JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
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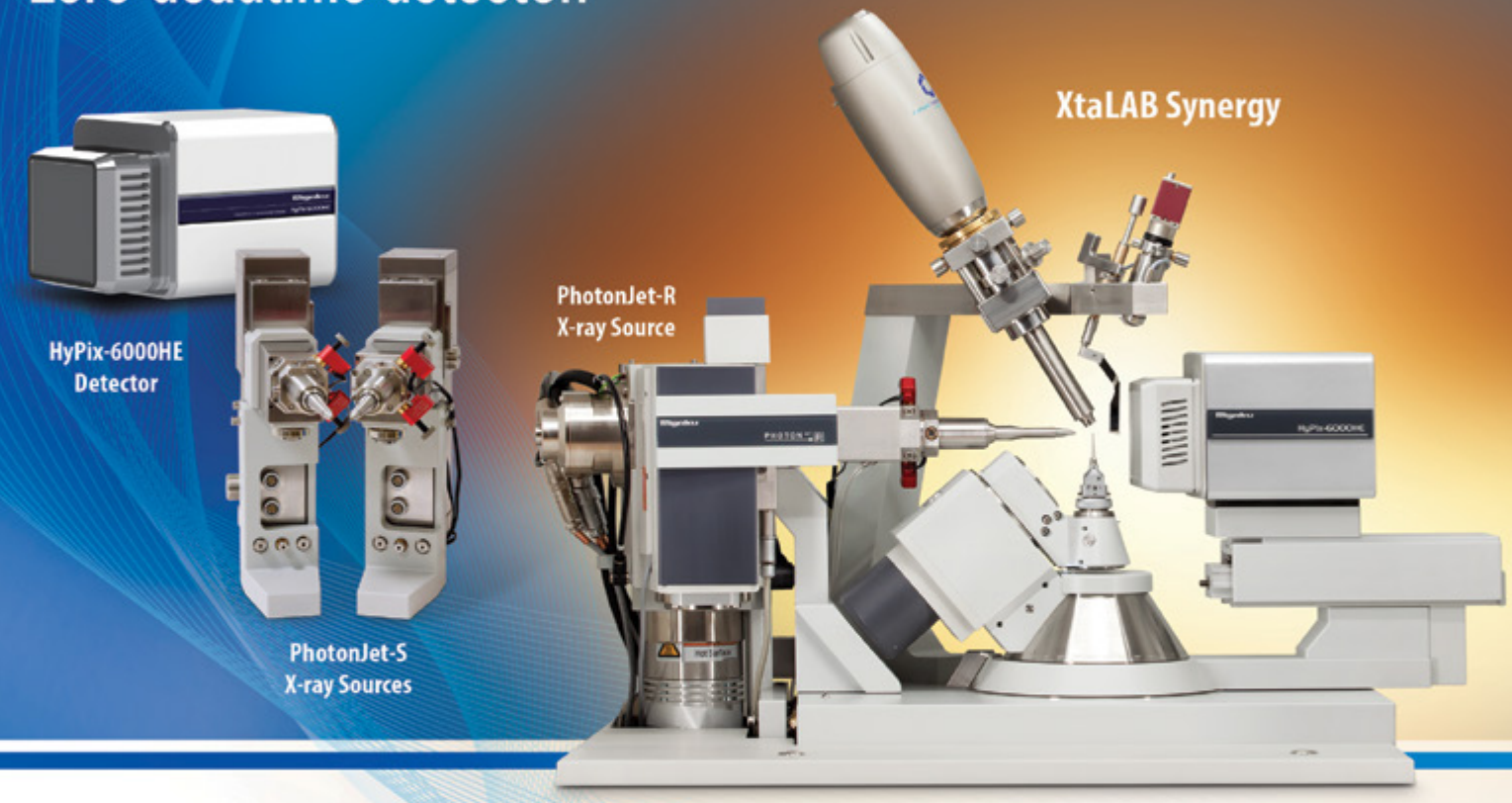

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