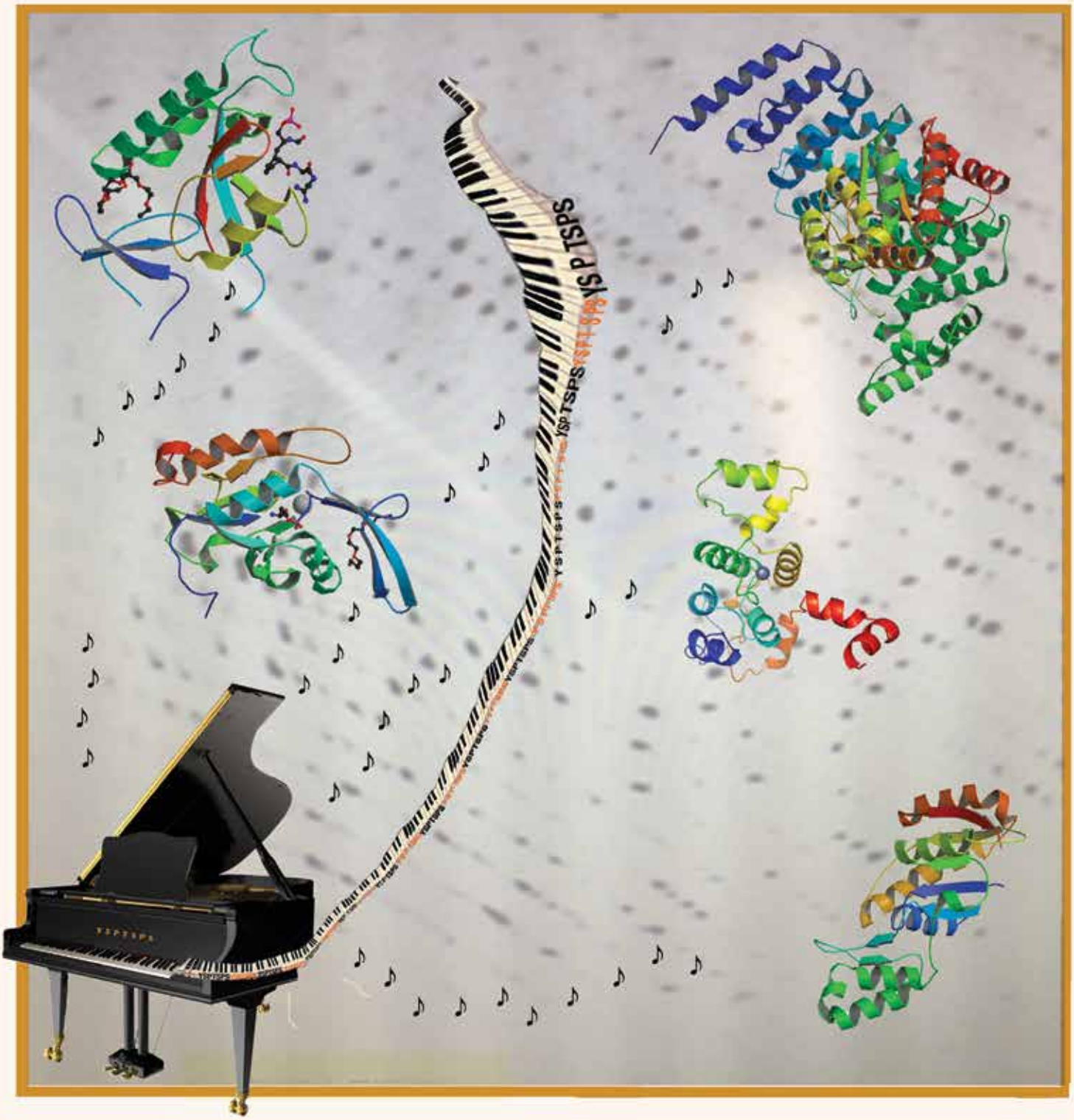
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 3

Fall 2015



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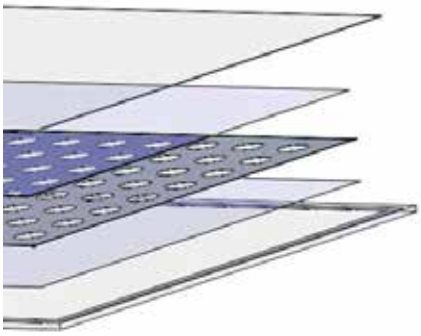

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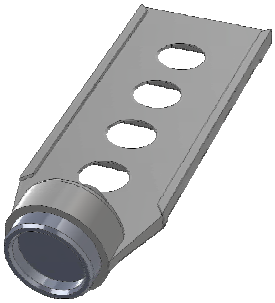

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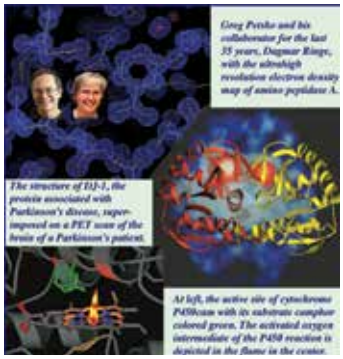

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Chris Cahill

President's Column

Greetings from Washington, DC! Summer is waning, and the city is filling back up with all those who fled the heat and took advantage of government breaks. If you are like me, your head might still be spinning from the outstanding Philadelphia meeting. What a terrific event; I cannot be more proud of the ACA at present. As always a huge Thank You goes out to the Buffalo staff and also to you, the Members, who make these meetings possible. This issue of *RefleXions* will of course be full of session and general meeting highlights and summaries, and I encourage you to give them a solid read. That said I do want to call out a few items of particular note. The first is that we had some great press coverage this year through AIP Media Services. Articles got picked up in newspapers around the world and in several languages. See the ACA webpage for a complete listing. Moreover, Twitter was lit up like I have never seen before – which actually was not too hard for me as I only just got an account!

Other items to note from Philadelphia are the Business Meeting and the First Annual Fellows and Past Presidents Reception. I think you will agree that the Business Meeting was particularly productive this year, at least for me, as we were able to place some collective concerns about the meeting structure and site selection into a greater, more comprehensive context. Without going back over too many details I believe we had a positive exchange resulting in some members of the vendor community volunteering to serve on the site-selection committee, along with an action item for Buffalo to distribute the site requirements. In this way Members can be a bit more aware of the infrastructural needs and footprint of an annual meeting. As such, I encourage everyone to put their thinking caps on and give some thought to potential locations beyond our usual spots. If nothing else, please give the siting document a read if only to gain some perspective as to the complexity of the process. Meetings are set for 2016 (Denver), 2017 (New Orleans) and 2018 (Toronto). Let's look to 2019 as the year to perhaps break the mold on location and/or type of venue. That means we need to get to work now as meeting locations are typically arranged three years in advance.

The ACA Fellows and Past President's Reception was a tremendous success on many fronts. The background to this event is that Council wished to engage some of the more senior members of the ACA, not only to recognize their contributions but also to pick their brains in the context of the Strategic Planning efforts. None of us on Council knew quite what to expect, but what transpired was a wonderfully productive discussion regarding areas of critical need and opportunity for the ACA. Approximately 20 participants split into groups and simultaneously identified two key focus areas for the ACA: relevance, and our ability to communicate the importance of science (not just crystallography) to a broader audience. What made this so timely is that it helped to crystallize (pun intended) an implicit acknowledgement of these needs by a range of our Members. The Philadelphia program was rich with 'Communicating Your Science' and career workshops, yet I believe we have a new 'call to arms' specifically in the area of communications. The SIGs and your Program Chairs for 2016 have been informed and engaged on this matter, and I think we can look forward to some significant emphasis on this in Denver.

Looking beyond the context of the meeting, communication naturally needs to be a year-round effort. We all need to be better at this. I encourage everyone to have an 'elevator speech' at the ready that explains what it is you do and why it is important. Be thinking of a range of target audiences, from your mom to a Senator to a non-scientific colleague. My personal hope is that ACA, with the help of other organizations that have more experience in this arena, can provide a forum for training in this capacity.

I would like to close with a glimpse at a big-ticket item on Council's plate, and one for which we could of course use your help. As many of you know, our two primary revenue streams are membership dues and income derived from the Annual Meetings. With declines in the former and increasing costs for the latter, we need to diversify our revenue streams and decrease our dependency on these core areas. I have much more to say on this topic, yet at this point I would like to leave it as an acknowledgement by Council that we need to generate additional income and that we are considering a number of options. Your thoughts will be welcome! Stay tuned for the next *President's Column* for more details.

Thanks again for a great meeting and best wishes for the remainder of 2015!

Chris Cahill

Michael James

News from Canada

In this issue of *RefleXions* the Canadian contribution will cover the biographies of two crystallographers. As with the last time we tried this there will be one from the East (Central) and one from the West. In addition, Jim Britten has written a short review of the CCCW15 workshop that was held in Ottawa this year.

It is a pleasure to introduce to the readership of *RefleXions* two mid-career crystallographers, one from McGill University in Montreal (Albert Berghuis) and one from the University of Alberta in Edmonton (Mark Glover). Both of these gentlemen run active and productive research programs in structural biology, and both hold Tier 1 Canada Research Chairs in Structural Biology.

Albert Berghuis

Albert Berghuis began his research career at the University of Groningen, the Netherlands. He received an M.Sc. in Chemistry under the tutelage of Wim Hol, who is now in the Department of Biochemistry at the University of Washington, U.S.A. Albert struck out to the 'New World' to complete his Ph.D. in the Biochemistry Department at the University of British Columbia, Canada, under the direction of Gary Brayer. Following the completion of his Ph.D., Albert travelled south to a postdoctoral fellowship

at the University of Texas Southwestern Medical Center with Steve Sprang.

Albert's first independent position was in the Department of Biochemistry, McMaster University in Hamilton, Ontario. It was while he was at McMaster that Albert developed his interest in combatting bacterial resistance to conventional antibiotics. In particular he concentrated on the aminoglycosides that target the 30 S ribosomal subunit and cause a misreading of the genetic code. This introduces an interruption of bacterial protein synthesis and subsequent cell death. In one of the first papers on the structures of the aminoglycoside antibiotic resistance enzymes, the Berghuis lab (Fong, D.H. and Berghuis, A.M., *EMBO Journal* **23**, 2323-2331 (2002)) showed how the aminoglycoside kinase APH(3')-IIIa is able to inactivate two closely-related antibiotics kanamycin A and neomycin B. The phosphate added to the 3'OH group is common to both antibiotics, but there are major structural differences in the remainder of the two molecules. The Berghuis group's work explained the extensive substrate promiscuity of these aminoglycoside antibiotic-resistance enzymes.

In a very illuminating review article, the Berghuis lab members (Shi, *et al*., *Front. Cell. and Infect. Microbiol*. **3**, 1-17 (2013)) discuss the prospects for combatting aminoglycoside kinase mediated bacterial resistance. The article discusses the history of the aminoglycosides and the details of the several mechanisms that bacteria use to circumvent the effects of the antibiotics. The most common method that bacteria use to resist the effects of the aminoglycosides is by covalent modification of the antibiotic using a variety of modifying enzymes. This review focusses on the aminoglycoside kinases (APH), a phosphotransferase that transfers the γ–phosphate from ATP (or GTP) to the 3' hydroxyl group on the aminoglycoside substrate. The large number of solved structures of APH enzymes has revealed a common architecture that resembles the eukaryotic protein kinase (ePK) enzyme family. In addition to the residues from the enzyme, there are 2 magnesium ions required for the transfer of the phosphate to the antibiotic substrate. The article clearly presents the structural details of the nucleoside-binding and triphosphate-binding pockets in the N-terminal lobe of the enzyme. The C-terminal lobe houses the catalytic site with the residues involved in the phosphate transfer and the substrate (aminoglycoside) binding pocket (Fig. A at left adapted from Fig. 2 in Shi *et al*.). In spite of a pessimistic outlook for the development of a pan APH inhibitor, there are excellent prospects for developing an inhibitor of those APHs belonging to the same subfamily. Efforts are underway to make use of the extensive structural data that have been amassed for the APH enzymes.

Fig. A: The structure of an APH enzyme. The nucleoside and triphosphate binding sites are in blue and yellow. The catalytic site is in green, and the antibiotic binding site is in purple.

Mark Glover

Mark Glover received his B.Sc. degree in Biochemistry and Chemistry from Dalhousie University. He moved on to the 'big city' of Toronto for his Ph.D. degree where he was co-supervised by David Pulleyblank and Jack Greenblatt in the Department of Biochemistry at the University of Toronto. A postdoctoral fellowship in Steve Harrison's laboratory at Harvard University cemented Mark's continuing interest in the structure of DNA and in the various proteins that recognize and bind to DNA. While he was in Harrison's lab, Mark determined the structures of the bZIP family of transcription factors Fos and Jun bound to DNA. Mark's first appointment as an independent research scientist was in the Biochemistry Department at the University of Alberta. Subsequently he has risen through the ranks to full Professor at the University of Alberta and holds a Tier 1 Canada Research Chair in Structural Molecular Biology.

The C-terminal repeats (BRCT) of the breast cancer protein coded by the gene BRCA1 have figured prominently in Mark's research program. BRCA1 is a tumor suppressor, and the BRCT domains are essential for the repair of double-strand breaks in DNA and in homologous recombination. These domains interact with phosphorylated target proteins containing the sequence phospho-Ser-X-X-Phe. The crystallographic study of the BRCT dimer (repeats of ~ 100 amino acids in length) has shown that the repeats pack in a 'head to tail' fashion (Williams, R.S. *et al*., *Nature Struct. Mol. Biol*. **11**, 519-525 (2004)). This association of the domains creates a hydrophilic binding pocket with a lysine residue to balance the charge of the phosphoserine. There is also a hydrophobic pocket at the interface of the domains, which is the binding site for the phenylalanine side chain of the phosphoserine peptide that was used for the crystallographic study. There have been a number of variants of the BRCT repeats from BRCA1 that have been associated with enhanced risks of cancer. These variants have diminished phospho-peptide binding as determined by this structural and biochemical study.

In a collaboration with Laura Frost and her lab in the Biological Sciences Department at the University of Alberta, Mark and his colleagues have done an elegant study of the cooperative DNA recognition by the plasmid conjugational factor, TraM (Wong, J.J. *et al*., *Nucl. Acids Res*. **39**, 6775-6788 (2011)). Bacterial conjugation involves the transfer of ss-DNA from a donor to a recipient bacterium, where the proteins involved in this transfer are produced by the plasmid encoded tra operon. TraM is one of the essential proteins for the conjugative transfer of F and F-like plasmids. It is this process that allows bacteria to rapidly spread virulence and antibiotic resistance factors among human pathogens (i.e., among MRSA strains). TraM forms a tetramer, and the N-terminal domains of each monomer interact with the DNA via a ribbon-helix-helix (RHH) domain. The DNA in the complex used for the structure determination was the sbmA site from the origin of transfer region (oriT) in the F plasmid. The crystal structure of the TraM-sbmA complex from the plasmid pED208 was determined by the molecular replacement method from an

Fig. B: The TraM tetramer bound to the smbA region of the pED208 plasmid.

earlier structure of TraM C-terminal domain. The interaction of TraM with the DNA introduces unwinding and kinking in the DNA. The asymmetric unit of the sbmA DNA/TraM has one strand of DNA and one TraM tetramer. The biologically relevant complex is generated by a crystallographic 2-fold axis that completes the sbmA duplex DNA and two TraM tetramers (Fig. B at left). Mark's lab has recently turned its attention to the structures of ubiquitin-conjugating enzymes and their roles in nuclear DNA damage signaling and cytoplasmic NF-κB signaling. Their most recent study involves the structure of covalent inhibitors of an E2 ubiquitin-conjugating enzyme UBC13.

CCCW15 – The 6th Canadian Chemical Crystallography Workshop, organized by Jim Britten and members of the Canadian National Committee for Crystallography, was hosted by the Department of Chemistry at the University of Ottawa from June 8-12 as a satellite of the Canadian Society for Chemistry annual meeting. The participants learned some basic crystallographic theory and procedures necessary for structure determination each morning, and they spent the afternoons working on structure refinements with the instructors. The main focus of the meeting was the use of Olex2 and Shelx for the solution and refinement of small-molecule and solid-state structures. Methods to handle disorder and twinning were on the top of everyone's to-do list. We also heard some terrific talks on high-pressure crystallography (Serge Desgreniers) and the integration of crystallography into an extensive chemistry research project (Jaclyn Brusso). Paul Boyle's popular crystal-growing presentation generated a lot of interest. Hilary Jenkins instilled an appreciation – not a fear – of checkcif in the minds of the students.

CCCW15, L to R: Jim Britten, Pavan Mandapati, Naser Rahimi, Sara Dickens, Ilia Korbokov (Local Chair), Chuck Campana, Hubert Bilan, Miriam Gillett-Kunnath, Nathan Yutronkie, Gabriel Brunet, Hilary Jenkins, Jaclyn Brusso, Katie Harrimen, Paul Boyle, Amélie Pialat, Serge Desgreniers.

The number of people registering for the workshop was a bit lower than usual; however, the participants benefitted from the extra one-on-one time available. Pavan Mandapati from the University of Manitoba appreciated the skill and confidence he gained at the meeting. Miriam Gillett-Kunnath completely redefined her approach to learning, teaching, and applying crystallography and was excited to bring her newfound knowledge back to the students at Syracuse University. The Bruker Pub night was, of course, the greatest social event in Ottawa for that week!

We can now announce that Jason Masuda and Kathy Robertson will be hosting CCCW16 at St. Mary's University in beautiful Halifax, NS from May 31-June 4, 2016.

Michael James and Jim Britten

Editor's Note: Michael James is currently Canadian Representative on the ACA Council. Jim Britten has formerly served in that capacity.

From the Editor's Desk

Errata: Frances Bernstein has called our attention to an error on p. 48 of the summer issue of *RefleXions*, where we misspelled Åke Kvick's name. Our apologies to Åke! Also in the summer issue, on p. 26, in the box on *Candidates for ACA Offices in 2016*, Joe Ferrara noticed that we interchanged the candidates' names for the Continuing Education and Data Standards & Computing Committees. This box should read: *Data, Standards & Computing*: Joe Ferrara & Allen Orville; *Continuing Education*: Danielle Gray & Mark Whitener. Also in this box, Paul Davie should not have been listed as a candidate for office in 2016. Paul's appointment to replace Tom Terwilliger on the *Continuing Education* committee will extend through the end of next year.

This issue features reports from the ACA's Annual Meeting in Philadelphia, held in late July. Connie Rajnak has put together the cover and **What's on the Cover** (see p. 7) featuring our 2015 Etter Early Career Award winner, Jessie Zhang, as well as the photo collages on pp. 14-15 and p. 51. Special thanks go out to Dick Bromund for providing us with his fabulous photos!

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, along with our student volunteers responsible for the session group photos and coordinated by Marty Donakowski with assistance from Kristina Vitale.

Our open-access journal, *Structural Dynamics*, published jointly by ACA with AIP Publishing, continues to grow and thrive. For additional information on *Structural Dynamics*, see the facing pp. 5-6. I encourage you to have a look at some of the outstanding papers appearing in the journal for yourself.

This issue of *RefleXions* has all our regular features including Daniel Rabinovich's **Spotlight on Stamps** column, new this year (see p. 56). This issue is quite full and so we've decided to hold the workshop reports from Philadelphia for our winter issue, along with those from our travel award winners. Stay tuned!

Tom Koetzle

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The linac coherent light source single particle imaging road map
A. Aquila, A. Barty, C. Bostedt, S. Boutet, G. Carini, *et al.*
Struct. Dyn. 2, 041701 (2015)
DOI: 10.1063/1.4918726

Perspectives for imaging single protein molecules with the present design of the European XFEL
Kartik Ayyer, Gianluca Geloni, Vitali Kocharyan, Evgeni Saldin, Svitozar Serkez, *et al.*
Struct. Dyn. 2, 041702 (2015)
DOI: 10.1063/1.4919301

Electronic damage in S atoms in a native protein crystal induced by an intense X-ray free-electron laser pulse
L. Galli, S.-K. Son, M. Klinge, S. Bajt, A. Barty, *et al*
Struct. Dyn. 2, 041703 (2015)
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Radiation damage in a micron-sized protein crystal studied via reciprocal space mapping and Bragg coherent diffractive imaging
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Struct. Dyn. 2, 041704 (2015)
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Improvements in serial femtosecond crystallography of photosystem II by optimizing crystal uniformity using microseeding procedures
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Possibilities for serial femtosecond crystallography sample delivery at future light sources[a)]
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Struct. Dyn. 2, 041709 (2015)
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Struct. Dyn. 2, 041716 (2015)
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Struct. Dyn. 2, 041717 (2015)
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Struct. Dyn. 2, 041718 (2015)
DOI: 10.1063/1.4922774

Microfluidic sorting of protein nanocrystals by size for XFEL diffraction
Bahige G. Abdallah, Nadia A. Zatsepin, Shatabdi Roy-Chowdhury, Jesse Coe, Chelsie E. Conrad, *et al.*
Struct. Dyn. 2, 041719 (2015)
DOI: 10.1063/1.4928688

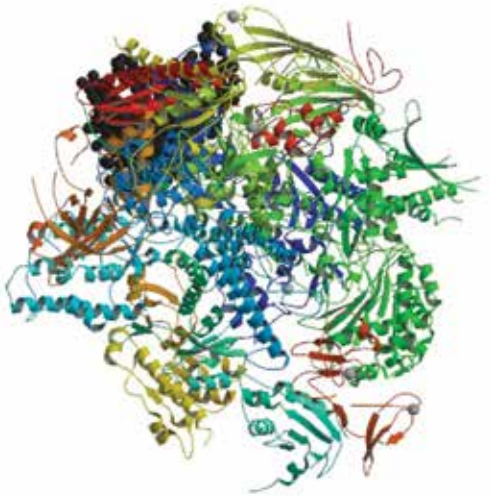
Serial femtosecond X-ray diffraction of enveloped virus microcrystals
Robert M. Lawrence, Chelsie E. Conrad, Nadia A Zatspin, Thomas D. Grant, *et al.*
Struct. Dyn. 2, 041720 (2015)
DOI: 10.1063/1.4929410

Yan (Jessie) Zhang, Assistant Professor of Biochemistry, Department of Molecular Biosciences, University of Texas, Austin, is the **2015 Etter Early Career Award** winner. The citation stated *'Jessie Zhang's research on transcriptional regulation could lead to a novel approach to cure neurodegenerative diseases such as Alzheimer's. Her studies focus on the pivotal role that the C-terminal domain of RNA polymerase II (CTD) plays in temporal control of transcription regulation in eukaryotes. Using X-ray crystallography and complexes with regulatory proteins, Dr. Zhang established that two CTD phosphatases (Scps and Ssu72) can result in dramatically different transcriptional fates by combinatorial reading of the post-translational modifications on CTD. Her lab has identified the first highly selective inhibitor for a serine/threonine phosphatase, Scp, which is now being optimized for neuron regeneration.'*

The conformational states of the CTD of RNA polymerase II, termed the CTD code, represent a critical regulatory check point for transcription.[1,2] As the template for all transcription factors to be recruited to transcription, CTD is totally missing (because of high flexibility) from the beautiful structure of wild-type RNA Polymerase II (below, right) solved by David Bushnell and Roger Kornberg (Stanford University)[3]. The CTD, found only in eukaryotes, consists of 26–52 tandem heptapeptide repeats with the consensus sequence, $Tyr_1Ser_2Pro_3Thr_4Ser_5Pro_6Ser_7$. It was Jessie's idea that these 7 repeating residues, YSPTSPS, correspond nicely to the musical notes Do-Re-Mi-Fa-So-La-Ti that in the key of C major are all the white keys in an octave. Her concept for the cover involved a piano in the corner; a keyboard that would overflow from the piano keyboard, labeled with the YSPTSPS repeating sequence, and all five of the structures solved in her lab that relate to CTD research floating as though they emanated from the piano.

The structures are (clockwise from the piano and listed by their PDB IDs): 3L0B;[4] 3TCZ;[5] 4IMJ;[6] 5C2Y;[7] 3OMW.[8,9]

By studying the biological molecules that regulate the post-translational modification states of CTD, Jessie and the members of her lab focus on how phosphorylation of CTD is regulated; how this phosphorylation affects the outcome of transcription, and how these processes are involved in important biological phenomena like neurogenesis. They aim to exploit the results from this research in the design of small-molecule effectors that can intervene in the CTD processes and thereby function as regulators of gene expression. Eventually, such compounds may lead to drugs that promote neuron regeneration to improve the life quality of patients with neurodegenerative diseases such as Alzheimer's disease and ALS.



Biological Assembly Image for 1N1K, Wild Type RNA Polymerase II, at 4.1 Å resolution, solved by the Kornberg Lab, Stanford University.

Protein chains are colored from the N-terminal to the C-terminal using a rainbow (spectral) color gradient.

1. Dahmus, ME (1996), Reversible phosphorylation of the C-terminal domain of RNA polymerase II, J Biol Chem, 271, pp 19009–12.

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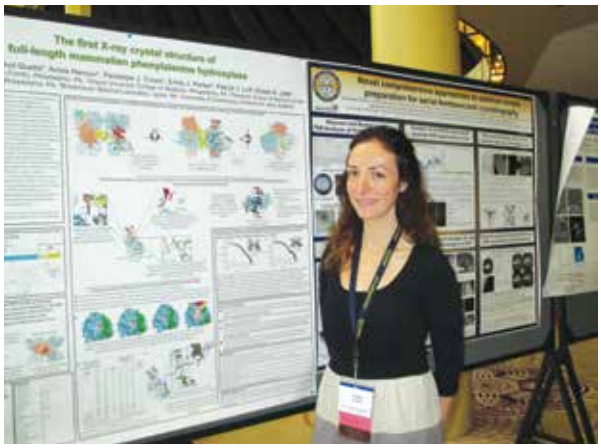
Pauling Poster Prizes

The **Pauling Poster Prizes**, established in honor of Linus Pauling, are given to the best *graduate or undergraduate* posters presented at the annual meeting of the American Crystallographic Association. Seven Pauling Prizes can be awarded at each meeting: three **ACA Pauling Poster Prizes** honoring Linus Pauling's contributions to science and U.S. crystallography; the **Herman R. Branson Pauling Poster Prize** honoring one of the first African American physicists to make crystallography the focus of his research; the **Muttaiya Sundaralingam Pauling Poster Prize** honoring Sundaralingam's ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids; the **Louis Delbaere Pauling Poster Prize** honoring Delbaere's contributions to science and Canadian crystallography, given to the best graduate or undergraduate poster from a Canadian laboratory; and the **IUCr Pauling Poster Prize** recognizing IUCr's support of graduate and undergraduate training in crystallography.

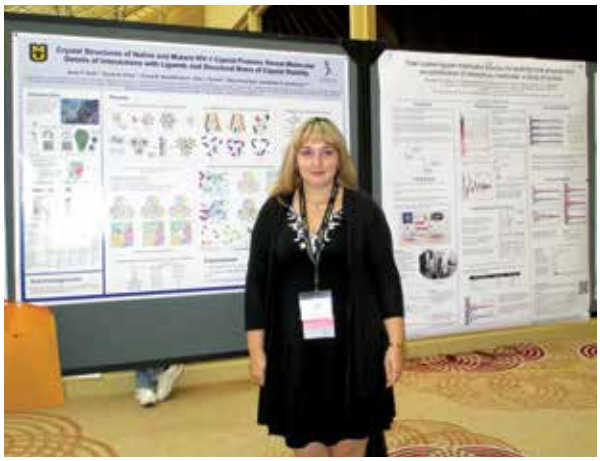
At Philadelphia, 43 graduate and undergraduate posters were evaluated for the Pauling Poster Prize by a panel of eight judges. Students were judged both on the work presented on their posters and on their general knowledge of the subject and crystallography. The posters and their presenters were all found to be excellent, making the task of determining the best posters very difficult. Below are the seven winners of the 2015 Pauling Poster Prize.

Emilia Arturo, Fox Chase Cancer Center/Drexel University (poster **S51**: *The First X-ray Crystal Structure of Full-Length Mammalian Phenylalanine Hydroxylase*) received an **ACA Pauling Poster Prize** for her work in the preparation, crystallization, and 2.0Å structure determination of the first full-length mammalian phenylalanine hydroxylase. This structure is important in understanding the allosteric regulation of the enzyme with potential application to common inborn errors of phenylalanine metabolism such as phenylketonuria.



Emilia Arturo

Anna Gres, University of Missouri – Columbia (poster **S13**: *Crystal Structures of Native and Mutant HIV-1 Capsid Proteins Reveal Molecular Details of Interactions with Ligands and Structural Basis of Capsid Stability*) received an **ACA Pauling Poster Prize** for her work on the HIV-1 Capsid Protein (CA), which is key to virion assembly and is a target for drug discovery. The structure of the native CA hexamer and an E45A mutant were presented together with complexes of CA with CPSF6 and the potent antiviral PF74 that prevents CPSF6 binding. The structures provide insight into the inherent structural plasticity of the capsid that modulates interactions among CA molecules, which in turn affects capsid stability.

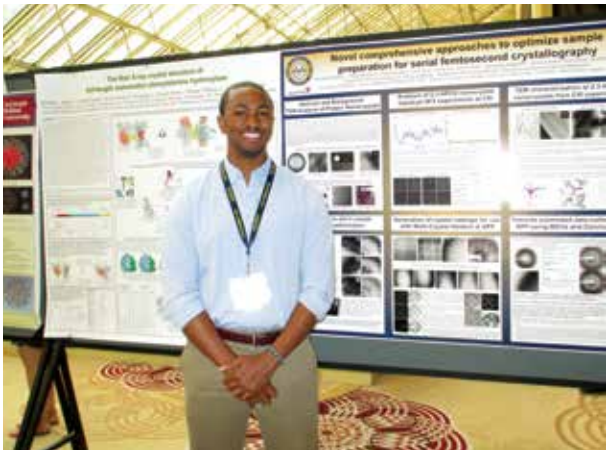


Anna Gres

Vicky Doan-Nguyen, University of Pennsylvania (Poster **S47**: *Synthesis and X-ray Characterization of Cobalt Phosphide Nanorods for Oxygen Reduction Reaction*) received an **ACA Pauling Poster Prize** for her work on cobalt phosphide (Co_2P) nanorods, a cheaper alternative to the typical platinum anode catalyst used in low-temperature fuel cells. Using a combination of experimental techniques coupled with modeling, Vicky investigated anisotropic Co_2P nanorod growth. Her results show that Co_2P nanorods are more durable than commercial Pt catalysts and give comparable performance.

Maxwell Terban, Columbia University (Poster **S57**: *Total Scattering Pair Distribution Function for Probing Local Structuring and Recrystallization of Amorphous Molecules: A study of lactose*) received the **Branson Pauling Poster Prize** for his studies on local structural correlations in amorphous lactose using the total scattering pair distribution function (TSPDF). Lactose is extensively used in food and pharmaceutical products as an excipient material in both amorphous and crystalline formulations. The studies focused on how the formulations of each type were produced. Results indicate that TSPDF can aid in making predictions on the characteristics and performance of different formulation designs.

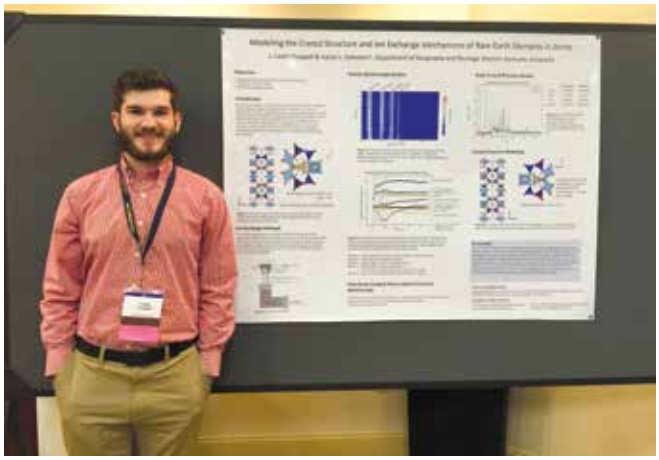
Christopher Barnes, University of Pittsburgh (shown on the following page, poster **S29**: *Novel Comprehensive Approaches to Optimize Crystal Growth and Nanocrystal Sample Preparation Using Transmission Electron Microscopy*) received the **Sundaralingam Pauling Poster Prize** for his work on using transmission electron microscopy (TEM) to characterize nanocrystals for serial femtosecond crystallography (SFX). His results demonstrate the utility of TEM analysis in predicting consistency of sample delivery and nanocrystal diffraction quality. Of note was the diamond-shaped multi-crystal holder and UV crystal imaging that he presented, which shows promise in significantly decreasing the number of crystals needed to complete a SFX dataset.



Christopher Barnes

Matthew McDougall, University of Manitoba, Canada (Poster **S52**: *The Incorporation of Polyaromatic Hydrocarbons into an S-layer Protein of the Hyperthermophilic Archaeon Staphylothermus marinus*) received the **Louis Delbaere Pauling Poster Prize** for his studies on the S-layer protein from *S. marinus*, a right-handed coiled-coil protein with potential biotech applications. Structures of both the sulfur bound complex in its native state and a complex with naphthalene were presented. The naphthalene complex is important since naphthalene is an EPA 16 priority pollutant polycyclic aromatic hydrocarbon (PAH) and the structure demonstrates the potential of the S-Layer protein for bioremediation applications.

Caleb Chappell, an undergraduate from Western Kentucky University (Poster **S25**: *Modeling the Crystal Structure and Ion Exchange Mechanisms of Rare Earth Elements into Zorite*), received the **IUCr Pauling Poster Prize** for his work on understanding the processes that direct ion diffusion and ion selectivity in zorite, a nanoporous sodium titanium silicate. The synthesis, crystal structure, and cation exchange mechanisms of sequestered yttrium were presented. Time-resolved Raman spectroscopy provided a means of following the ion exchange process *in situ*. Results show a more open nanoporous channel structure that may have applications in improved gas sensing and catalytic cracking technologies.



Caleb Chappel (photo courtesy of Krystle McLaughlin)

The following posters also received honorable mention:

Suman Pandey, Indian Institute of Technology (Poster **S39**: *Structural Basis for the Substrate Specificity of Periplasmic Glucose Binding Protein ppGBP from Pseudomonas putida CSV86*) presented the crystal structures of the apo and glucose/galactose bound forms of the periplasmic glucose binding protein from *P. putida* CSV86. The work provided the structural basis of substrate specificity that has implications for reagentless biosensor development, and the structures will also help in understanding glucose transport in *Pseudomonas* sp.

William Booth, University of South Carolina (Poster **S27**: *Nicotinamide Adenine Dinucleotide Biosynthesis in Streptococcus pyogenes*) described his work on the structural studies of the proteins NadC, NadD and NadE from *S. pyogenes*, which are involved in NAD^+ biosynthesis. The crystal structures of NadC and NadE were presented. These structures together with that of NadD will be used to develop new antibacterial compounds for the inhibition of the NAD^+ biosynthesis in Group A Strep, which annually causes over 500,000 deaths worldwide.

Fraser Ferens, University of Manitoba, Canada (Poster **S05**: *Biophysical Analysis of a Natively Folded VDAC*) reported a method for the extraction and purification of a voltage-dependent anion-selective channel (VDAC) collected from its native *Neurospora crassa* mitochondrial membrane. This approach does not require the refolding of the expressed protein common to recombinant expression. The purified protein was then characterized for its usefulness for structural studies.

We would like to express our thanks to the students and their mentors for their hard work in carrying out the research presented at the ACA.

I would also like to thank the Pauling Poster Prize judges (**Nikoletta Bathori**, **Louise Dawe**, **John Helliwell**, **Shuishu Wang**, **Victor Young**, **Katrina Forest** and **Andrew Howard**) for a job well done.

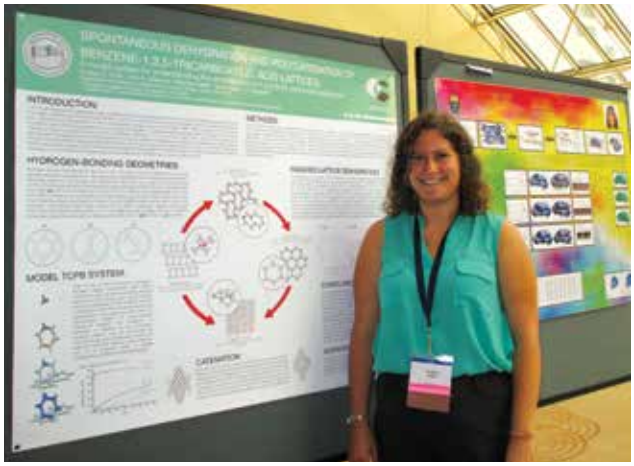
John Rose
Pauling Poster Prize Chair

CrystEngComm Poster Prize

The **CrystEngComm Poster Prize**, sponsored by the Royal Society of Chemistry, is awarded to the best *graduate or undergraduate* poster in the field of crystal engineering/supramolecular chemistry. The 2015 judges were **Kristin Kirschbaum**, **Marcus Bond**, and committee chair **Andrey Yakovenko**.

Andrea Goltz from Youngstown State University was given an RSC book voucher for her winning poster **M62**: *Spontaneous Dehydration and Polycatenation of 1,3,5-Benzenetricarboxylic Acid (H_3BTC) Lattices: A model system for understanding the crystallization of 1,3,5-tris(4-carboxyphenyl)benzene (tbdc)*. In her poster, which is displayed in the photo on the following page, Andrea described a study of the tbdc crystallization pathway via combination of TGA, single-crystal, and powder diffraction crystallography. In this study she was using H_3BTC as a model of a 3-fold rotationally symmetric acid. Four different forms of

H_3BTC were characterized by single-crystal X-ray diffraction in this work. An announcement of Andrea's award will be posted on the *CrystEngComm* website.



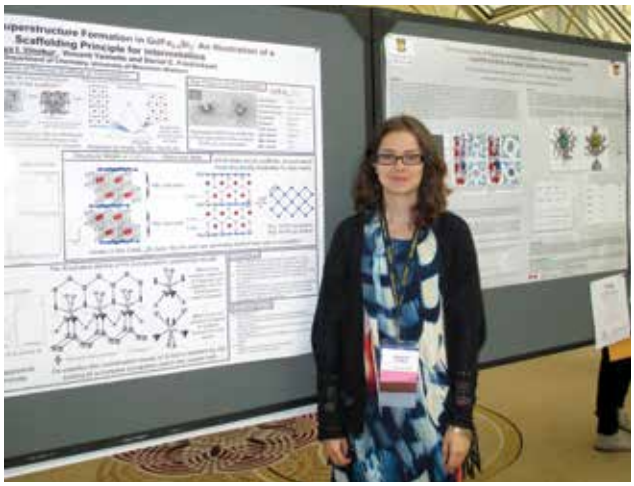
Andrea Goltz

In addition the judges would like to give an honorable mention to **Nicole Vanagas** from Georgetown University for her work presented in poster **M-63**: *Structural Chemistry of Tetravalent and Hexavalent Actinide-Furoic Acid Complexes*.

Andrey Yakovenko

Journal of Chemical Crystallography Poster Prize

The **Journal of Chemical Crystallography Poster Prize**, sponsored by Springer's *Journal of Chemical Crystallography*, is given to the best student (*graduate or undergraduate*) poster presentation in the area of chemical crystallography or small molecule structure determination and analysis. **Anastasiya Vinokur**, University of Wisconsin – Madison (poster **M03**: *Superstructure Formation in $GdFe_xSi_2$ (x~0.7): Scaffolding as a design principle in intermetallics*) is this year's winner.



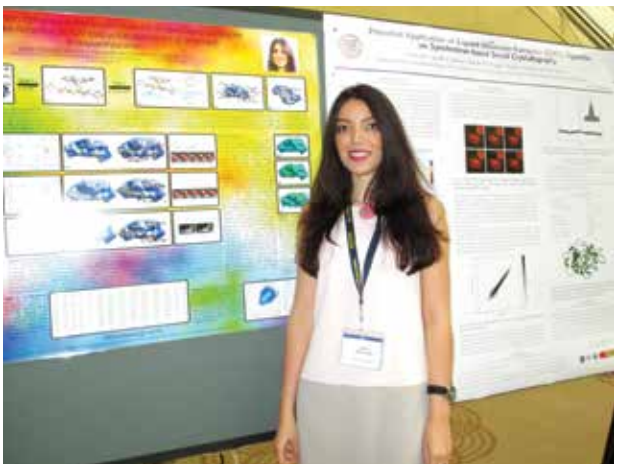
Anastasiya Vinokur

Alyssa Adcock of Georgetown University received honorable mention for her poster **M25**: *Synthesis and Characterization of a Bismuth (III)-Organic Hybrid Material*.

The judges for this year's *Journal of Chemical Crystallography* Poster Prize were **Judith Gallucci**, **David Grossie**, and committee chair **Christine Beavers**.

Structural Dynamics Poster Prize

The **Structural Dynamics Poster Prize** is sponsored by our open-access journal, *Structural Dynamics*, published jointly by ACA with AIP Publishing. The Structural Dynamics Prize is given for excellence in research on structure determination and dynamics of systems, enabled by the emerging new instruments (e.g., XFELs, high harmonic generation, electron sources, etc.) and new experimental and theoretical methodologies and is open to students (*graduate and undergraduate*) and postdocs. The winner receives a cash award of $250. This year's recipient is **Sanaz Khorisani**, University of the Witwatersrand, South Africa, for her poster **M35**: *Dynamic Reaction Pathways in the Single-Crystal-to-Single-Crystal Solid-State Diels-Alder Reaction of NN'-bis(cyclobutylimino)-1,4-dithiin with 9-Vinylanthracene*.



Sanaz Khorisani

Ti-Yen Lan, Cornell University, received honorable mention for poster **M-43**: *Potential Application of Expand-Maximize-Compress (EMC) Algorithm on Synchrotron-Based Serial Crystallography*.

The judges for this year's Structural Dynamics Poster Prize were **Edward Collins**, **Marvin Hackert**, **Yasufumi Umena**, and committee chair **Edward Snell**.

Oxford Cryosystems Low-Temperature Poster Prize

This prize, sponsored by Oxford Cryosystems, is open to all participants and is awarded to the best poster describing work in low-temperature crystallography. The 2015 judges were **Dominika Borek**, **Katrina Forest** and committee chair **Robyn Stanfield**.

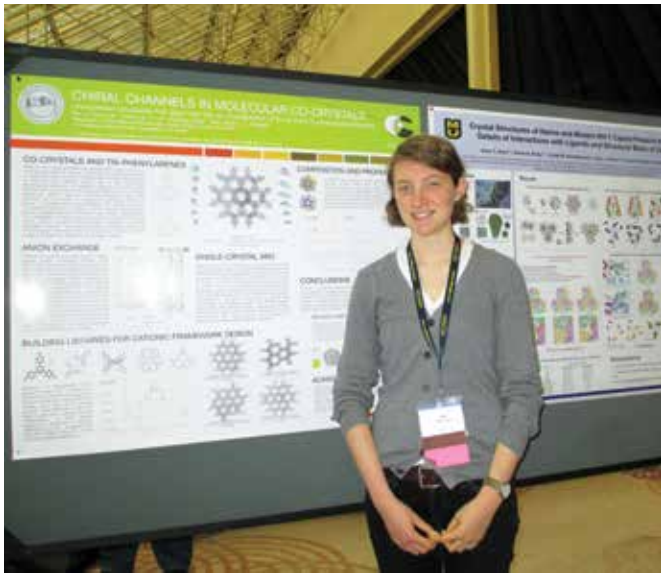
The 2015 winner was **Kristen Kirschbaum**, University of Toledo, for her poster **M29**: *The Structural Beauty of Nanoparticles. The so far Largest Crystal Structure of a Gold Nanoparticle: $Au_{133}(SC_6H_4{}^tBu)_{52}$* This beautiful crystal structure consists of a highly ordered geometric arrangement of five nested shells of gold atoms, with the single central gold atom surrounded by consecutively larger shells of 12, 42, and 52 gold atoms, and with a final outer shell of 26 gold atoms mediating staple motifs with 52 thiolate ligands. The highly ordered thiolate-Au-thiolate motifs form four helical stripes on the exterior of the spherical Au_{107} kernel.

Robyn Stanfield

MiTeGen-Society of Physics Students Undergraduate Poster Prize

The **Undergraduate Poster Prize** is co-sponsored by the Society of Physics Students (SPS) and MiTeGen, who generously donated a portion of the $250 cash prize, along with $250 in MiTeGen credit for crystallography supplies. This prize, established in 2014, recognizes the best *undergraduate* poster presentation and will be awarded annually. The 2015 judges were **Jacqueline Vitali** and **Krystle McLaughlin**.

At ***#ACAPhilly***, we awarded the Undergraduate Poster Prize for the second year. We had more than double the number of undergraduate researchers presenting posters at ACA 2015 as compared to ACA 2014! This year's winner was **Ren Wiscons** from Oberlin College for her poster **S07**: *Chiral Channels in Molecular Co-Crystals*.



Ren Wiscons

With so many great undergraduate posters, the judges also would like to give honorable mention to another poster presenter, **Caleb Chappell**, Western Kentucky University, for his poster **S-25**: *Modeling the Crystal Structure and Ion Exchange Mechanisms of Rare Earth Elements in Zorite*. (*Editor's Note*: Caleb is the recipient of this year's **IUCr Pauling Poster Prize**, see p. 9.)

We hope that the Undergraduate Poster Prize continues to inspire and encourage young undergraduate researchers in the field of crystallography to attend ACA.

Krystle McLaughlin

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 2015 were **Blaine Mooers**, **Pat Weber**, and committee chair **Barry Finzel**.

This year the prize went to **Marina Ivanova**, a 3rd year graduate student working at the Francis Crick Institute in London, U.K. While the selection committee found excellence in the science and poise of all the presenters, we were particularly impressed by the quantity and diversity of the work performed by Marina during her study of *Molecular Interactions within the Crumbs Cell Polarity Complex*, poster **S26**. She performed all the molecular biology, fluorescence polarization, and crystallographic experiments toward the structural and functional characterization of PDZ domains in protein partners that act just inside the cell membrane to polarize cells undergoing asymmetric cell division.

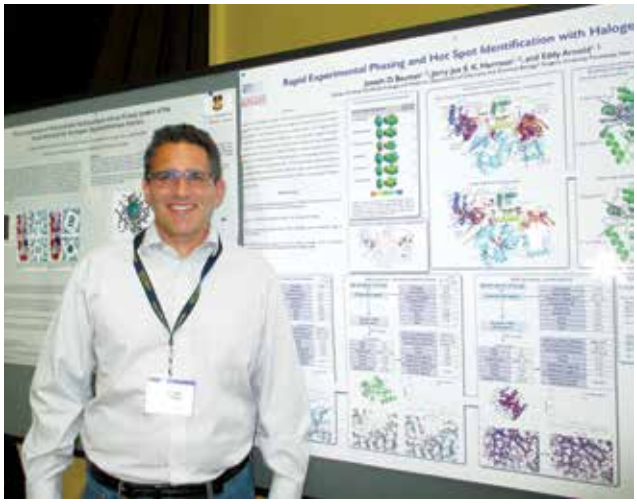
Kunhua Li, University of Florida, deserves honorable mention for his excellent progress toward solving the difficult structure of the glycosylated Y3 protein from the fungus *Coprinus comatus* (poster **S21**: *High Resolution Crystal Structures of Antiviral, Glycosylated Y3 Protein from the Fungus Coprinus comatus*.

Barry Finzel

Taylor & Francis Biomolecular Crystallography Poster Prize

The **Taylor & Francis Biomolecular Crystallography Poster Prize**, open to all participants, 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.

Joseph Bauman received the award this year for work he did in Eddy Arnold's lab at Rutgers on fragment-based screening using compounds that contain an anomalous scattering center (poster **M27**: *Rapid Experimental SAD Phasing and Hot-spot Identification with a Halogenated Fragment*). Bauman discovered that promo-pyrazole binds specifically to several sites in several proteins, suggestive of a new useful heavy-atom derivative.



Joseph Bauman

The judges for the 2015 **Taylor & Francis Prize** were **David Dranow**, **Pat Weber**, and committee chair **Elizabeth Goldsmith**.

Elizabeth Goldsmith

Editor's note: Photos of poster prize winners courtesy of Kristina Vitale except where otherwise indicated.

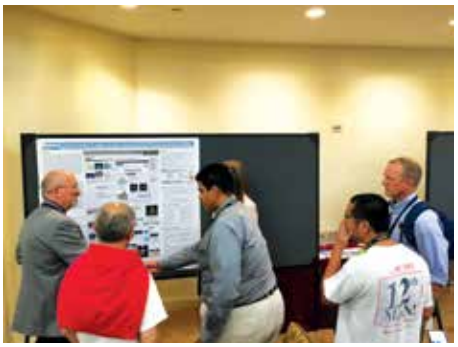
Alex Alvarado and Nicole Werpachowski with Sean Bentley

Reception and Symposium for Undergraduate Students

The second annual **Undergraduate Student Reception** was held at ACA 2015, in an ongoing collaboration with the **Society of Physics Students (SPS)**. Attendees, many of them students and mentors, were treated to lunch and a short program. Director of the SPS **Sean Bentley** provided the welcome remarks and spoke about the benefits of SPS membership. Organizer **Krystle McLaughlin** and YSSIG Chair **George Lountos** then reported on the new expanded partnership of YSSIG and SPS for next year's meeting in Denver, including a **Career Toolbox** workshop implemented by SPS. Next, ACA CEO **Bill Duax** gave a spirited talk on his very interesting life's journey in the world of crystallography. Bill's talk was filled with fun stories about research, car surfing, and being Hillary Clinton's unofficial photographer, as well as accompanying pictures from the Nobel Prize ceremony he attended and subsequent reenactments in Buffalo. Bill also tried to help students with the question, 'What to do with your life?'. Some answers: 'Make the world a better place'; 'Love what you do and do what you love'; and, 'Keep smiling'. The Q&A period started with a somersault by Bill, to the delight of everyone in attendance. The reception culminated with a mini-poster session for undergraduate researchers in attendance at ACA, allowing them to present their work in this highlighted special session.

Krystle McLaughlin

Bill Duax



Photos courtesy of Krystle McLaughlin

Contributors to this Issue

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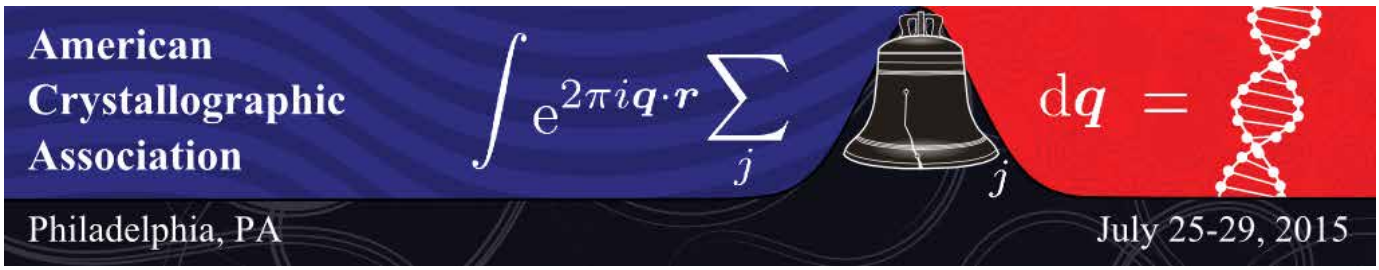


The **2015 ACA Meeting in Philadelphia** kicked off on Saturday, July 25, with workshops on **Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials**, on **Rietveld Refinement Analysis**, and on **Small Angle Scattering: Structural Biology and Soft Matter**. The **Opening Reception Exhibit Show** was held Saturday evening and 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 **B. Warren Award** for 2015 was presented to **Laurence Marks**. **Gregory Petsko** received the **M. J. Buerger Award**, and **Yan (Jessie) Zhang** received the **Margaret C. Etter Early Career Award**. Jessie's work is featured on our cover (see also **What's on the Cover** on p. 7). **Juan Manuel García-Ruiz** delivered a fascinating plenary lecture, *The Impact of Crystals and Crystallography in Art and Culture*. Juanma also treated meeting attendees to a screening of his documentary film, *The Mystery of the Giant Crystals*. The **Transactions Symposium**, *Crystallography for Sustainability*, was chaired by **Cora Lind-Kovacs** and **Robin Rogers**.

The meeting wrapped up on Wednesday evening with ACA's annual **Awards Banquet**, featuring the **Past President's Address** by **Martha Teeter**. The evening's program chaired by **ACA President**, **Chris Cahill**, included the introduction of the **2015 Class of ACA Fellows**: **Zbigniew Dauter**, **David Eisenberg**, **Hakon Hope**, **John Helliwell**, **Tom Koetzle**, and **David Rose**; and presentation of the **ACA Service Award** to **Ilia Guzei**. The ACA honored this year's **14 Poster Award Winners** along with eight students selected to receive an honorable mention from among the truly exceptional array of posters (see pp. 8-11 for news on the Poster Awards).

Louise Dawe and **Kraig Wheeler** were **Program Chairs** for the meeting; **Ilia Guzei** was **Posters Chair**; **Marty Donakowski** managed the **Session Photos** with assistance from ACA's **Kristina Vitale**; and **Richard Bromund** and **Virginia Pett**, ACA's **Videography Team**, recorded the award and plenary lectures.

Leo Straver, at left, with ACA Posters Chair Ilia Guzei relaxing at Saturday evening's Opening Reception Exhibit Show

(L-R) ACA CEO Bill Duax & Alex McPherson discussing a point in front of the Registration Desk. ACA's Marcia Colquhoun & Patti Coley are attending to business at the desk.

Plenary Lecturer Juanma García-Ruiz

ACA Vice President Tom Terwilliger, at left, with Peter Müller

Stan Rajnak, at left, with ACA RefleXions Cover Editor Connie Rajnak

View of attendees at the Opening Reception Exhibit Show, with ACA Past President Martha Teeter in the right foreground and Cora Lind-Kovacs at center

Photos on this page by Dick Bromund
Philadelphia Meeting Logo Design: Jason Mercer

Photos by Dick Bromund

Photos by Dick Bromund

P1: Warren Award

*The **B. Warren Award** for 2015 was awarded to **Laurence Marks**, Professor of Materials Science and Engineering at Northwestern University, for 'his contributions to electron crystallography and surface science, using both electron and X-ray diffraction.' The Warren Award, which was established in 1970 by students and friends of Professor Warren on the occasion of his retirement from MIT, recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques.*

It was with great pleasure that I was able to hear Laurence Marks address the ACA after receiving the Warren Award with his award lecture, *Understanding Oxide Surfaces: From structures to catalysis*, and treat us to a retrospective of many years of study of surface reconstructions for titanates. I may have been a particularly receptive audience to this talk, since my own Ph.D. studies were in surface science. However, I fled that field soon after for the greater rigorousness and conclusiveness of crystallography. In his address Marks showed how he and his students have used electron microscopy to examine a number of metal oxide surfaces and have developed techniques that allow exquisite structural descriptions of these systems.

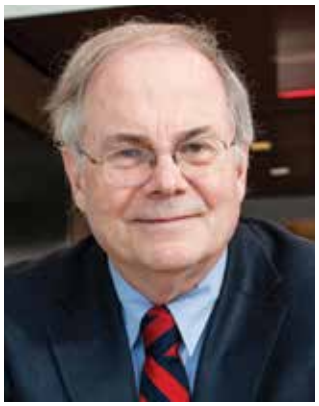
While crystallographers like to think about the structures from single crystals as if they extend to infinity, in truth everything is finite and there is always an interface. There is no reason that the atoms at a crystal-vacuum boundary will retain the same structure as the bulk. In fact, it is probably true that atomic structure at any surface will never be exactly the same as the bulk. Marks showed us how extremely complex superlattice patterns are seen, indicating that a reconstruction is occurring at the oxide surface.

One of the more challenging aspects of surface science is that a surface remains pristine only for minutes and, even then, only if ultra-high vacuum techniques are used. In the work of Marks and his group, an electron microscope and vacuum system are integrated and electron diffraction patterns are collected after surfaces are prepared and carefully annealed. Structures are solved using both direct methods and iterative techniques. Density Functional Theory computations provide a basis for understanding the energetics for different surface-reconstruction models.

Marks provided an atlas of elegant reconstructed surfaces that have been found and structurally determined for different lattice planes from a single material, $SrTiO_3$, as well as describing several order-disorder transitions. I lost track of the number of structures that were presented, but the talk showed that even a 'simple' material has a wealth of detail that is revealed when it is closely examined.

I have never regretted returning to crystallography after my graduate work, but it was a delight to see the road I did not take, in combining both fields. I think everyone in the audience left with a view of how much structural richness there is to be found at surfaces. I commend Laurence Marks for his beautiful work, an exciting talk and the contribution he has made to the structural science that delighted B.E. Warren, for whom this prize was named.

Brian Toby



P2: Buerger Award

*The **M. J. Buerger Award** for 2015 was awarded to **Gregory Petsko**, Arthur J. Mahon Professor of Neurology and Neuroscience at Weill Cornell Medical College. The Buerger Award recognizes mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA, and is awarded in memory of the late Martin J. Buerger, Institute Professor Emeritus of MIT and University Professor Emeritus of the University of Connecticut. Greg's award citation reads, 'Professor Greg Petsko has made "contributions of exceptional distinction" to the study of proteins and enzyme mechanisms by X-ray crystallography, to the application of Structural Biology to the medical sciences, to the training and education of researchers and undergraduate students, to the mentoring of a generation of Structural Biologists, and to the research community in general, through service on government and other advisory boards and committees, and through his unique communication skills to the broader scientific community as well as to the lay public.'*

Greg Petsko's Buerger Award lecture was, as all anticipated it would be, thoughtfully prepared, carefully organized, and presented with eloquence and good humor. The lecture was at times moving and inspirational as it featured the career of Tom Alber who passed away from Lou Gehrig's disease. Tom, Greg's first graduate student at MIT, later became professor at the University of California, Berkeley and, like Greg, was a renowned crystallographic presence in his own right. Not incidentally, I suspect, Greg now directs an institute dedicated to the elucidation and potential treatment of the neurological diseases, one of which ultimately claimed Tom's life. In addition to his expressed admiration for Tom, Greg's lecture was rich with praise for the many collaborators and students who marked his research career. He reserved particular appreciation for his long-time research partner Dagmar Ringe and Ilma Schlichting, obviously a favorite student. Dagmar and Greg's work was featured on the cover of the spring 2015 issue of *ACA RefleXions*.

Greg emerged as a postdoctoral fellow from (Sir) David Phillips' laboratory at Oxford University with a profound appreciation of the potential role of macromolecular structure and protein crystallography in understanding enzymatic catalysis. Once independent, he pioneered investigations into structural enzymology, developing, as he described, an arsenal of techniques for trapping substrate or ligand complexes, and enzymatic intermediates in the crystalline state. Greg began his explorations with considerable success, along with trials and

difficulties, using the proteolytic enzyme elastase. The focus of his most extensive research, however, was cytochrome P450, and a primary approach was the application of low-temperature and cryogenic crystallographic techniques. Many of the methods that we use today were invented and refined in Greg's laboratory at MIT and Brandeis University. The lecture included an extended discourse on how these approaches were employed to work out the enzymatic pathway of P450 and the importance of concepts like the glass transition temperature and the intrinsic flexibility of proteins and enzyme active sites. The methodologies initiated and developed in Greg's laboratory have been recognized as major contributors to our understanding of enzymatic catalysis. Indeed, in enzymology today, a knowledge and detailed understanding of the underlying molecular structure as derived by X-ray crystallography is the first imperative.

An interesting consequence of Greg's experiences with low-temperature, high-resolution crystallography was his increasing awareness, now becoming widespread, that protein structures determined under cryogenic conditions may differ, sometimes significantly, from the more relevant structure that exists at physiological temperature. Greg finished his talk by suggesting that caution in interpreting cryogenic structures was certainly in order, and that it would perhaps be appropriate and useful if all macromolecular structures deposited in the Protein Data Bank ultimately were to be accompanied by structures determined at room temperature. He further suggested that this might now, or in the near future be possible using the free electron laser source.

In sum, Greg Petsko's award lecture was heartfelt, inspiring, generous, and a credit to the name Martin Buerger. It was, furthermore, a fascinating adventure in the challenges and triumphs that mark the tortuous journey of innovation and discovery so familiar to us crystallographers.

Alex McPherson

P3: Etter Early Career Award

The **Margaret C. Etter Early Career Award** *for 2015 was awarded to* ***Yan (Jessie) Zhang****, Assistant Professor of Biochemistry, Department of Molecular Biosciences, University of Texas, Austin. 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.*

Jessie highlighted her research in her award lecture, *Nature, Imitation Game: Decipher the combinatorial CTD code for eukaryotic transcription*. Her work is featured on our cover. See p. 7 for Jessie's award citation and for information about her award-winning research. See pp. 38-39 for additional information and a report on this year's **Etter Award Symposium, 3.1.1**.

P4: The Impact of Crystals and Crystallography in Art and Culture

Juanma García-Ruiz, at right, with ACA Program Co-Chair Louise Dawe

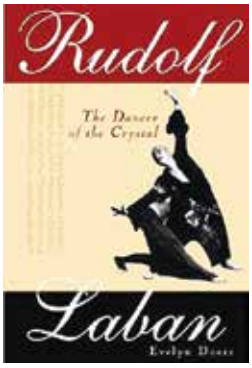
Juan Manuel (Juanma) García-Ruiz, a research professor of the National Research Council (CSIC) at the University of Granada, Spain, and founder of Triana Science & Technology (***http://www.trianatech.com***/), joined North American crystallographers in Philadelphia in July. Invited to speak to the U.S. National Committee for Crystallography by the current chair Joseph Ng, and to ACA2015 delegates by program co-chair Louise Dawe, Juanma gave a fascinating plenary lecture on the last day of the ACA meeting: *The Impact of Crystals and Crystallography in Art and Culture*. In addition to the lecture, he displayed the exhibit *CRISTALES: A world to discover* (***http://cristales2014.org***) near the registration desk throughout the ACA meeting, and screened the documentary *The Mystery of the Giant Crystals* (***http://www.iycr2014.org/learn/watch/giant-crystals***) for conference delegates and registered guests.

Juanma began his plenary lecture by describing the crystallographic instruments and techniques that are an invaluable contribution to art preservation and quickly moved on to the core of his lecture – that, beyond these technical tools, ideas about crystals have been highly influential in the history of art and in the development of our minds. Based on his studies of primitive life he found that our minds have been shaped by the belief that a sharp boundary exists separating two distinctly different worlds of symmetry: the realm of biology dominated by the symmetry of curvature and branching (fractals), which is related to sensuality and passion, and the realm of minerals dominated by the symmetry of crystals, the straight line and the faceted shapes evoking rationality and intelligence. This boundary has pervaded the landscape of arts and philosophy for centuries. Crystals played an important role in defining that boundary – they fascinate; see the schoolchildren in the image below.

Antonella Guagliardi explaining crystallization to Italian children. Photo by Martha Santana.

Turn to p. 18

It seems that this influence appeared very early, even before the birth of our consciousness. Crystals were first among the objects collected by hominids hundreds of thousands of years ago because crystals are singular entities, mathematically and physically different from any other object in nature. Early on crystals were thought to have magical powers and were used for their healing properties. A smoky quartz crystal found in the 6000-year-old funerary site of Alberite in Spain was notable because such crystals did not exist in that area – so it must have been transported at least 400 kilometers. When, at the end of the 18th century, René Haüy realized that crystals have internal order, philosophers thought that meant that there is an, *order in our world, hidden but perfect, like in crystals. It appears that finally we can understand the world*. Crystals started to populate literature (Jules Verne's *Journey to the Center of the Earth*, George Sand's *Voyage dans le Cristal*, Mary Shelley's, *Frankenstein*); sculpture (David DiMichele's *Construction* installation), painting (cubism and purism), dance (see image at the left) and architecture. Many of you will remember the 2009 ACA meeting in Toronto and the wonderful new 'Crystal' addition to the Royal Ontario Museum. Other spectacular buildings that celebrate crystals are the *Crystal Cathedral* and *Le Kinémax*, but the architectural landscape of modern cities is dominated by crystalline symmetry (see images below).

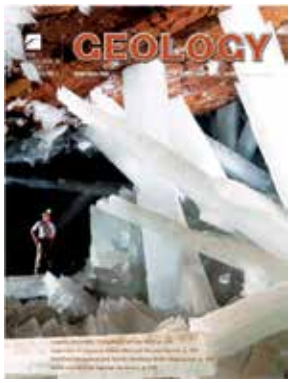


Cover of the book, 'Rudolf Laban: The Dancer of the Crystal,' by Evelyn Dörr

Le Kinémax, the flagship pavilion of 'Futuroscope,' the French theme park in Vienne, about 6 miles north of Poitiers, was designed by the architect Denis Leming, who led the project to build the theme park.

Growing crystals in Philadelphia. Photo by Juanma García-Ruiz.

Juanma summed it all up with: '*The notion of crystal transcends scientific thinking to also inspire the arts, from literature to painting, from architecture to dance, from music to filmmaking*.'



The April 2007 cover of *Geology* (see at left) featured an article by Juanma and coworkers on the formation of natural gypsum megacrystals in Naica, Mexico. The documentary, *The Mystery of the Giant Crystals*, that he showed later on the day of his lecture is a research tale on crystals written for all audiences. Exploration in the Naica mine in Mexico revealed several caves containing giant, faceted, and transparent single crystals of gypsum ($CaSO_4 \bullet 2H_2O$) as long as 11 meters. These large crystals must have been formed at very low supersaturation. The 2007 *Geology* article suggested that the megacrystals were formed by a self-feeding mechanism driven by a solution-mediated, anhydrite-gypsum phase transition. Apparently the crystals grew from low-salinity solutions at a temperature of ~54 °C, slightly below that at which the solubility of anhydrite equals that of gypsum. The authors' fluid inclusion study showed that there was a very narrow temperature range in the caves, and nucleation kinetics calculations indicated that the self-feeding mechanism probably accounted for the formation of the giant crystals.

Connie Rajnak

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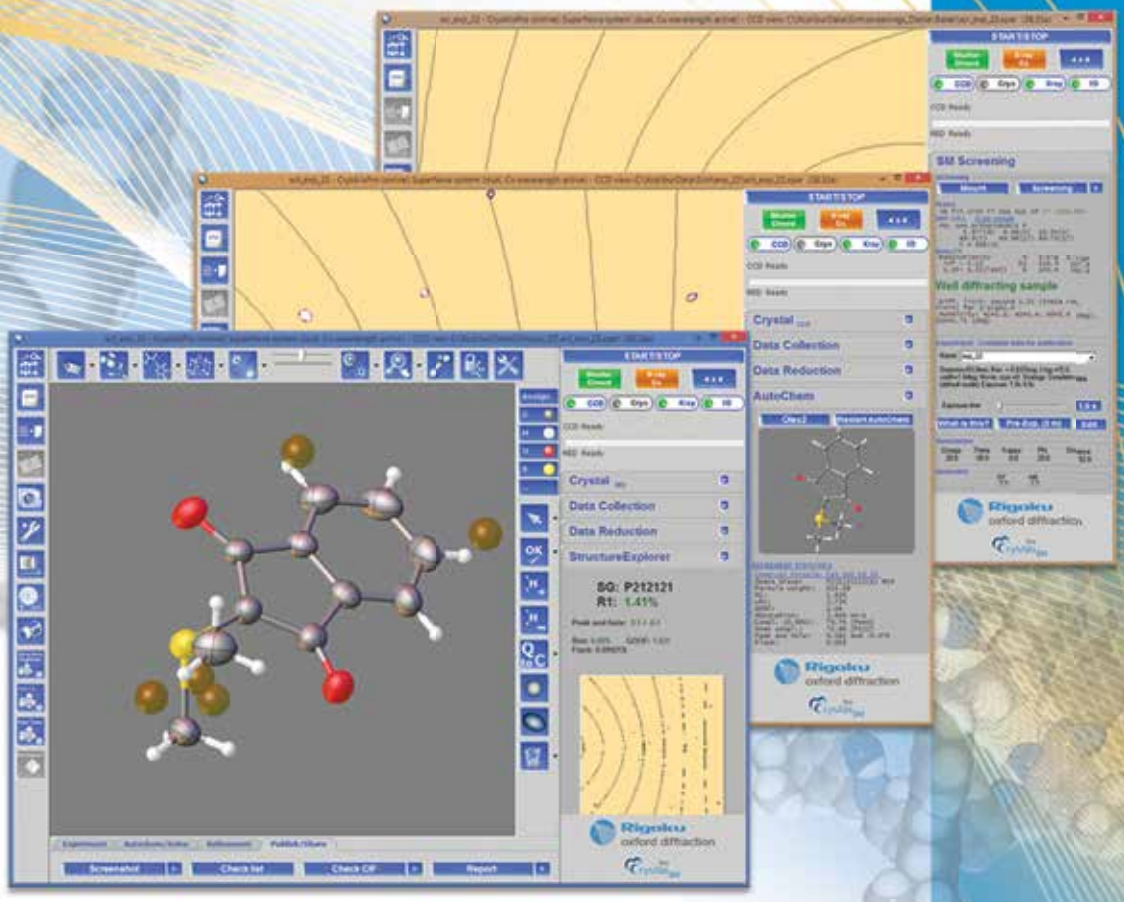

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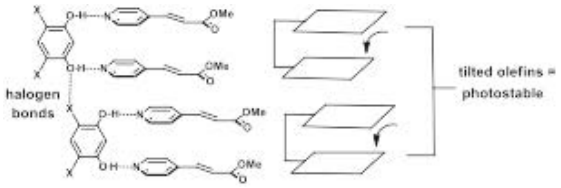
TR: The Transactions Symposium: Crystallography for Sustainability

L-R: Cora Lind-Kovacs, Ashfia Huq, Holger Kleinke, Anja Mudring, Len MacGillivray, Tomislav Friščić, John Helliwell, Hans-Conrad zur Loye, Robin Rogers

The 2015 **Transactions Symposium** was focused on *Crystallography for Sustainability* to discuss cutting edge crystallography-based research related to global aspects of the sustainability of world resources, including green chemistry, the globalization of chemistry, and responsibilities and opportunities to serve the broader public. The discussions included aspects such as the lead role of crystallography in the design of materials and in the design of processes that reduce energy consumption, protect the environment, or provide new greener routes to chemicals and materials.

Len MacGillivray, U Iowa, opened the symposium and quickly captured the audience with his applications of crystal engineering to the solid-state synthesis of organic materials. The long-range order of the molecules in the solid state, and the specific interatomic distances and relative orientations of reactive groups, can determine whether co-crystals can undergo solid-state reactions. The focus of Len's lecture was on [2+2] photodimerization of resorcinol co-crystals with other organic moieties. While many compounds are prone to photodimerization, Len showed that secondary forces like halogen or hydrogen bonding could be exploited to produce photostable co-crystals of pyridinyl and resorcinol moieties.



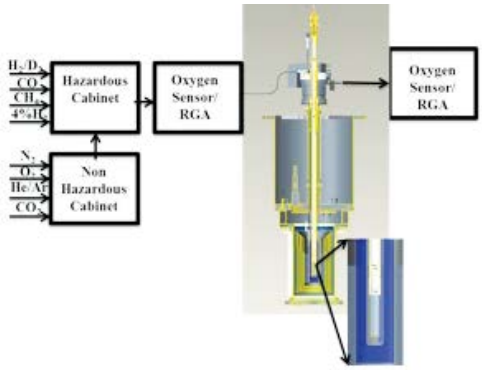
The symposium continued with **John Helliwell** from U Manchester, U.K., who shared some broader thoughts on crystallography and sustainability. John began by asking which of the UN's Millennium Development Goals are directly or indirectly addressed by crystallography. The most obvious contribution lies in the development of better medicines, which in turn can also help reduce child mortality rates. Crystallography also has a long-standing tradition of promoting gender equality, which is evident in the inclusion of women in crystallographic research since the earliest days of our science, as well as the fact that there have been several female IUCr Presidents and Nobel Laureates. Through the IUCr and regional associates, crystallography also fosters the development of global partnerships. The sustaining and passing on of knowledge is ensured through the establishment of databases, which have recently shifted to also offer archives for preservation of raw diffraction data. Finally, John emphasized that a number of famous crystallographers like Kathleen Lonsdale, Dorothy Hodgkin and Linus Pauling took a strong stance for world peace.

After the morning coffee break, **Tomislav Friščić** from McGill U, Canada, introduced the audience to an unconventional approach to solid-state synthesis using mechanochemistry. This method allows the complete elimination of solvents, making it attractive with respect to green chemistry principles such as the elimination of solvent waste.

The morning session ended with **Hanno zur Loye**'s (U South Carolina) presentation on materials discovery via crystal growth, which is an active area of research that has led to the preparation of many novel materials along with the determination of their crystal structures. One sub-area of this field is the preparation of organic/inorganic hybrid materials containing metals in reduced oxidation states. Hanno's group has developed an environmentally friendly new synthetic technique, the low temperature two-step hydrothermal method, to prepare new reduced hybrid materials. This two-step approach, where the reduction of the metal cations is performed in a first step and the crystal growth is performed in a second step, can lead to vastly improved yield in certain situations. This approach is particularly useful for systems where the *in situ* reduction is kinetically too slow versus the crystallization of an unwanted fully oxidized species. In this work, naturally occurring carboxylic acids, such as oxalic acid and tartaric acid, were used as reducing agents in an aqueous reaction environment.

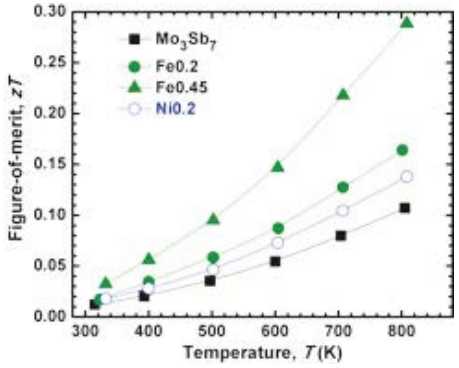
The afternoon session started with a focus on characterization techniques that are useful in studying and improving materials related to energy challenges. **Ashfia Huq** from Oak Ridge National Lab showed how powder neutron diffraction is a unique method for visualizing the pathways for light atoms like lithium,

hydrogen or oxygen in energy materials. Setups at the POWGEN instrument at the Oak Ridge Spallation Neutron Source (SNS) include the ability to study materials under operating conditions using a sophisticated gas handling system in combination with a furnace (see the illustration below). This allows reliable determination of site occupancies, including those responsible for ionic conductivity. The distribution of vacancies, and anisotropic displacement parameters of light atoms that indicate the direction of ionic movement, can give insights into underlying mechanisms and help optimize materials.

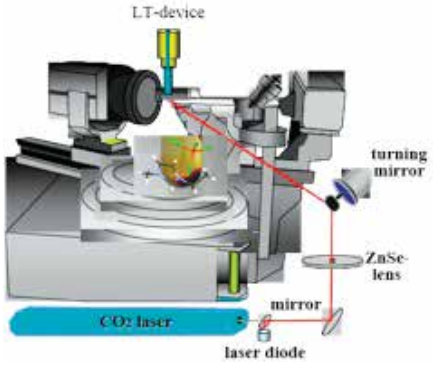


Peter Kalifah from Stony Brook U continued the focus on crystallographic method development for the study of energy materials by showing the application of advanced powder diffraction methods to semiconductors that can catalyze solar water splitting.

Holger Kleinke from the U Waterloo, Canada, showed how structure-property relationships are crucial in the understanding and design of thermoelectric materials related to Mo_3Sb_7. Thermoelectric materials can convert waste heat into electricity, thereby contributing to a higher sustainability of today's society. Advanced thermoelectrics are heavily doped, narrow-gap semiconductors with heavy elements and complex crystal structures. As Mo_3Sb_7 is a metallic material, it needs to be modified via chemical substitution to obtain the missing valence electrons to become semiconducting. Holger's group recently achieved this via Sb/Te exchange, but tellurium is too toxic and rare for environmentally friendly applications. To overcome this problem, Mo_3Sb_7 was modified with iron and nickel. Crystallography served as an important tool to control and verify these modifications, as well as to analyze the resulting changes. It was found that iron works better than nickel, as it prefers the Mo sites over the cubic holes, mostly for steric reasons. This led to a roughly tripled thermoelectric figure-of-merit of tellurium-free Mo_3Sb_7 (see figure below).



The final talk of the symposium highlighted **Anja Mudring**'s (Iowa State U) work on ionic liquids (ILs). ILs, which are salts with a melting point lower than 100 °C, have received a tremendous amount of continuing interest both in academia and industry over the past two decades. Because of their often-low vapor pressure and inflammability ILs are frequently discussed in the context of green chemistry. However, ILs are not green *per se* – but they can be made green and a number of applications are now established that meet the criteria for a green(er) process. It is now realized that their modular character allows engineering an IL for a certain application, for example as active pharmaceutical ingredients. Yet predictions about which ion combinations to choose that give rise to a room temperature IL (RTIL) with the desired properties are difficult. Analysis of their complex structural behavior by means of X-ray structure analysis is challenging but allows for important insights. Since RTILs are liquid at room temperature it is not an easy task to crystallize them for X-ray structure analysis. Anja discussed crystallization techniques for ILs, and showed an example where X-ray structure analysis



Apparatus for crystallizing ILs in situ on an X-ray diffractometer

of a set of ILs made it possible to gain valuable insights into property-relationships in ionic liquids and helped to formulate design principles for RTILs. On the whole, Anja's contribution gave insights into the liquid-solid phase transition of ionic liquids from the viewpoint of crystallography, with the goal to contribute to a better understanding of this intriguing and exciting class of compounds.

Cora Lind-Kovacs and Robin Rogers

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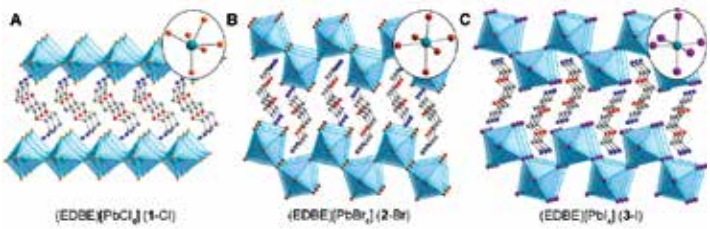
1.1.1: Crystallography of Emergent Phenomena

L-R: Efrain Rodriguez, Jai Prakash, Jared Allred, Keith Taddei, Huibo Cao, Hemamala Karunadasa

The **Crystallography of Emergent Phenomena** session showcased research where crystallographic tools played a primary role in determining the mechanism and true behavior of 'complex' materials, i.e., those compounds where the properties cannot be understood as coming from one ingredient but instead emerge from the collective interaction of the whole. Some highlights of the session follow.

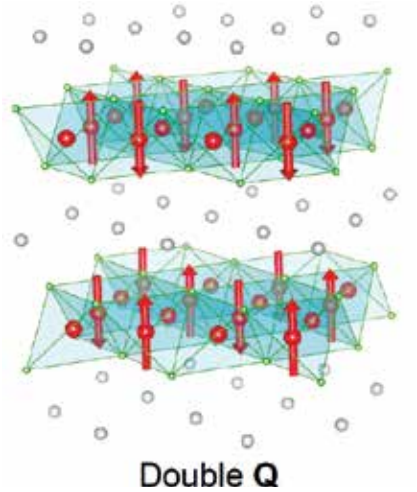
The relationship between structure and light absorption/emission was highlighted by **Hemamala Karunadasa**, Stanford U. For a class of hybrid organic/lead halide perovskites – compounds where organic molecules span 2D sheets of an inorganic material – it was found that certain members exhibit an unusual photoluminescent property when illuminated with blue light: broad-spectrum light emission.

The relationship between the structure and properties of related structures was shown. For example, various analogs exhibit different 2D planes extracted from perovskite and different types of distortion in the lead coordination environment, as shown below. In-depth photochemical and substitutional studies indicated that



the emission is intrinsic to the bulk crystal rather than induced by surface defects. More specifically, there is evidence that the broad spectrum is effected both by the relatively squishy lattice and from 'self-trapped electrons.' White-light emitting phosphors have many advantages over current technologies where multiple single-color phosphors are used in tandem. Still, these new materials have room to grow. While the compounds are stable after several months of continuous illumination, their low quantum efficiency (<10%) would need to be improved in order for them to be useful in an application.

Keith Taddei, Northern Illinois U, was chosen by the Neutron Scattering SIG to receive the **Etter Student Lecturer Award** for his contribution on the iron-based superconductors $Sr_{1-x}Na_xFe_2As_2$. The complex interaction between order parameters was investigated by combined X-ray and neutron powder diffraction. This combination enabled the tracking of subtle phase transitions from high to low symmetry and back again as a function of temperature and composition. The result was a complex phase diagram with two types of magnetism competing against superconductivity and each other. The two prevailing theories can individually explain the observed magnetism: either the physics is dominated by local-type interactions or by delocalized band-like physics. Since the latter implies wave-like states that might destructively interfere, Mössbauer spectroscopy was used as a local probe to look for 'nodes.' These are places where the component wavefunctions cancel one another out, so that there is no effective magnetic field. Indeed, exactly 50% of the iron sites were shown to be non-magnetic, as shown below



and as predicted by the magnetic wave-like model. This highlighted the importance of combining careful diffraction experiments with complementary local probes.

Jared Allred

1.1.3: Application of SANS/SAXS to Structural Biology

L-R: Adam Round,William Heller, Jill Trewhella, Nikolina Seculic, Joseph Curtis, Susan Krueger, Sangita Sinha

William Heller, Oak Ridge National Lab, reported on the application of small-angle neutron scattering (SANS) to the study of cellular membranes, which includes proteins, lipids and other molecules. This is an area that continues to challenge structural biologists because of issues such as membrane protein solubility and the complex phase behavior of lipids. The Sinbidis Virus, Light Harvesting Complex II, Bacterial Photosystem I, and antimicrobial peptides, were used as examples to illustrate how contrast variation methods using isotopic exchange together with neutron scattering experiments made it possible to gain unique structural insights not accessible by other approaches.

Sangita Sinha, North Dakota State U, presented her group's research on the structure and function of BECN1, a key component of the autophagy nucleation complex. This complex is involved in the degradation and recycling of unwanted, damaged, or harmful cytoplasmic components. Sangita presented an integrative approach to the study of this protein that included bioinformatics, X-ray crystallography, small-angle X-ray scattering (SAXS), circular dichroism (CD), and molecular dynamics (MD). Together, these results revealed key insights into the structure and dynamics of the protein, revealing the presence of a transient structure that changes into an ordered arrangement upon binding to partner.

Sangita's talk was followed by **Nikolina Sekulic**, Perelman School of Medicine, U Pennsylvania, who reported on contrast variation studies of centromeric mononucleosomes. Centromeres are vital to the proper segregation of chromosomes, and are defined by a variant histone protein called CENP-A and slightly A-T rich repetitive DNA sequences. Using analytical ultracentrifugation and SANS contrast variation, a more extended conformation of CENP-A derived nucleosomes in solution was determined relative to the canonical form. These results reveal the role of DNA in the physical basis of how the CENP-A histone distinguishes centromeres from the rest of chromatin.

In the next talk, **Jill Trewhella**, U Sydney, Australia, demonstrated the utility of small-angle scattering to the study of macromolecular structure in the presentation of work done by her group on proteins from HIV, including matrix (MA) and its interaction with calmodulin, and HIV reverse transcriptase. Both cases illustrated how the marriage of the complementary information from solution scattering with available crystallographic information, hydrogen-exchange mass spectrometry, fluorescence, and other approaches together could provide unique insights into the structure and dynamics of these proteins.

Adam Round, ESRF, France, reported on innovations at the synchrotron SAXS beam line BM29, including SEC-SAXS, streamlined data management and analysis with the ISPyB database, and microfluidic devices. To make data acquisition more efficient, droplet microfluidics were implemented and their utility illustrated with regards to adjustable additive concentrations, radiation damage, and background scattering. As a proof-of-principle, *in situ* crystallization of glucose isomerase was performed to show that crystals could be grown and transported within the droplets, allowing for the study of nucleation in different additive conditions.

Susan Krueger, NIST Center for Neutron Research (NCNR), reported on the application of SANS and contrast variation to the study of disordered proteins in the context of two-subunit complexes, using the example of Skp OmpW bound to Skp OmpA. Using the program SASSIE, Monte Carlo sampling of backbone dihedral angles within protein models was used to generate ensembles of energetically relevant conformations for the disordered regions of the complex, using structural models that satisfy the contrast variation data obtained.

Susan's colleague, **Joseph Curtis** of NCNR, closed the session by providing a report on the progress of the CCP-SAS initiative, an NSF-funded joint U.K./U.S.A. collaboration. The goal of this effort is to produce a new generation of open-source software to facilitate the atomistic modeling of macromolecules using SANS/SAXS data. These web-based applications include the SASSIE/SCT module and the modeling of analytical ultracentrifugation data using US-SOMO. The software will be open-source, easy to use, and stable. Research examples using these new tools were provided.

Kushol Gupta and Alvin Acerbo

1.2.1: From Fingerprinting to Full ID: PXRD

This session was intended to bring new aspects of the use of powder diffraction to a more general audience. We were able to bring a great variety of speakers, thanks to our sponsors, **Bruker AXS**, **PANalytical**, and **Rigaku/Oxford Diffraction**. The session was exciting right from the start with a great talk by **Andrew Brunskill**, Merck Research Labs, where he discussed several techniques and demonstrated the power of PXRD to characterize compounds relevant to pharmaceutical industry. **Simon Bates**, Triclinic Labs, provided an exceptional lecture on the ability of PXRD to perform various quantitative analyses on component mixtures, emphasizing the use of the chemometric method. Simon discussed the matrix effects that occur in the pharmaceutical industry. **Julie Quinn**, PANalytical, discussed the use of conventional PXRD instrumentation to perform Pair Distribution Function (PDF) studies for the analysis of non-crystalline materials. Julie presented basic information and some great examples of how PDF is used to evaluate solid materials. Though possibly not yet routine, PDF can provide a new method of analysis in PXRD. **Raj Suryanarayanan**, U Minnesota, provided a new twist in the use of PXRD. By analyzing pellets, he has begun to understand the chemistry and effects from pressing drugs into pellets. Use of microdiffraction with an area detector provides new insights into the crystallization of pharmaceuticals during tablet production. Raj's use of PXRD in this study shows what one can accomplish using X-ray diffraction. The last talk of the session was given by **Jim Britten**, McMaster U, Canada, and provided the audience with a great overview of how one can use single-crystal diffractometers and area detectors to perform multiple PXRD techniques. Jim outlined the positives and negatives of these techniques and provided many exciting examples of experimental results.

Overall the session introduced the audience to a wide range of PXRD experiments that they could consider employing in their own research.

Richard Staples

1.2.2: Engaging Undergraduates with Crystallographic Research

L-R: Jim Golen, Alexander Nazarenko, Joe Tanski, Paul Cook, Christine Phillips-Piro, Roger Rowlett, Dean Johnston

In a half-day session, speakers focused on the use of X-ray crystallography in their undergraduate research programs, how to incorporate X-ray crystallography into the undergraduate curriculum, and how to launch a successful research program incorporating chemical crystallography at a primarily undergraduate institution.

The talks in this session featured a mixture of both small molecule and protein crystallography. **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. **Christine Phillips-Piro**, Franklin & Marshall College, discussed her research using X-ray crystallography to study the interaction of unnatural amino acids with proteins, as well as some of her ideas about the key factors in setting up and running a productive protein crystallography lab at a predominantly undergraduate institution. **Jim Golen**, U Massachusetts Dartmouth, relayed the story of a diffractometer acquisition through the NSF-MRI program for an instrument that is being used as a regional resource in southeast Massachusetts, and gave several examples of the undergraduate research results that are being obtained. **Dean Johnston**, Otterbein U, described the pedagogical approach of using mini research projects, based on student proposals, to isolate and structurally characterize coordination compounds with his inorganic chemistry class or with undergraduate research students. **Paul Cook**, Grand Valley State U, discussed in detail his experience of addressing the challenges of setting up a macromolecular crystallography research program at a predominantly undergraduate institution. To complete the session **Joe Tanski**, Vassar College, gave a description of his research program in the field of titanium mediated asymmetric catalysis through the lens of the crystal structures obtained at all stages of the project.

Joe Tanski and Roger Rowlett

L-R: Marilyn Olmstead, Bruce Foxman, Christine Beavers.

Ben Hish, at left, with Helen McDonnell

Photos by Dick Bromund

1.3.1: Career Odyssey

The **Career Odyssey** session, held on Sunday afternoon, featured four panelists from varied career paths. The session started out with the panelists describing their career path, responsibilities in their current positions and what helped them to survive in them. This was followed by a Q&A session and open discussion. The Career Odyssey session was followed by the **YSSIG Mixer** held at the City Tap House. Our Career Odyssey panelists included **Cora Lind-Kovacs**, **Christine Beavers**, **Celeste MacElrevey**, and **Steven Sheriff**.

L-R: Celeste MacElrevey, Christine Beavers, Smita Kakar, Cora Lind-Kovacs, Steven Sheriff

Cora Lind-Kovacs is a Professor at U Toledo. Cora shared her perspective as an investigator managing graduate students and postdocs in her laboratory, and as a faculty member teaching undergraduates. She suggested that senior postdocs aspiring to an academic career should learn people-management skills and have mentors who are more experienced than they are. These can be your Ph.D. advisors, department chairs, or someone else who is more experienced than you. When asked, 'What is one thing you wish you were taught in graduate school?' Cora replied, "Nobody taught me how to teach undergraduates; coming from Germany, there was a clash of cultures in the beginning when I started teaching. I wish someone had taught me that." What Cora especially likes about her job is flexibility to set her own schedule.

Christine Beavers is a beamline scientist at ALS. Christine said that although hers is a high burnout rate job, she manages to find time for vacation and to pursue her interests. The one thing she wishes she was told in graduate school is, 'Graduate school is not about what you learn, it's about whether to learn to learn and learn to network.' Christine likes her job because it never gets boring; she gets to meet new people who use her beamline, and she can travel places around the world.

Celeste MacElrevey is a pharmacokineticist at Nuventra Inc., a contract research organization. Celeste has a vast experience and has established an LLC consulting company. She enjoys the 'variety' in her job and the satisfaction to further someone's research goal. Celeste suggests students to try new things and to never give up and keep trying.

Steven Sheriff is a senior research fellow at Bristol-Myers Squibb. Steve suggested that being flexible is an important way to survive. He also suggested that managing people is a part of any job and one should learn how to do that. Steve enjoys doing science and discovering what is not known.

Overall, the session was very informative and interactive. Students and postdocs left the session with encouragement and motivation to pursue their goals. You can read more about the panelists at ***http://www.amercrystalassn.org/documents/2015%20Meeting/SpeakerBios_2015_SK.pdf***. Also, a summary of questions and answers can be found at ***http://www.amercrystalassn.org/documents/2015%20Meeting/SpeakersQs_Career_odyssey_2015_SK.pdf***. (Note that Jason Stagno unfortunately could not participate in the session.)

Smita Kakar

L-R: back row – Fernando Uribe-Romo, Stephen Fitzgerald, Mircea Dincă, Matthew Hudson; front row – Tabbetha Dobbins, Andrey Yakovenko, Craig Brown

2.1.1: Porous Materials at the Nano and Meso-scale

This session was designed to illustrate the power of diffraction to elucidate important structural aspects of materials that have some form of porosity. Tools that enable these observations range from powder and single-crystal diffraction to illuminate the atomic scale structure, through to small-angle scattering, which gives the broadest view of porosity over many nanometer length scales. A wide range of possible technological applications was evidenced throughout the talks, illustrating the deep connection between structural form and function in modern materials development. Some highlights of the well-attended session that stimulated significant discussion throughout the meeting are presented here.

While a few talks described the tremendous interest in metal-organic frameworks (MOFs) as sorbents for gas storage and separation applications, **Mircea Dincă**, MIT, detailed his recent progress in applying concepts of photophysics and charge-transport phenomena to the design of new MOFs exhibiting these

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2.1.1: Porous Materials at the Nano and Meso-scale, ctd.

properties. For the latter aspect, three potential mechanisms for electron hopping in molecular systems were described: through space; through bonds; and redox hopping. While they are all conceptually difficult to design into a porous framework *a priori*, the Dincă lab has synthesized some examples of these. Rational insights from the π-π stacking structures observed in organic superconductors were applied to the design of a tetrathiafulvalene MOF with a chiral organization of stacking ligands separated by about 3.8 Å. The exceptional chemical and structural flexibility of MOFs were used to tune the electronic overlap, and hence improve electrical conductivity by two orders of magnitude, via synthesis of the MOF with different divalent metal cations of differing ionic radii. Another example, with a six orders of magnitude improvement in conductivity, came from modifying the ligands of the well-known MOF-74 system. Here the electron-hopping mechanism was demonstrated by tuning the orbital energy levels for the ligand by replacing coordinating oxygen atoms with sulfurs. The resulting structural analogue has Fe cations coordinated to S atoms forming infinite chains and a much better electronic overlap facilitating the electron-hopping mechanism.

Stephen Fitzgerald, Oberlin College, presented a moving tribute to the late **Jesse Rowsell**, Oberlin College. This was clearly an emotional time for Stephen and several students in the audience. The academic legacy of Jesse is tremendous. Just one manuscript from his early graduate work has been cited over 1500 times, and he was one of the first to study the MOF-74 system for hydrogen storage applications, a fact that connected Jesse to Stephen's current research. Besides the evident intelligence of Jesse, Stephen revealed many aspects of Jesse that showed him to be empathetic, driven, creative, and beyond loyal to the students to whom he taught materials chemistry and inorganic chemistry. Jesse was constantly trying to improve not only their learning experience, but also expanding science education to the public. Stephen continued with an amazing high-level discussion and clearly delivered talk concerning the last project that Jesse was tackling. This was no mean feat for a lay crystallographer as it involved discussing the intricacies of self-assembly of an 8-fold polycatenated hydrogen-bonded framework, and the ensuing polymorph induced 56 independent molecules in the asymmetric unit cell! Just as impressive is the fact that this material is also permanently porous with a surface area over 1000 m^2/g.

Craig Brown and Fernando Uribe-Romo

2.1.2: Crystal Engineering Form & Function

L-R: Tomislav Friščić, Nikoletta Bathori, Nadrian Seeman, Jason Benedict, Adam Matzger, Mircea Dincă, Peter Wood, Len MacGillivray

This session showcased current research in the field of crystal engineering with an emphasis on the relationship between the structure and the function of crystalline forms. The session very successfully captured the broadness of contemporary crystal engineering, from functional co-crystals to photo-responsive metal-organic frameworks (MOFs), all the time attracting a considerable audience of more than 50 attendees.

The first half of the session kicked off explosively with a talk by **Adam Matzger**, U Michigan, who illustrated the potential of co-crystals to improve the properties of energetic materials. Adam illustrated examples where the sensitivity or the power could be tuned effectively using co-crystallization (see: *J. Am. Chem. Soc.* **2015**, *137*, 5074; ***dx.doi.org/10.1021/jacs.5b00661***).

Len MacGillivray, U Iowa, then continued the theme of co-crystals by introducing us to the use of co-crystallization and photochemical transformations to control the assembly of molecules in organic solids to affect electrical properties (see: *J. Am. Chem. Soc.* **2014**, *136*, 6778; ***dx.doi.org/10.1021/ja4131774***). Len's lecture explained how organic co-formers such as resorcinol can be used to engineer the stacking arrangement of π-rich compounds like thiophenes into organic semiconductor co-crystals (see also Len's talk in the **Transactions Symposium**, p. 20).

The final talk in the first half of the session was given by the invited *CrystEngComm* lecturer, **Mircea Dincă**, MIT. By presenting a highly interdisciplinary study heavily dependent on careful structural characterization, Mircea presented a view of MOFs as tuneable, macromolecular-like systems that can be used to achieve unusual metal coordination geometries (see: *J. Am. Chem. Soc.* **2013**, *135*, 12886; ***dx.doi.org/10.1021/ja4064475***). A notable example of this was engineering highly unusual nickel(II) centers tetrahedrally coordinated with oxygen ligands within the MOF-5 scaffold. Beyond engineering unusual coordination environments, this study revealed unexpected genuine dynamics and unusual defects in this familiar structure.

The second half of the session started with a presentation from a true legend of crystal engineering, **Nadrian Seeman** of New York U. Ned's lecture attracted a huge audience who got a glimpse of his outstanding work in generating wide-open and programmable structures based on self-assembled DNA-based building blocks (see: *Science*, **2015**, *347*, 1260901; ***dx.doi.org/10.1126/science.1260901***).

Further in the topic of molecular materials, **Nikoletta Bathori**, Cape Peninsula U Technology, South Africa, brought us back full circle to co-crystals and their pharmaceutical applications, showing some fascinating structures and clear trends between melting points and solubilities, which promise to place us one step closer to a rational design of crystals with desired pharmaceutical properties (see: *CrystEngComm*, **2014**, *16*, 9992; ***dx.doi.org/10.1039/c4ce01298d***).

The session concluded with a talk by an inspired rising star of crystal engineering, **Jason Benedict**, U at Buffalo, who presented pioneering work on combining the modular and open structures of MOFs with the photoswitchable behavior of diarylethylenes. Jason presented a structurally challenging new family of switchable MOFs accomplished by a unique combination of organic synthesis and coordination-driven self-assembly (see: *Chem. Commun.* **2013**, *49*, 8012; ***dx.doi.org/10.1039/c3cc44119a***).

All the speakers were acknowledged for their effort by a small bottle of original Canadian maple syrup. If a single statement conclusion is ever needed for this session, it would most likely be that crystal engineering is a vigorous discipline, advancing more rapidly than ever!

Peter Wood and Tomislav Friščić

2.1.3: General Interest I

L-R: Michael Ruf, Brian Toby, Emil Espes, Stacey Smith, Chuck Campana, Zheng-Qing Fu, Andreas Kleine. Photo courtesy of Stacey Smith.

This session highlighted recent developments in instrument and software technology.

Michael Ruf, Bruker AXS, opened the session with a description of the long-awaited APEX3 software package released by Bruker AXS just before the start of the conference. In addition to the new icons, Michael highlighted the new structure solution and refinement plugin and demonstrated the improved twin-handling tools. **Andreas Kleine**, Incoatec, then described the magic behind their microfocus X-ray sources and scatterless pinholes, ending with a discussion of what it takes to upgrade existing systems to these new technologies. **Emil Espes**, Excillum AB, updated us on the liquid metal jet X-ray source technology. An exciting new development is the use of a Ga-In alloy as the cup of liquid metal, which would allow both the Cu-like wavelength (from Ga) and the Ag-like wavelength (from In) to be used in diffraction experiments on the same instrument, if the system is set up with dual ports and separate Montel optics to select those wavelengths. With brilliances close to those of first-generation synchrotron sources, protein data can be collected in-house to nearly the same resolution as synchrotron data (1.85Å vs. 1.75Å). **Chuck Campana**, Bruker AXS, followed Emil, describing several examples of analyses completed with the metal jet system on a Bruker D8 Venture. **Zheng-Qing Fu**, U Georgia, then presented work in which he used shutterless data collection with a CCD detector to extract an extremely weak but successful native SAD signal. **Brian Toby**, Argonne National Lab, rounded out the session with an update of what's new in the development of GSAS-II. Brian highlighted the improved user interface and graphing capabilities of GSAS-II as well as the dual powder and single crystal and dual X-ray and neutron diffraction refinement capabilities, though TOF analysis is still a work in progress. Other recent updates include twin handling and constraints.

Stacey Smith

2.1.4: Publication Practices

This year's **Publication Practices** session cast a contemporary and forward-looking focus on the publication of small-molecule crystal structures. The exponential growth in the number of small-molecule structures being published – and of those that are not being published – continues to influence all aspects of the publication process, from best-practice procedures in the conduct of structure analyses to the proper presentation of reports to the curation and archiving of results. The speakers in this session, co-organized with the able assistance of YSSIG volunteer Kimberly Lincoln, touched on all aspects of the process.

The natural first decision regarding publication of a structure is whether to publish or share it at all. **Suzanna Ward**, of the CCDC, presented an estimate of the number of 'zombie' or unpublished, unshared structures. How might science benefit from having these structures available to everyone? The CCDC private-communication mechanism is an excellent way to enhance the public availability of structures that are not published in journals. Suzanna raised the question of how to provide incentive for private communication. There is information about structure deposition here: ***http://www.ccdc.cam.ac.uk/Community/Depositastructure/Pages/StructureDepositionInformation.aspx***.

Sandy Blake, U Nottingham, U.K., Section Editor at *Acta Cryst., Section B*, presented what many thought was a much-needed talk about the current missions of the IUCr journals, especially the division of labor among *Acta Cryst*. Sections B, C and E. In brief, the journals have been redefined: There are new journal directions, new designs, and new web sites. Section B is creating an individual brand that includes commentary on outstanding articles. Section C, which has been rebranded as 'Structural Chemistry,' has new types of articles, including lead articles, feature articles and scientific comment, as well as a much more flexible submission process that includes the use of Word and OpenOffice documents for the text. This removes an earlier requirement to include all text, including rich text, in the CIF, which led an unquantifiable number of authors to consider other avenues of publication for their results. An editorial from earlier this year gives more information on the direction of Section C:

http://journals.iucr.org/c/issues/2015/01/00/me0560/me0560bdy.html. *Acta Cryst.*, *Section E*, which in its prior format was popular among authors but which has not been indexed by the Web of Science since 2012, has been relaunched to publish the much more substantial Research Communications, which have much in common with the Structure Communications previously published by Section C. The Data Report format of Section E will be supplanted by the new *IUCr Data*.

Ton Spek, U Utrecht, the Netherlands, the 2010 ACA Trueblood Award laureate, had a clear message – that when reporting single-crystal structure determinations the unmerged reflection data should be included in the report. At present the most common vehicle for doing so is the embedded reflection file in the CIF produced by structure refinement software. This permits any unusual features of the structure and above all, claims of unexpected chemical features, to be investigated in detail. Ton demonstrated his point using two clear examples of re-examined results including one chemically intriguing result published in a high-impact journal.

Phil Fanwick, Purdue U, reflected on his vast experience as a chemist, chemical crystallographer, service crystallographer, author, reviewer and editor, using the appropriate title *Crystallography from all Sides*. One of Phil's best pieces of advice was directed at reviewers (but could apply as well to editors): 'You can re-refine a structure but do not try to make it your own.' Phil gave several other examples of what might be called 'veteran practitioners' wisdom.'

The **Publication Practices** session drew a large audience, and each of the talks generated substantial discussion.

Note from the organizers: Trying to put together a high-quality, well-rounded, and above all useful program on the current scientific publishing scene necessarily involves inviting speakers from various parts of the globe. We are grateful to those who traveled significant distances to participate. And we thank **Crystallographic Resources, Inc.** and their Chief Scientific Officer **Richard Staples** for generous support of this program.

Kimberly Lincoln and Larry Falvello

2.1.5: Structural Dynamics

This session was devoted to the topic area of *Structural Dynamics*, the ACA journal co-published with AIP Publishing (see pp. 5-6), and included work on metals, materials, small molecules, and proteins. The talks followed nicely from the Buerger Award Lecture by Greg Petsko, which highlighted the role of dynamics in protein function.

The **Structural Dynamics** session had a mixture of technique and result-oriented talks, beginning with beautiful and elegant results of **Marius Schmidt**, U Wisconsin – Milwaukee, on a full kinetic description of the photocycle of photoactive yellow protein, including experimental crystallographic movies of transitions around the cycle. **Philip Coppens**, U at Buffalo, took dynamic analysis to the inorganic chemistry level, showing how to treat diffraction data properly in terms of scaling to reveal transient electronic structure in Ag-Cu crystals. **George Phillips**, Rice U, who also served as Session Chair (along with Co-chair Keith Moffat, U Chicago), presented a perspective on new challenges of using X-ray lasers and a progress report on his student Jonathan Clinger's work on the development of a new photo-signaling system for time-resolved studies. The next talk, by **Mariano Trigo** of SLAC, shifted back to hard condensed matter, with a fantastic description of phonon dispersion as measured in real time with a pump-probe examination of Brillouin zone coverage between Bragg spots. The subject then turned back to proteins, with a talk by **Travis Gallagher** of NIST on designed flexibility in antibodies. Following this, the program turned to metallo-organic chemistry, with a fine study on the construction of a special chamber that allows compounds to be easily exchanged in frameworks (MOFs) and the viewing of the substitutions in nicely controlled ways, presented by **Jordan Cox** of U at Buffalo. The session closed with a talk by applied mathematician **Ali Dashti**, U Wisconsin – Milwaukee, on the use of powerful manifold embedding methods in revealing conformational landscapes of ribosomes and the ryanodine receptor.

The papers in this session nicely illustrated the range of topics that overlap the *Structural Dynamics* journal areas.

George Phillips

David Rae

L-R: Carol Brock, Jenny Gliusker, Amy Katz

Bill Furey, at left, with B. C. Wang

Photos by Dick Bromund

2.2.1: Advances in Multi-crystal Approaches and Serial Crystallography

L-R: back row – Danny Axford, Cornelius Gati, Nadia Zatsepin, Qun Liu; front row – John Spence, Jennifer Wierman, Gleb Bourenkov, James Holton

With the design of novel X-ray light sources, X-ray beams with unique properties such as extremely high peak brilliance, femtosecond pulse duration, and full spatial coherence became available. To make full use of these improvements in protein crystallography, it was necessary to develop novel techniques for data collection, namely by distributing the dose over many (small) crystals. This session, **Advances in Multi-crystal Approaches and Serial Crystallography**, covered a range of such newly available techniques and their impact on crystallography. The session included topics ranging from merging data from a handful of incomplete datasets collected at a synchrotron, up to the extreme case of serial femtosecond crystallography (SFX) at hard X-ray free-electron lasers, where a single crystal only withstands the X-ray pulse for fractions of a second before it is completely destroyed, so that only one diffraction pattern can be collected per crystal.

The talks, from world-leading experts in the field, had an emphasis on allowing even entry-level crystallographers to follow the discussion of new possibilities, limitations and challenges. Given the user-oriented theme of the session, which covered cutting-edge techniques, the auditorium was more than fully occupied. The first talk, presented by **John Spence**, Arizona State U, introduced the broad spectrum of ongoing and recent exciting SFX experiments, as well as methodological developments and limitations of the technique, and clearly was a highlight of the session. The following presentation by **James Holton**, U California, San Francisco, covered the very relevant problem of anisomorphism in multi-crystal data merging and its utilization to overcome the crystallographic phase problem. **Jennifer Wierman**, Cornell U, introduced a novel algorithm to overcome the problem of indexing diffraction patterns with extremely low photon counts, which are out of reach for conventional autoindexing programs. **Gleb Bourenkov**, European Molecular Biology Lab, Hamburg, Germany, and Danny Axford, Diamond Light Source, U.K., described novel data collection schemes for micron-sized crystals with the major advantage of using easily accessible synchrotron light sources, which is a particularly important aspect for the user community. Finally, **Qun Liu**, NY Structural Biology Center, presented his exciting work on the topic of experimental phasing using multi-crystal approaches at synchrotron light sources, as well as obtaining phase information from SFX data sets using native S-SAD, which is particularly challenging and hence a very important problem.

Overall the session was very well received and, for many, one of the highlights of the ACA meeting. It was a great honor to have the opportunity to assemble such an exciting schedule during one of the most important meetings in the topic of crystallography worldwide. We are all very much looking forward to seeing new exciting results and methodological breakthroughs in this vibrant field, which will enable even more experiments than currently possible.

Nadia Zatsepin and Cornelius Gati

Virginia Pett with Bill Duax at the opening reception

IUCr President Marv Hackert, at left, with Arthur Monzingo

Photos by Dick Bromund

2.2.2: Materials Discovery and Crystal Growth

L-R: Paul Forster, Jared Allred, Efrain Rodriguez, Patrick Woodward, Jennifer Aitken, Kirill Kovnir, Susan Latturner, Joshua Goldberger

This session brought together some of the top materials and solid-state chemists in the field to demonstrate how crystallography is key towards promoting materials discovery. The focus of the session was on inorganic solids such as transition metal oxides, chalcogenides, and some new main group compounds as well.

In the opening talk of the session, **Patrick Woodward**, Ohio State U, showcased his work on how cation ordering in layered perovskite oxides can influence the octahedral tilting and thereby change their functionality. Guided by symmetry relations among the perovskites, Woodward demonstrated how the chemistry of these layered perovskites can lead to functional properties. **Kirill Kovnir,** U California, Davis, presented his work on main group element clathrate materials. The clathrates prepared by Kirill are typically pnictides with transition metals as part of the cages. 'Rattling' around inside these cages are heavy alkaline earth metals such as Sr and Ba, which give these clathrates the unique thermal conductivity properties that make them candidate materials for next generation thermoelectrics. **Joshua Goldberger**, Ohio State U, presented some impressive chemistry in preparing two-dimensional materials by dimensionally reducing their three-dimensional parent phases. From this strategy he has prepared Group IV analogues to graphane, such as germanane, which is an interesting semiconductor with a direct band gap.

From Duquesne U, **Jennifer Aitken** showed new compounds from main groups such as $CdGeP_2$ that are derivative of the diamond structure. Such compounds are semiconductors and hold promise in a broad range of areas such as photovoltaic and luminescent applications. **Susan Latturner**, Florida State U, presented a series of intermetallic phases prepared through exploratory synthesis. Susan's investigations into magnetic ordering in these complex systems were facilitated by reactions carried out in metal fluxes.

Jared Allred, Argonne National Lab, reported on a new ternary iron chalcogenide with unconventional magnetic behavior at higher temperatures. In the compound $(BaF)_2Fe_{2-x}Q$ for Q = S and Se, strong antiferromagnetic coupling is observed between the Fe–Fe dimers along the edge sharing FeQ_4 tetetrahedra, yet the system exhibits weak ferromagnetism at relatively high temperatures. **Julien Makongo Mangan**, U Delaware, presented his work on the synthesis and crystal chemistry of a series of pnictides. In the series $A_{14}Cd_{1+x}Pn_{11}$ for A = Sr, Eu and *Pn* = As,Sb, Julien presented how both electronic structure calculations and ion size effects were key to understanding their properties including their non-stoichiometry.

Efrain Rodriguez and Paul Forster

2.2.3: How I Spent My Summer Vacation: Experiences Derived from Small Molecule Summer Schools

This session, **How I Spent My Summer Vacation: Experiences Derived from Small Molecule Summer Schools**, included six oral presentations from ACA summer school students. These presentations included former students from the past five years that represented a cross section of academic faculty, postdoctoral researchers, and graduate students. Furthermore, half of the presentations were chosen from submitted abstracts. Presentations ranged from small molecule crystallography, to crystal engineering, to mineralogy, and even the diagnosis of a new disease given the name 'Adult Onset Crystallography (AOC).'

Stephanie Hurst, Northern Arizona U, discussed her efforts to secure funding for the purchase of a single-crystal X-ray diffractometer. The plan put forth in her proposal is for an instrument to be housed at NAU and available for a host of schools in the 'crystallographically isolated' Colorado Plateau area. Stephanie also discussed her work with tropylium complexes and tropylium derivatives as well as the synthesis and characterization of dibenzoxanthene derivatives, which involve collaborations respectively with the ALS Synchrotron and with **John Lee**, U Tennessee, Chattanooga.

Lauren Mitchell, currently a postdoctoral researcher at U.S. Naval Academy, discussed work that she performed while a graduate student at U Texas at Austin. At UT, Lauren had the opportunity to use her department's diffractometer to solve structures for 10 different synthetic groups. The focus of her presentation was on work with iridium complexes of highly-conjugated, bidentate cyclometallating ligands. These complexes were prepared for their luminescent properties to be utilized in

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2.2.3: How I Spent My Summer Vacation, ctd.

OLEDs, and crystallography was exploited in an attempt to relate structure to their quantum efficiency.

Christopher Durr, currently a postdoc at Ohio State U, discussed his work utilizing crystallography to develop a project that was otherwise non-existent within his research group. Christopher's research originally involved the preparation of X–Y (where X–Y = Mo–Mo, W–W, or Mo–W quadruple bond) complexes with novel bridging acetate ligands to be used to capture light energy in solar-energy conversion. Taking crystals of synthetic intermediates and using knowledge gained during his summer school experience he was able to look not only at just the isolated single molecule but at the packing within the crystal lattice as well. This revealed intermolecular halogen-halogen interactions that extended through the lattice. He then used these results to develop crystal engineering by changing the interactions between the molecules.

Dean Johnston, Otterbein U, discussed a combination of incorporation of his benchtop diffractometer into his department's undergraduate curriculum (i.e., course development), research with undergraduates, and collaborations with other institutions. Incorporation into the classroom initially was done at the sophomore level in an inorganic laboratory and then extended to a full course in crystallography at the senior level. A symbiotic relationship was developed between teaching crystallography and undergraduate research with particular interest in the structure of polynuclear molybdate and tungstate anions.

John Lee discussed his use of knowledge gained at the summer school in application to undergraduate research. As a new faculty member with no prior formal X-ray crystallography training he used the ACA summer school experience to start an undergraduate research program in synthetic inorganic and organometallic chemistry centered around his department's benchtop diffractometer. John discussed the preparation and characterization of a series of organometallic ruthenium piano-stool complexes with different phosphines and phosphites with varying amounts of fluorine. Here they were able to use a combination of results, which included single-crystal X-ray crystallographic data, to make a rational choice for a complex to take forward for catalytic studies.

Nichole Valdez, currently a graduate student at U Idaho studying both chemistry and geology, discussed using X-ray crystallography as a technique to characterize minerals. Nichole showed several examples including how Olex2 could be used to observe both extended structure and polyhedra. The second half of her presentation included a chemistry portion where she is currently looking at polyoctahedral silsesquioxanes and hexamolybdates in collaboration with Peter Müller, MIT.

In conclusion, the first annual reunion for former ACA summer school participants was successful. The presentations were given from a spectrum of career points from student to postdoc to junior faculty and senior faculty. This allowed for great networking between the speakers in addition to opening the door to a new venue (i.e., several were first-time attendees) for faculty and students to present their work.

John Lee and Amy Sarjeant

2.2.4: SAS with Membranes and Membrane Proteins

L-R: Mark Lensink, Frederick Heberle, Drew Marquardt, Volker Urban, Shuo Qian, Ryan Oliver

Membranes and membrane proteins continue to present new and unexpected challenges to researchers seeking to understand their structure and organization. For example, one of the challenges is to understand membrane protein structure in a membrane context. At the same time, membrane plays an important role in defining membrane protein structure and other regular cell activities. SAXS and SANS are at the leading edge of these efforts, allowing for structural studies in biologically relevant solutions or membrane-mimetic conditions. Especially, SANS with contrast variation technique provides methods for these systems without the use of extrinsic probes. This session focused on current and emerging methods to study membranes and membrane proteins with scattering and other complementary techniques.

Volker Urban, Oak Ridge National Lab, presented the use of biocontinuous microemulsions as a biomembrane mimetic system for membrane proteins developed with collaborators from Douglas Hayes's group at U Tennessee, Knoxville. Volker showed how a biocontinuous microemulsion system was used

in a SANS study of the incorporated antimicrobial peptide melittin; the results were comparable to other studies of melittin in liposomes. **Ryan Oliver**, a recent graduate of U Virginia in transition to a postdoctoral position at Oak Ridge National Lab, presented his Ph.D. thesis work on determining micelle and bicelle structure with SAS. Ryan's systematic studies on detergents and lipid-detergent mixtures provide important references to optimize membrane protein folding in solution for SAS experiments. **Marc Lensink** of CNRS, an invited speaker from France, presented the latest developments in probing membrane protein structure with SAS and molecular modeling. Their strategy of combining explicit atomic detergent modeling with SANS measurements holds significant potential for structural studies of other detergent-solubilized membrane proteins.

After coffee break, **Drew Marquardt**, U Graz, an invited speaker from Austria, focused on the methods and structures of asymmetric liposomes. The effort of developing well-controlled asymmetric liposome bilayers constituted a significant step toward a more realistic model membrane system for biophysical and membrane protein studies. To wrap up the session **Shuo Qian**, Oak Ridge National Lab, presented a recent realization of performing membrane diffraction on typical SANS instruments. The large unit cell of lipid 'quasi-crystals' encountered in modeling membrane fusion is ideal for small-angle diffraction. The resulting SANS structure was consistent with the X-ray structure that was solved earlier and clearly revealed the water distribution in a membrane fusion intermediate structure.

Shuo Qian

2.2.5: Mechanistic & Spectroscopic Structural Enzymology

Brian Mahon, U Florida, presented a carbonic anhydrase IX (CA IX) surface variant structure. CA IX is an established biomarker and drug target for several aggressive cancers. Wild type CA IX has been difficult to crystallize, so they designed a construct that crystallizes more easily and shows highest activity at physiological pH. Its crystal structure was determined at 1.6 Å. They characterized the ordered water network in its active site. Also, differential scanning calorimetry results show that this construct is thermostable between pH 7-9.

Diana Tomchick, U Texas Southwestern Medical Center, shared results on the identification of flavin trafficking protein (Ftp) in syphilis spirochete (*Treponema pallidum*). Two subclasses of Ftp proteins have been identified: FAD binders and FAD hydrolyzers. FAD pyrophosphatase is a metal-dependent enzyme that hydrolyzes FAD into AMP and FMN in the periplasm. FAD binding and enzyme activity is dependent on two Mg^{2+} ions binding to its catalytic center. The Tomchick group's results show via mutagenesis that a single amino acid substitution converts it from an FAD-binding protein to an Mg^{2+}-dependent FAD pyrophosphatase (*T. pallidum*-like). Furthermore, Diana shared that covalent flavinylation occurs on components of bacterial RnF and/or NqR redox systems

Raymond Trievel, U Michigan, surveyed the role of S-adenosyl-L-methionine (AdoMet)-dependent methyltransferases in metabolism and signal transduction. These enzymes belong to multiple distinct classes sharing a catalytic mechanism that arose through convergent evolution; however, the fundamental determinants underlying this shared methyl transfer mechanism remain undefined. Biochemical and structural characterization of a model lysine methyltransferase and active site mutants that abolish carbon–oxygen hydrogen bonding to AdoMet illustrate that these interactions are important for high-affinity AdoMet binding and transition-state stabilization. Corroborative crystallographic and NMR dynamics studies of the wild-type enzyme demonstrate that the carbon–oxygen hydrogen bonds constrain the motion of the AdoMet methyl group, facilitating its alignment during catalysis. Together, the structural survey and the experimental and computational results illustrate that methyl carbon–oxygen hydrogen bonding represents a convergent evolutionary feature of AdoMet-dependent methyltransferases, mediating a universal mechanism for methyl transfer. (See also the description of poster **S28**, under **General Interest Posters** on pp. 37-38.)

Flora Meilleur, North Carolina State U and Oak Ridge National Lab, discussed the application of neutron crystallography to GTPase and redox enzymes. Neutron protein crystallography allows the experimental location of hydrogen atoms at resolutions (~2.2 Å) typical of protein crystallographic structures. The sensitivity of neutrons to hydrogen arises from their interactions with atomic nuclei; this is in contrast to X-rays, which interact with atom electron clouds. The data presented by Flora were collected on the IMAGINE beam line at the High Flux Isotope Reactor of Oak Ridge National Lab. Key features of the neutron scattering length density maps illustrated how neutron protein crystallographic data contribute to a more complete description of chemical reactions catalyzed at enzyme active sites.

Mohammed Taha

Stephan Ginnell, at left, with Patrick Loll. Photo by Dick Bromund.

2.3.1: Professional Development: Communicating Your Science

L-R: back row – Jarrod French, Joseph Gindhart, Darcy Gentleman, Celeste MacElrevey, Andrew Torelli; front row – Amalia Issa, Katherine Sippel. Photo courtesy of Andy Torelli.

This year the Young Scientists Special Interest Group (YSSIG) hosted the first in what we hope will be an annual series of sessions on professional development. It was an extremely exciting and informative session that brought together experts from diverse career paths to share insights and advice on how to effectively communicate to specific audiences.

Darcy Gentleman, Manager, Engagement and Science Communications at the American Chemical Society, shared news of the Chemistry Champions project he is spearheading to empower and engage young chemists across the nation by challenging them to explain their research in a simple way to diverse audiences. Darcy also underscored the importance of 'knowing your audience' with accounts of his work interacting with members of Congress and their staff to educate and inform policymakers about topics broadly relevant to chemistry. **Amalia Issa**, Professor and Chair of the Department of Health Policy and Public Health at University of the Sciences in Philadelphia, expanded on Darcy's segue to communicating with legislators, and outlined the design and delivery of successful presentations in this context. Amalia provided a framework for effectively translating research and communicating your message to policy makers and the general public. **Celeste MacElrevey**, a pharmacokineticist with Nuventra Pharma Sciences, shared her experiences and insights into the intricacies of communicating in a regulatory forum. Celeste outlined the major developments that have influenced regulatory principles over the past several decades and discussed the challenges of maintaining good laboratory practices while working within the guidelines set by the FDA and EPA that shape regulatory filings. We also heard from **Joseph Gindhart**, a program director in the Division of Cell Biology and Biophysics at NIH. Joseph discussed the merits of communicating with your program officer (PO) throughout the NIH grant cycle and detailed how to identify the appropriate PO, when to contact them, and what details and information they can help you with. He also highlighted the power of using the NIH Research Portfolio Online Reporting Tools (RePORT) to find research programs and NIH personnel online with research interests that overlap your own. The session ended with a very informative talk by **Katherine Sippel**, a contract science writer and editor from BioScience Writers, on strategies to improve written communication. Katherine's talk included specific advice and tips to clarify writing, such as removing redundant and unnecessary text, and choosing appropriate power words. Katherine also emphasized the need to use simple words and to balance adjectives and prepositions. A highlight was her explanation of the serial position effect of free recall. This theory explains why it is important to place the major message at the beginning and end of a sentence or paragraph.

Overall, this session was extremely successful and received tremendous positive responses from those who attended. Our diverse set of speakers provided informative and thoroughly captivating presentations that sparked exciting discussions during and after the session. It is clear from the questions asked, and feedback received, from the young scientists in attendance that these speakers addressed crucial issues and provided valuable advice on various fundamental aspects of communicating science. For those who were not able to attend our session, copies of the presentations given by our speakers will be posted in the Young Scientists Zone on the ACA website. As the session organizers, and on behalf of the YSSIG, we would like to thank **Laboratory Product Sales** of Rochester, NY, and the ACA for their very generous support.

Jarrod French and Andy Torelli

2.3.2: Would You Publish This?

L-R: back row – Frank Fronczek, Carl Schwalbe, Lee Daniels, Allen Oliver, Brian Dolinar; front row – Carla Slebodnick, Louise Dawe, Christine Beavers. Photo courtesy of Louise Dawe.

Would You Publish This? returned after a two-year hiatus, co-chaired by Louise Dawe, Wilfrid Laurier U, Canada, and Brian Dolinar, U Wisconsin – Madison, and with generous support from **Crystallographic Resources, Inc.** **Allen Oliver**, Notre Dame, introduced the evening with an editor's perspective on the value of considering X-ray structures in their research context. **Carl Schwalbe**, Aston U, U.K., brought forward the question of how to share data with possibly limited research impact, but that has been generated from public (tax) funds. During the course of the evening **Carla Slebodnick**, Virginia Tech, **Lee Daniels**, Agilent, and **Christine Beavers**, Lawrence Berkeley National Lab, led the audience in engaging discussions on publishing structures with a variety of problems, and the importance of supporting characterizations. **Frank Fronczek**, Louisiana State U, closed the evening by discussing a situation where excellent refinement values were obtained for a chemically unreasonable structure.

Louise Dawe

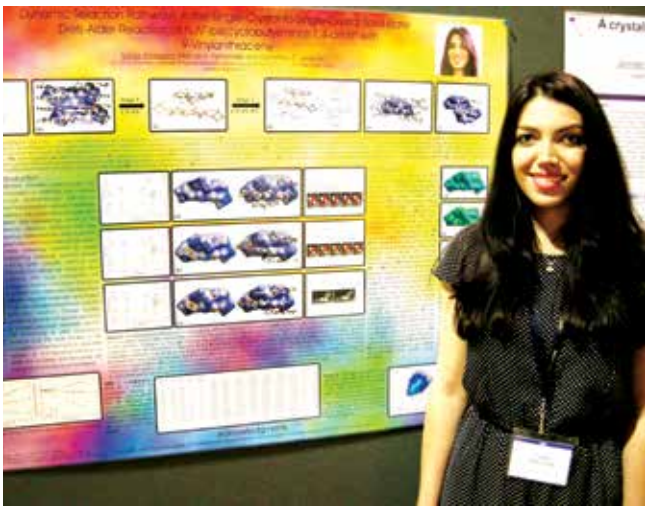
General Interest Posters

Picking posters to summarize from the wealth of beautifully presented fascinating science on show in Philadelphia is inevitably dictated by one's personal predilections. As a small-molecule crystallographer, I was fascinated by three posters applying this technique to solid-state reactions and two posters using concepts or data from small-molecule studies to inform protein crystallography.

Poster **M23**: *Doping Effects on Thymine Monohydrate Crystals*, presented by **Elizabeth Koch**, Georgetown U

As a constituent of DNA, thymine has been very well studied; but it still holds surprises. It crystallizes both in anhydrous form (CSD Code THYMIN01, denoted T) and as the monohydrate (THYMMH, denoted TMH). Because the TMH crystal has obvious water channels, it would seem that the dehydration observed in air starting at about 50°C could occur simply by ejection of water molecules from the channels and closure of the resulting gaps. Although hot-stage microscopy confirms that the fastest dehydration occurs along the *c*-axis, which is the water channel direction, the actual mechanism must be more complicated because the direction of hydrogen bonds between heterocycles changes between the two forms. Instead, a pure single crystal of TMH forms an opaque polycrystalline block of a disordered phase, T_d. The structure of this intermediate phase has now been determined from synchrotron data collected at APS. Thymine molecules in T_d sit on a special position, providing alternative positions for O2 and hence the hydrogen bonds it accepts. Sublimation at about 190°C then converts T_d to T. Next, doped crystals were grown from saturated aqueous solutions of thymine (0.04 M) also containing 1 of 24 different dyes at low concentration (10^{-6} – 10^{-7} M). TMH crystals were obtained with 19 of the 24 dyes, while with the other 5 dyes crystals of T were the result. The doped TMH crystals had the same plate-like morphology as pure TMH crystals but were obviously colored. Analysis by differential scanning calorimetry showed that the already low concentration of dye in the crystallization mixture had been reduced by a factor of about 100 in the doped crystals. Nevertheless, the dehydration temperature had increased by an average of about 12.8°C. Large increases in dehydration temperature were observed whether the dyes were cationic, neutral, or anionic. Kinetic parameters suggest that dehydration of the pure material occurs by a one-dimensional diffusion mechanism; however in the doped systems the dehydration occurs by a three-dimensional diffusion mechanism. The supposition is that the dye molecules interfere with this mechanism by steric hindrance, retarding either the egress of water or the collapse of the host. Future work, again making use of synchrotron radiation, will try to locate the dye binding sites.

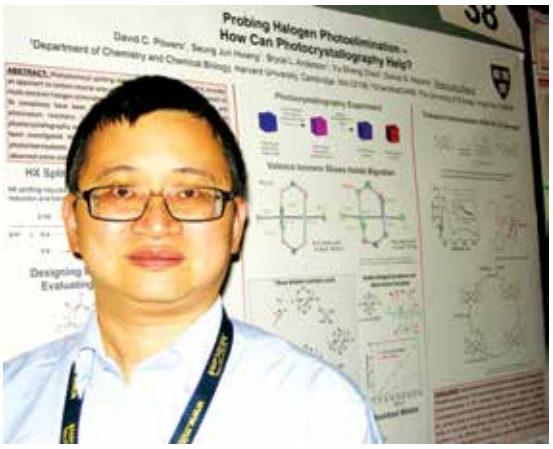
Poster **M35**, *Dynamic Reaction Pathways in the Single-Crystal-to-Single-Crystal Solid-State Diels-Alder Reaction of N,N'-bis(cyclobutylimino)-1,4-dithiin with 9-Vinylanthracene*, presented by **Sanaz Khorasani**



Sanaz and colleagues at U Witwatersrand in South Africa have been looking at a single-crystal-to-single-crystal reaction with interesting kinetics. Diels-Alder cycloaddition occurs within a crystal of the 1:1 charge-transfer complex (CT) composed of stacks of alternating *N,N*'-bis(cyclobutylimino)-1,4-dithiin and 9-vinylanthracene molecules, where the orientation of the vinyl influences the reaction pathway. It starts by forming a single product, P1 (product 1). After the reaction has converted about 34% of CT to P1, additional P1 continues to form but another product P2 begins to appear. At 88% conversion, reaction ceases with 71.5% P1 and 16.5% P2 having formed. The space group remains unchanged, but as conversion proceeds from pure CT to the 88% limit, the *a*-axis lengthens by 1.2%, the *b*-axis lengthens by 0.3%, and the *c*-axis contracts by 0.7%. In the CT crystal the reactant molecules alternate in a stack along the *a*-axis. Simplistic consideration of the distances between the bridgehead carbon atoms of a single vinylanthracene molecule and potential reaction partner atoms in the acceptor molecules above and below in the stack shows that they are 3.46 and 3.52 Å in the pairing that would lead to P1, 3.47 and 3.64 Å in the pair for P2. Because all of these values are comfortably within Schmidt's criterion requiring the reacting atoms to be closer than 4.2 Å, deeper analysis is needed to explain the selectivity in favor of P1. Hirshfeld surfaces for the CT with the surrounding packing environment show no obstacles to the formation of P1 as the vinyl group points away from these reacting molecules. However, the vinyl group is oriented between the reacting molecules that lead to P2 preventing its formation. The packing environment also prevents the vinyl group from undergoing the rotation required

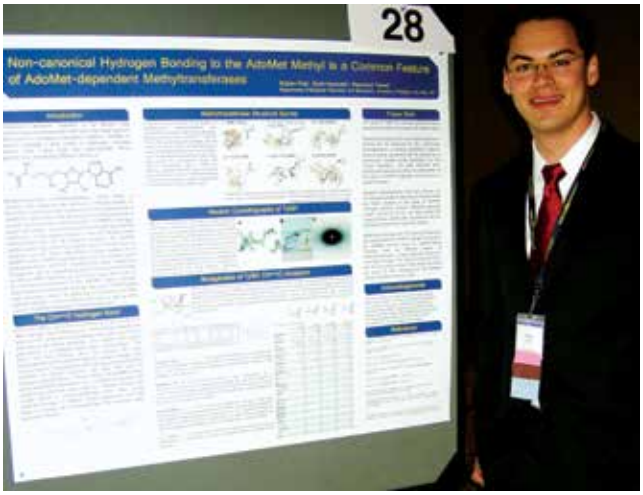
to form P2 during the early stages of the reaction, but the vinyl group rotates out of the way when sufficient space is created around it during the formation of P1 molecules in surrounding stacks, which allows the formation of P2. Hirshfeld surfaces based on the reacted crystal coordinates for later stages of conversion (around 67% and around 88% respectively) indicate the presence of very close contacts as the reaction nears completion. The compatibility of packing arrangements for CT, P1, and P2 was further tested with PIXEL (intermolecular energy) calculations. A hypothetical P1 only crystal is much more stable than a hypothetical P2 only crystal. This suggests that the final crystal structure is dominated by P1 while P2 and the CT molecules are probably arranged in an ordered manner in the reacted crystal that prevents close contacts, indicating significant cooperativity between the molecules during the reaction.

Poster **T38**, *Probing Halogen Photoelimination – How Can Photocrystallography Help?*, presented by **Shao-Liang Zheng**, Harvard U



In nature, oxygenic photosynthesis involves the splitting of water into oxygen and hydrogen, the latter product eventually bringing about the reduction of CO_2. For the reaction $2H_2O \rightarrow 2H_2 + O_2$ the standard Gibbs free energy change per electron is +28.4 kcal/mol. However, the splitting of HCl according to the equation $2HCl \rightarrow H_2 + Cl_2$ would capture even more free energy, $\Delta G°$ per electron being +31.3 kcal/mol. The photolysis of bimetallic rhodium-containing complexes with Cl ligands together with phosphinomethylamine ligands has been investigated by photocrystallography. Diffraction data are collected in the dark and again when the crystal on its goniometer head is irradiated with a laser. A photodifference map demonstrates halide migration. Analysis of transient absorption spectra shows that photolysis of Rh_2[I,III] and Rh_2[II,II] valence isomers proceeds via a common intermediate. Encouraging though the results with rhodium may be, the scarcity and expense of this element would preclude its use on a large scale. A far more realistic prospect for free-energy capture is the recently discovered photoelimination of halide from mononuclear Ni(III) complexes. High-yielding Cl_2 elimination has been achieved from such a complex with 3 Cl ligands and a bis-(diphenylphosphino)ethane ligand. Although this substance has not yielded diffraction-quality crystals, its bromo analog has, revealing a distorted square-pyramidal complex. The apical Ni(III)-Br bond is a few hundredths of an Ångstrom longer than the basal bonds. A difference map was based on diffraction data collected from a crystal of the analogous bis-(diphenylphosphino) ethylene complex before and then while undergoing laser irradiation at λ = 365 nm. It showed that in the photoproduct the apical bond had lengthened by almost 1.25 Å. Thus there is a stereoelectronic preference for apical Ni-X photoextrusion. A plausible mechanism suggests that the apical halide atom, as it breaks free of the Ni atom, is abetted in its escape by interaction with one of the aryl rings of a diphenylphosphine moiety.

Poster **S28**, *Non-canonical Hydrogen Bonding to AdoMet is a Common Feature of AdoMet-dependent Methyltransferases*, presented by **Robert Fick**, U Michigan



The proposal of C-H…O hydrogen bonding by June Sutor in 1963 met with a great deal of prejudiced opposition, even though it now forms an essential part of the analysis of the intermolecular interactions of small molecules. Work in the research group of Raymond Trievel, see p. 33, has demonstrated the significance of C-H…O interactions in macromolecular recognition, specifically the S_N2 mechanism of methyl transfer from S-adenosyl-L-methionine (AdoMet) catalyzed by AdoMet transferases. AdoMet is the most common biological methyl donor. It donates the methyl group to a wide variety of recipients, in reactions catalyzed by enzymes that are structurally unrelated. Nevertheless, they exhibit a conserved catalytic mechanism. A survey of high-resolution structures in the PDB of methyltransferases with bound AdoMet showed that, based on distance and angle criteria, the methyl carbon atom of AdoMet was close enough to active site oxygen atoms that C-H…O hydrogen bonding could be inferred. Methyl groups are generally considered to be weak C-H…O donors, but attachment to the positively charged S atom in AdoMet should activate the H atoms. Of course, no methyl hydrogen atoms were actually located; however, the inference was reinforced by various analytical techniques and by quantum mechanical calculations. Robert's poster reported progress in verification by more direct means. Now that crystals have been grown of TyIM1 protein plus AdoMet with its methyl group deuterated, neutron diffraction should be able to reveal these D atoms and their interactions. Measurement of neutron diffraction data from this material to about 6 Å on HFIR at Oak Ridge provides proof of principle. Additional mutagenesis studies also provide support: Tyr-14 –> Phe removes one hydrogen bond acceptor and is predicted to decrease substrate affinity based on quantum

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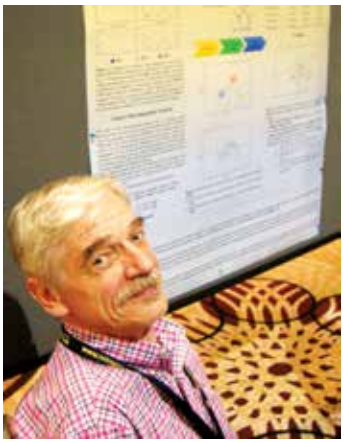
General Interest Posters, ctd.

mechanical calculations. Mutating Ser-120 –> Ala removes an acceptor for the two methylene groups flanking S^+, thought to be involved in substrate/product discrimination. The double mutant lacks two hydrogen bond acceptors. These mutants have been structurally characterized to validate their use in biochemical studies.

Poster **T41**, *Protonation Changes Geometry of Histidine Rings*, with first author Miroslawa Dauter, presented by **Zbigniew Dauter**, National Cancer Institute, Argonne, IL



The imidazole ring in histidine contains two nitrogen atoms, ND1 and NE2, either or both of which may be protonated. Changes in protonation state affect the geometry of the ring. Only in very rare cases can the relevant hydrogen atoms be located in a protein, but sometimes hydrogen bond donors or acceptors in the environment may give a clue. On the other hand, the Cambridge Structural Database contains a large number of imidazole structures for which the protonation state is clear and the geometry has been accurately determined. In 1991 Engh and Huber compiled a set of stereochemical restraint target values for use in protein structure refinement, EH91, based on the small-molecule data available at that time. A decade later, the revised EH99 set was compiled, based on more voluminous data. The present authors have incorporated the wealth of new small-molecule data to produce a definitive set. The geometry around an unprotonated nitrogen atom may be affected by metal binding or hydrogen bond acceptance, but these factors had much less effect than protonation. Trigonometric impossibility was found in the tabulations of EH91 and EH99 geometry for protonation at ND1. In fact, this error has had little practical effect since the popular programs for routine refinement assume double protonation regardless of other clues! As one might expect, protonation of either nitrogen atom has the greatest effect on the bond distance to the intervening carbon atom and the endocyclic bond angle at that N atom. Discriminative analysis has produced two functions of these geometric variables, *his1* and *his2*, such that a two-dimensional plot of these values for the small-molecule imidazole structures reveals three well-defined clusters corresponding to the different protonation states. When the same functions are plotted for atomic-resolution (better than 1 Å) protein data from the PDB, the clusters blur together. However, this appears to be a consequence of always using restraints for doubly protonated histidine. To test the discrimination analysis, a recently released 0.99 Å structure, PDB ID 4rj2, was re-refined with histidine restraints removed. For most of the histidine residues a clear indication of the protonation state appeared after re-refinement. It then becomes possible to re-apply restraints specifically appropriate to that state.

I conclude by abusing the privilege of a roving reporter to give a brief mention of my own poster, **S20***: 'H...H Clashes in Published Carboxylic Acid Structures.' I found 31 catemeric carboxylic acid structures in the Cambridge Structural Database with OCOH…HOCO contacts so close that they triggered a CheckCIF Class A alert. Some of these were published in journals as respected as Acta Crystallographica, Section C! Although the SHELXL manual carries an explicit warning, it is all too easy to rely on the automatic placement of hydrogen atoms without examining the difference electron density, the interatomic distances, or the CheckCIF output – any one of which would have pointed out such a clash arising from the placement of two hydrogen atoms along the same hydrogen bond. Thanks to the watchful eyes of* ***Richard Marsh****, missed symmetry elements have been exposed and there are even signs of an 'inverse Marsh effect' where authors, fearful of getting Marshed, have treated pseudo-symmetry as exact symmetry. At previous ACA meetings we have had spirited presentations by* ***Bernhard Rupp*** *reminding us that binding sites in proteins want to bind something, if only buffer components; and it is all too easy, by a process of wishful thinking, to interpret such peaks as one's new wonder drug. I think it is only a matter of time before getting caught making such an error will be called 'getting Rupped.' I doubt if placing hydrogen atoms in clashing positions will be called 'getting Schwalbeed' – but please check that CheckCIF output carefully!*

Carl Schwalbe

3.1.1: Etter Early Career Symposium

The **Etter Early Career Symposium**, sponsored by the Young Scientists Scientific Interest Group (YSSIG), is held yearly to honor the memory of Margaret C. Etter. The symposium immediately followed Jessie Zhang's Etter Award Lecture, in which she presented the work from her laboratory that aims to understand and decipher the combinatorial CTD code for eukaryotic transcription. Since the assembly of transcription apparatus is regulated by information programmed in the C-terminal domain (CTD) of RNA polymerase, Jessie's group has studied the phosphorylation state of this domain extensively. She presented several structures and biophysical studies of the CTD that provide insights into how the phosphorylation state affects the outcome of transcription. Jessie's work is featured on our cover. See also p. 7, **What's on the Cover**, for her award citation and for more information about her award-winning research.

The Etter Early Career Symposium featuring student and postdoc presentations opened with a presentation by **Matthew Whitley**, U Pittsburgh School of Medicine. Matthew presented a combined small-angle X-ray scattering and NMR analysis of the conformational ensemble present in the partially denatured state of V75D mutant intermediate of human γD-crystallin. Using the experimental data to lead computational modeling of the structural assembly, he provided the structural insides of a non-native state of γD-crystallin mutant.

Powder Diffraction SIG **Etter Student Lecturer** awardee, **Daniel Mast**, U Nevada, spoke about a structural investigation of technetium metal at high pressure and variable temperature via high-resolution X-ray powder diffraction. The equation of

state has been determined up to 150GPa and agrees with results of DFT calculations.

Jennifer Gadient, U Toledo, presented the results of *in situ* high-pressure measurements for a number of negative thermal expansion materials with general formula $A_2M_3O_{12}$. Jennifer showed that in case of different trivalent metal species (M = Mo or W), different high-pressure phase transitions can be observed.

Aaron McGrath, U California, San Diego, presented several crystal structures that provided structural insights into ligand entry, malleable binding, and induced helical movement in P-glycoprotein. The crystal structures provide information that will enhance the understanding of how this protein binds metabolites and drugs.

The YSSIG **Etter Student Lecturer** awardee, **Katarzyna Handing**, U Virginia, presented crystal structures that analyzed the binding of zinc to serum albumin that sheds light on metal transport and distribution in mammals. **Lisa Mueller**, U Wisconsin – Milwaukee, continued the session by discussing her efforts to understand the structure and function of the acetoacetate decarboxylase-like superfamily and presented crystal structures of the Sbi00515 protein in complex with substrates, providing insight into the catalytic mechanism of the enzyme.

General Interest SIG **Etter Student Lecturer Pawel Janowski**, Rutgers U, discussed his current research efforts on how molecular dynamics can be utilized as a powerful tool in improving the analysis of crystallographic data. To wrap up the symposium, Light Sources SIG **Etter Student Lecturer Pascal Krotee**, U California, Los Angeles, described the use of electron diffraction to obtain crystal structures of Type-II diabetes-related peptides from very small crystals.

George Lountos and Andrey Yakovenko

3.1.2: Local Structure and Complex Materials

Olaf Borkiewicz, Argonne National Lab, showcased novel sample environments for examining devices *in situ* and their usefulness in studying energy storage materials such as those found in batteries. Hard X-rays have been very successful in elucidating failure modes and operational modes in new candidate materials for insertion and interconversion electrodes such as FeF_2. When battery cycling produces crystals too small for standard crystallography, pair distribution function analysis has revealed the whole story and explained the loss in electrochemical capacity after initial cycling.

Kirsten Jensen, Columbia U, presented a relatively new experimental method: computed tomography pair distribution function (ctPDF) analysis. Kirsten demonstrated the power of this technique, reporting on the spatial mapping of the internal crystalline and amorphous phases inside a traditional AAA battery without even having to open up its case. Then, in an unexpected twist, she introduced us to the important role that this technique can play in historical preservation. Using ctPDF, fragments of the hull of the Mary Rose (Henry VIII's warship sunk in 1545 and recovered in 1982) have been examined to identify sources of sulfuric acid that are decomposing the hull of the ship.

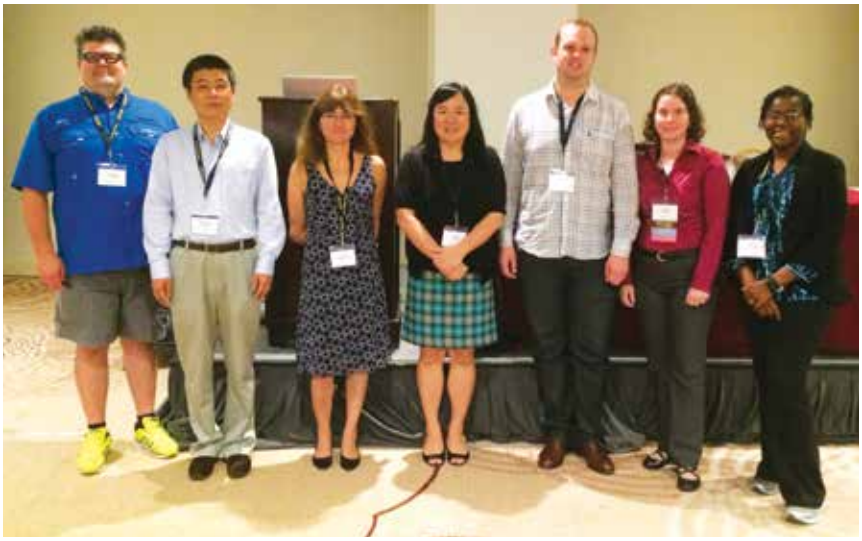
Igor Levin, NIST, discussed advances in reverse Monte Carlo modeling using multiple data types simultaneously, for example in fitting one model to X-ray and neutron PDF, EXAFS, and diffuse electron diffraction data. Igor described how this method was used to solve some mysteries regarding anomalous structure property relationships in $Ca_xBa_{1-x}TiO_3$ and $Ba_{1-x}Bi_xTi_{1-x}Sc_xO_3$ perovskite high-dielectric ceramics.

Katharine Page, Oak Ridge National Lab, opened her talk by providing an update on recent advances in data reduction on the total scattering instruments at the Spallation Neutron Source. Katharine then discussed novel modeling strategies for a new family of 2D and nanostructured compounds, MXenes. These materials present a complex challenge in the need to simultaneously describe the interlayer bonding, and particle shape and size, as well as correlations between particles – a full tour de force in atomistic modeling of complex data sets.

Martin Donakowski, Naval Research Lab, presented new data on a family of RuO_2-derived nanostructured composites that are enabling the development of ultracapacitor technology. Marty's results stimulated a productive discussion on the complex relationship between Ru–O and Ru–Ru bonding that can exist in these important families of functional materials.

Graham King and James Neilson

3.1.3: Hot Structures I – Intracellular Protein Regulons



L-R: Christopher Colbert, Huanchen Wang, Kristina Djinovi-Carugo, Hyun-Joo Nam, Richard Bunker, Chelsy Prince, Oluwatoyin Asojo. Photo courtesy of Hyun-Joo Nam

Richard Bunker, Friedrich Miescher Institute, Basel, Switzerland, discussed the crystal structure of COP9 signalosome, an elaborate ~350 kD eight-protein hetero-complex regulating the cullin-RING ligase (CRL) complexes (see illustration on top of p. 40). CRL ubiquitin ligases modify crucial cellular regulators and route them to proteasomes. Richard presented details of the crystallographic analysis and

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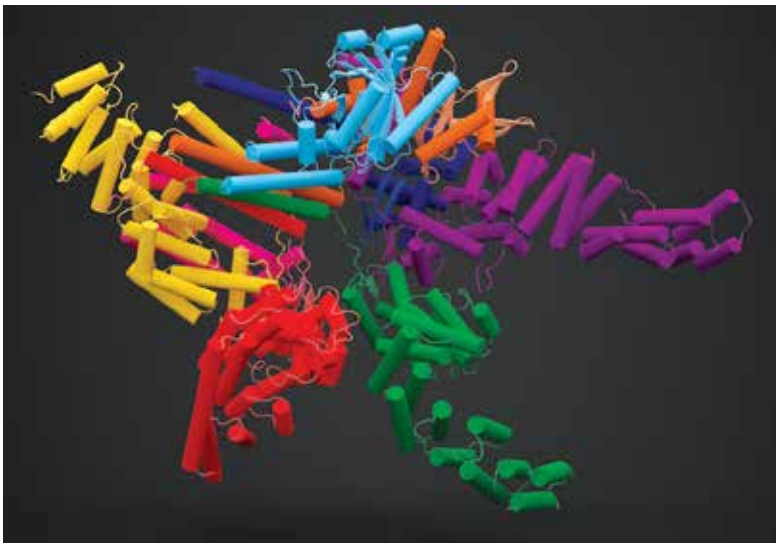
Hot Structures I, ctd.

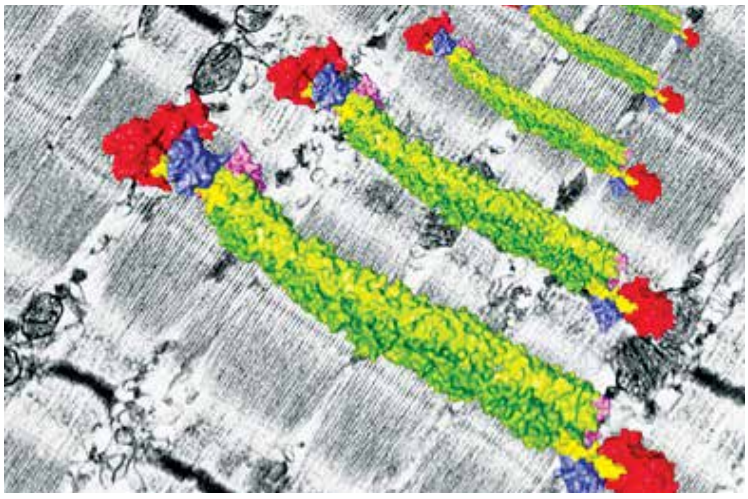


Cartoon representation of the human COP9 signalosome (CSN), an elaborate eight-protein (~350 kDa) protein hetero-complex that is a master regulator of intracellular protein degradation (from PDB entry 4D10). CSN is an essential eukaryotic complex with specialized isopeptidase activity that regulates the largest class of ubiquitin (E3) ligases – the cullin-RING ligase complexes (CRLs) – of which humans have several hundred. Ubiquitin ligases confer substrate specificity to ubiquitination, the process of post-translationally modifying proteins with the small protein, ubiquitin. For proteins ubiquitinated by CRLs, which include crucial regulators of DNA repair, growth, and development, this typically leads to their turnover by the 26S proteasome. Courtesy of Richard Bunker.

comparisons with electron microscopy data. Functions of each submit were discussed based on the mutational studies.

Chris Colbert, North Dakota State U, described the crystal structure of the cytoplasmic domain of PupR, a TonB-dependent transporter (TDBT) in *Pseudomonas putida*. PupR stimulates its own transcription upon iron binding at the extracellular segment by releasing the Sigma Factor bound to its cytoplasmic domain. Chris reported that the PupR cytoplasmic domain forms a dimer of three-helical bundles that suggest sequestering mechanisms of the Sigma Factor.

Kristina Djinovi-Carugo, U Vienna, Austria, presented results on α-actinin, a major actin cross linker in muscle and other cellular structures (see illustration below). Kristina described the high-resolution structure of the 200-kDa α-actinin-2 dimer from striated muscles, and discussed mechanistic insights of α-actinin interactions with sarcomere proteins such as titin. A phosphoinositide-dependent mechanism may be responsible for the interactions based on biochemical and cell-biophysics data.



Surface representation of the α-actinin dimer (Cell, 2014, http://dx.doi.org/10.1016/j.cell.2014.10.056) against a background of muscle sarcomeres viewed under the electron microscope. The sarcomeres display a typical striated pattern and are connected via joint Z-discs, seen as dark black and grey diagonal stripes. Courtesy of Mathias Gautel and Andrea Ghisleni, Kings College London (U.K.); Nikos Pinotsis and Kristina Djinovic-Carugo, MFPL, U Vienna.

Oluwatoyin Asojo, Baylor College of Medicine, reported the high-resolution structure of SALO, an 11kD protein from sand fly salivary gland homogenate. Oluwatoyin described the ongoing effort in vaccine development against *Leishmaniasis* transmitted through sand fly vectors, and purification of SALO as a candidate. SALO inhibits classical pathway (CP)-mediated hemolysis and C4b deposition.

Huanchen Wang, NIH, presented structural studies of IP6K and PPIP5K, two kinases involved in cellular signal transductions. These kinases add diphosphate groups to inositol rings at two different positions leading to different signal transduction pathways. Huanchen discussed a 'catch-and-pass' reaction mechanism employed by PPIP5K and IP6K. Inhibitor development is in progress.

Chelsy Prince, Queens University, Canada, presented the crystal structure of LapB, a key regulator of lipopolysaccharide synthesis (LPS) pathways in *E. coli*. The protein is composed of 9 tetratrico peptide repeats (TPR) motifs and a rubredoxin-type metal binding domain. Chelsy discussed insights into its functional mechanisms as docking sites for proteins in LPS pathways, based on mutagenesis data.

Hyun-Joo Nam

3.1.4 & 3.2.4: Standard Practices in Crystallography I & II: Data Collection Strategies and Data Reduction

This very well attended full-day session (consistently 130 to 150 attendees) was organized by Peter Müller, MIT, and was the first of a series of educational sessions sponsored by the ACA's Continuing Education and Data Standards and Computing Standing Committees. The session was co-sponsored by the General Interest, Service Crystallography, Small Molecules, and BioMac SIGs. Photos of the speakers and organizer are shown facing on p. 41.

The first three talks were dedicated to SAD phasing. **Dorothee Liebschner**,

L-R: back row – George Sheldrick, Dorothee Liebschner, Gerard Bricogne, Tobias Weinert, Mitchell Miller, Dominika Borek; in front – Peter Müller. Photo courtesy of Peter Müller.

L-R: back row – George Sheldrick, Zbigniew Dauter, Bruce Noll, Leo Straver; front row – Peter Müller, Dominika Borek, Chelsy Prince, Dorothee Liebschner. Photo courtesy of Peter Müller.

KEK, Tsukuba, Japan, **Tobias Weinert**, Paul Scherrer Institut, Switzerland, and **Chelsy Prince**, Queen's University, Canada, talked about *The Challenges of Soft X-rays: Data collection above 3 Å wavelength*, *Fast Native-SAD Phasing for Routine Macromolecular Structure Determination*, and *Tricks for Success using Zinc SAD Phasing*, respectively. The last talk before lunch by **Dominika Borek**, UT Southwestern Medical Center, had the title *Theory and Practice in X-ray Diffraction Data Processing* and was an excellent introduction to the details of data reduction.

After lunch, the focus of the session shifted to more general aspects of data collection strategy with interesting talks by **Mitchell Miller**, Rice U, **Gerard Bricogne**, Global Phasing Ltd., Cambridge, U.K., and **Zbigniew Dauter**, National Cancer Institute, Argonne, IL, who lectured about *Filling the Gaps: Data collection strategies for collecting diffuse scatter and Bragg data from low symmetry space groups*, *Back to the Future: Revisiting and improving interleaved protocols for experimental phasing, from design to processing*, and *Data Collection Strategy for Macromolecules*, respectively.

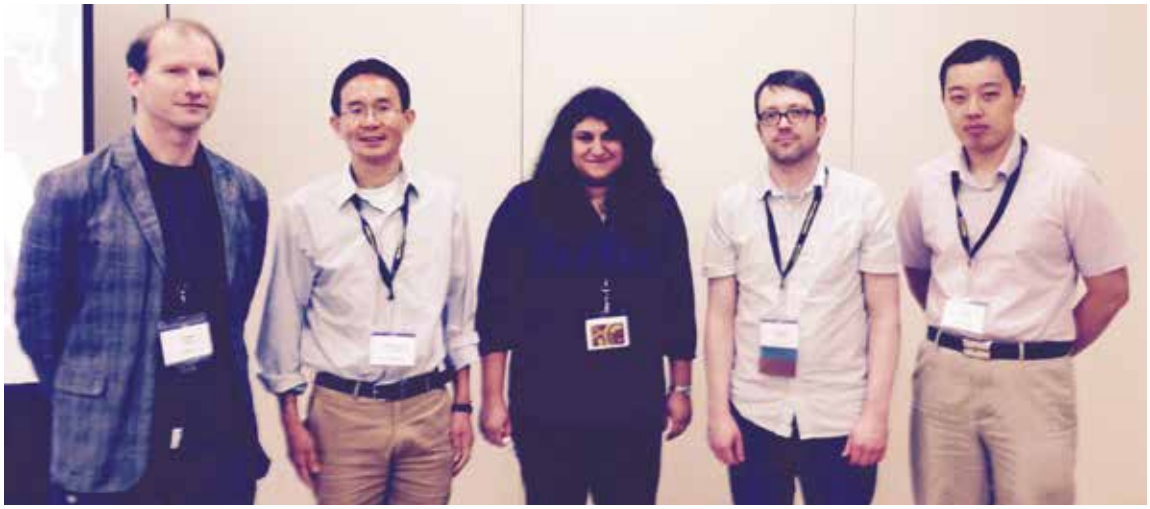
After the afternoon coffee break, **Bruce Noll**, Bruker AXS, and **Leo Straver**, Zoetermeer, Zuid-Holland, the Netherlands, presented a number of concrete examples how the data collection strategy influences the outcome of a diffraction experiment. Their respective talks had the titles *Fast Screening and Data Collection with the PHOTON 100 Detector*, and *Case Specific Optimization of Data Collection Strategy*. The final talk of the session was presented under the title *Data Scaling with SADABS and TWINABS*. In a fascinating and detailed presentation, **George Sheldrick**, U Göttingen, Germany, described how modern absorption correction and scaling is performed on the software level. This presentation dovetailed nicely with the lecture delivered before lunch by Dominika Borek, thus nicely rounding out the session.

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 first in a hopefully long series of **Standard Practices in Crystallography** sessions. Next year, at the annual ACA meeting in Denver, the second **Standard Practices** session will be on **Structure Refinement and Validation**. Invited speakers will include George Sheldrick, Ton Spek, and Tom Terwilliger.

Finally, it should be mentioned that **Bruker AXS** provided financial support for the session. Thanks to Bruker's generosity, many speakers from overseas could come to the meeting and Chelsy Prince received a student travel stipend.

Peter Müller

3.1.5: Structural Modeling for SAS



L-R: Thomas Weiss, Xiaolin Cheng, Farzaneh Tondnevis, Frederick Heberle, He Song. Photo courtesy of Xiaolin Cheng.

This session featured talks highlighting how the combination of solution small-angle scattering (SAS) data with detailed computational modelling can be used to uncover the underlying structure(s). The session was opened by **Xiaolin Cheng**, Oak Ridge National Lab, who showed how high-performance computing molecular dynamics simulations together with neutron contrast variation data can be used for elucidating the lateral organization in biologically relevant lipid membranes. Xiaolin further discussed remaining challenges and possible approaches to address them. **Hailiang Zhang**, NIST, then followed with a presentation on the application of molecular Monte Carlo calculations run on highly parallel GPU architectures for interpreting SAS data. Furthermore this simulation code is interfaced with a user friendly web-based GUI front-end (SASSIE-web), making it widely accessible. A presentation by **Frederick Heberle**, Oak Ridge National Lab, followed Hailing's talk and focused on the spatial organization and raft formation in asymmetric lipid vesicles. Fred showed how neutron scattering with contrast matching can be applied to decipher the mechanisms of leaflet coupling in asymmetric lipid bilayers and raft formation.

He Song, NIH, described the solution structure of the full-length *Saccharomyces cerevisiae* RNase III (Rnt1p) with and without RNA. Together with previously reported data this elucidated the full functional cycle of Rnt1p enzyme. In the final talk of the session **Farzaneh Tondnevis**, U Florida, described her work in elucidating the structure of the *E. coli* clamp loader clamp complex using small-angle X-ray scattering. The structure provides insights into the topological arrangements of the sliding clamp with respect to the clamp loader and exhibits high similarities to a T4 clamp loader clamp complex crystal structure previously reported. However, in contrast to the previously reported crystal structure, the solution structure shows an opening of the sliding clamp sufficiently large for DNA loading.

Thomas Weiss and Xiaolin Cheng

3.2.1 & 4.1.4: Important Science from Small Molecule Structures

L-R: Bruce Foxman, Marilyn Olmstead, Christine Beavers (at rear), Javier Campo, Xiaoping Wang (at rear), Matthew Wander, Garry McIntyre (at rear), Larry Dahl, Feliu Maseras (at rear), Alberto Albinati (at rear), Larry Falvello

The two-session program on **Important Science from Small Molecule Structures** played to two large audiences who engaged the speakers in lively discussions. The very well attended program was varied, with physics and chemistry well represented, and with presentations involving both theory and experimentation. Speakers came from all stations of professional development, from graduate students to established veterans.

The international physics community was represented in talks

by **Javier Campo**, Aragón Materials Science Institute (ICMA), Spain, and by **Garry McIntyre**, Australian Nuclear Science and Technology Organisation, on magnetic chirality and aperiodic crystals, respectively. The pre-eminence of neutron diffraction in both of these areas was clear. Neutron diffraction also filled an important part of the presentation by **Xiaoping Wang**, Oak Ridge National Lab, on a single-crystal-to-single-crystal transformation in a complex relevant as a possible catalyst in H_2 fuel cells. Xiaoping, who is Instrument Scientist at the Spallation Neutron Source, gave an introduction to time-of-flight neutron diffraction and also explained why iron-based catalysts are particularly desirable, using a periodic table weighted by relative abundance at the earth's surface. (To view this periodic table, enter 'periodic table by abundance' in your favorite search engine.)

Transformations also played principal roles in talks by **Christine Beavers**, Lawrence Berkeley Lab, and **Bruce Foxman**, Brandeis U. Bruce returned to a favorite theme, establishing mother-daughter orientation relationships in phase transitions. See Bruce's web site at ***http://people.brandeis.edu/~foxman1/*** for his program TOPO, which analyzes topotactic relationships. (And there is plenty of other good information, as well as tutorials, at the same site.) Christine introduced a single-crystal-to-single-crystal transformation in a spin-crossover system and went on to describe how she had successfully integrated a four-component system – an exercise in which her abundant crystallographic experience came in handy.

Theory entered the program in talks by **Matthew Wander**, Brigham Young U, and **Feliu Maseras**, ICIQ: Catalan Institute for Chemical Research, Spain, both involving bonding models. Matthew's focus was the Bond Valence Model and derivatives, while Feliu discussed the AIM (atoms in molecules) approach and applications to computational homogeneous catalysis, and perhaps left the audience with doubts about the universality of the 'direct connection' between bond critical points and the existence of chemical bonds.

The disorder that plagues fullerenes, and how it was removed in C_{70} structures, was the theme of a talk by **Marilyn Olmstead**, U California, Davis, a member of the ACS Class of 2014 Fellows. Marilyn and coworkers recently described ordered co-crystals of C_{70} with two different bromobenzene derivatives, in which Br…Br halogen bond formation underpins the resulting ordered fullerene structures. See *Crystal Growth & Design* **2015**, *15*, 2480-2485 for more.

Actinides were the central focus of talks by **Kara Knope**, Georgetown U, and **Suzanne Bart**, Purdue U. An understanding of actinide-organic interactions (Kara) could have useful implications in environmental transport of actinides. The organometallic chemistry of uranium (Suzanne) has potential for opening new avenues for studying fundamental chemical transformations because of the size and reducing capability of uranium. Such fundamental advances could have an extended utility because the wider family of organometallic compounds finds applications in the pharmaceutical and fine chemical industries, among others.

In his lecture on the theme of multiferroics, with switchable electric and magnetic ordering, **Peter Stephens**, Stony Brook U, provided cautionary comments on the pitfalls of structure refinement using powder diffraction data. Peter issued a plea to editors to consult experts in the field before publishing refinements based on powder data. An interactive exercise with the audience demonstrated that many of us do not have a clear view of how to judge the quality of a refinement to powder data.

Ivica Đilović, U Zagreb, Croatia, gave a talk on remarkable supramolecular chemistry involving host-guest complexes and a polyamine host that takes part in dynamic molecular recognition. For earlier results see *Angew. Chem. Int. Ed.* **2013**, *52*, 5504-5508 DOI: 10.1002/anie.201301032.

The Cambridge Structural Database (CSD), now 50 years old, was the main feature of two engaging talks at the end of the second session. **Carol Brock**, U Kentucky, provided what may have been the most memorable quote of the sessions, stating that the hypothesis for her CSD-based study on packing in high-Z' organic structures was that, "I am going to find something interesting." The results derived from Carol's study were indeed interesting, including a large number of high-Z' structures with translational modulation, an abnormal distribution of space group frequencies, and the common appearance of layered structures and polytypes. **Colin Groom**, CCDC, U.K., closed the program with a talk on important science derived from 787,912 structures in the CSD – a number that had changed from the value of 764,371 current at the time that Colin had submitted the abstract for this talk. An introduction to the philosophy and origins of the data base led in to a description of frontier knowledge-based studies, including an example of how the solubility of a compound can be improved solely by understanding its crystal structure. Colin also described how the difficult task of crystal structure prediction can be aided by knowledge-based descriptions of accessible conformations and interaction mapping.

Larry Dahl, U Wisconsin – Madison, ACA Fellow, member of the U.S. National Academy of Sciences, and winner of the 2010 F. Albert Cotton Award in Synthetic Inorganic Chemistry (an ACS national award), closed the first session with an enthusiastic presentation of his work on Pd-based hetero- and homometallic clusters stabilized by CO and PR_3. These clusters can be formed by up to 165 metal atoms.

It was a special pleasure to attend talks by two young scientists, **Kamran Ghiassi**, U California, Davis, and **Brian Dolinar**, U Wisconsin – Madison, whose highly professional presentations on their research were right at home alongside the talks by the seasoned veterans on the program. We are confident that with young researchers such as these in the community, there will be plenty more material for future **Important Science**… sessions.

We are especially grateful for financial support from **Crystallographic Resources, Inc.** and **Richard Staples** for this program.

Paulina Gonzalez, Alberto Albinati, and Larry Falvello

3.2.2: Powder Pair Distribution Function and Pharmaceuticals

The session, **Powder Pair Distribution Function and Pharmaceuticals**, was jointly sponsored by the Powder and Industrial SIGs and highlighted recent developments in the use of the atomic pair distribution function (PDF) approach applied to study amorphous and nanocrystalline pharmaceutical drugs. X-ray powder diffraction (XRD) is a backbone of sample characterization in the pharmaceutical industry. The powder patterns are used as fingerprints for the presence of target drugs in specific solid forms (structures) and for characterizing these forms, an important task not least because the efficacy and safety of the drug depends on its solid form. This works rather well when all the drug components present are crystalline. When some or all of them are amorphous, or nanocrystalline, this approach breaks down and additional approaches are needed, of which PDF analysis is one.

The session caught the excitement in this very new field. The talks were a mixture of pharmaceutical industry presentations, describing the critical need for this kind of analysis plus initial steps into implementing it in the industrial environment, and talks from academics who are more focused on developing the methodologies and applying them. The field has come a long way from early attempts to extract something useful by Fourier transforming conventional XRD data from laboratory Cu Kα sources, and there was a real sense that in the not too distant future these methods may be applicable to real industrial problems. After presenting a brief history of this field **Simon Billinge**, Columbia U, showed how, using synchrotron radiation, extremely small signals from dilute nanocrystalline drug products in aqueous suspension could be reliably extracted from the large backgrounds coming from the solvent, allowing the structure and morphology of the drug to be studied in the real dosage form for the case of an inhaler drug compound. In a similar fashion, **Eugene Cheung**, Amgen, showed how similarly small signals yielded critical information about recrystallization nuclei forming in the early stages of recrystallization from the amorphous form. In this case it was for an excipient (packaging material), not the drug itself, but understanding how drugs recrystallize from the amorphous state is a critical safety issue if drugs are brought to the market in the metastable amorphous form. Eugene also highlighted the importance of bringing to bear complementary experimental information, in this case NMR data, for a proper understanding of these complex problems. Another critical question for the industry is the effect of processing on the structure and properties of pharmaceuticals, and **Ahmad Sheikh**, AbbVie, gave beautiful examples where PDF could tell whether or not (depending on the particular case) certain processing steps such as milling modified the atomic scale structure of the drug. If these methods are going to be of widespread use in the industry, it will be important not only to use high power synchrotrons, with all the challenges of getting access to them, but also appropriate laboratory instruments that firms can have sitting at their own research facilities. Valeri Petkov, Central Michigan U, showed that rather high quality PDFs may be obtained from such devices, and are useful for many applications if not yet for the most sensitive work described above.

Obtaining quantitative structural models of molecules from PDF data is a difficult task, for the common reason that the atoms in the molecule need to be moved somewhat together to maintain the integrity of the molecule whilst allowing it to change position and orientation in the unit cell, but also because the PDF signals from the intra-molecular atomic distances and the inter-molecular ones have very different widths. **Pavol Juhas**, Brookhaven National Lab, presented impressive recent developments in the structural modeling of organic molecules from PDF data, where a number of previously known molecular structures have actually been solved directly from PDF data for the first time. This opens up the possibility in the future of solving structures of nano-sized drug clusters that cannot be solved crystallographically. The session ended with a characteristically entertaining jaunt through not PDF but regular powder diffraction, applied to solve troublesome issues with supposedly known structures of pharmaceuticals, presented by **Jim Kaduk**, IIT.

Simon Billinge

3.2.3: Hot Structures from Membrane Systems

L-R: Jessica Thomaston, Elisabeth Lowe, Jason Moore, Elise Blankenship, David Lodowski, Yu-Chung Chang, Bil Clemons. Not shown: Martin Caffrey. Photo courtesy of David Lodowski.

With the implementation over the past decade of new X-ray sources and membrane protein crystallization methodologies, we have seen an exponential increase in the number of structures from challenging membrane systems. Elucidating membrane protein structures advances our understanding of mechanisms of transmembrane signaling, transport, and secretion and is critical to understanding human health and disease; furthermore, these structures represent key targets for the development of therapeutics. This session highlighted recent structures comprising transport of solutes across the membrane, as well as transmission of signals

across the membrane by a variety of signaling systems.

Elisabeth Lowe, Newcastle U, U.K., presented the structure of the unusual sensor domains from Bacteroides hybrid two-component systems, which regulate expression of genes involved in polysaccharide breakdown in the gut. The ligand-bound and apo structures suggest a scissor-like mechanism for propagating a signal across the bacterial inner membrane.

Bil Clemons, Caltech, presented his group's work studying the eukaryotic targeting of tail-anchored membrane proteins, providing an overview of their structural work in fungal systems. Bil then expanded to demonstrate the overarching similarities with the human system despite the addition of the metazoan protein Bag6. The story culminated in a new structure of human TRC35 complexed with its binding site on Bag6.

Martin Caffrey, Trinity College Dublin, Ireland, presented the structure of the outer membrane porin AlgE, involved in the transport of alginate transport, which is an important component of biofilms produced by *Pseudomonas aeruginosa* – a major pathogen that contributes to the demise of cystic fibrosis patients. Martin also highlighted the development of the lipidic cubic phase technique and its impact upon the structure determination of AlgE and other membrane proteins such as channels and GPCRs.

Jessica Thomaston, U California, San Francisco, highlighted the roles of ordered water within the influenza M2 proton channel, and the establishment of a continuous network of ordered solvent extending from the gating histidine to the N-terminus. This was accomplished utilizing lipidic cubic phase crystallization techniques to solve high-resolution structures of M2 under both cryogenic and room-temperature data collection conditions.

Elise Blankenship, Case Western Reserve U School of Medicine, presented a 2.3-Å resolution structure of native-source rhodopsin, stabilized in an active-state conformation competent for G-protein binding. The structure exhibits a well-ordered water-mediated hydrogen bonding network not present in the ground state, which directly links the chromophore (ligand) binding site to the site of G-protein binding over 30 Å away and may underlie the transmission of the activation signal across the membrane.

Yu-Chung Chang, Fox Chase Cancer Center, presented the structure of the complex between RIAM and talin, which reveals both hydrophobic and electrostatic interactions along with a unique kinked helical conformation in RIAM talin binding site 1. The disruption of this kinked conformation abolishes talin recruitment and integrin activation, thus revealing structural and mechanistic insights into talin recruitment by RIAM.

Jason Moore, U Pennsylvania, reported a crystal structure of the membrane proximal FNIII domains of Tie2 and, along with biophysical and cell culture experiments to evaluate structure based mutations, an interface essential to Tie2 dimerization and signaling. Mechanistic insights were thereby revealed into the Tie family of receptor tyrosine kinases and their role in angiogenesis.

David Lodowski

3.2.5: Evolving Techniques for SAS

L-R: Hiroshi Okuda, David Green, Wim Bras (at rear), Kamila Wiaderek, Daniel Sunday (at rear), Brian Collins, Peter Mario Worsch (at rear), Tobias Madl (at rear), Cheng Wang. Photo courtesy of Cheng Wang.

Since the early attempts in the late 1930s, small-angle scattering (SAS) has evolved as a widely-used, high-resolution, nondestructive structure probe for a broad range of applications in materials science, structural biology, and environmental research. Over the past decade, with the development of 3rd generation synchrotron sources, spallation neutron sources, and free electron lasers, as well as advanced detectors, there have been many exciting new developments; for example, the application of resonant X-rays to provide both chemical and spatial information on materials, the development of advanced *in situ* sample environment techniques, and of high-pressure applications, as well as the use of coherent X-rays to capture the temporal correlation for kinetics and dynamics, such as fluctuation scattering. These developments have been accompanied by further improvement of high-performance computation tools for scattering modeling and data analysis.

This session aimed to bring experts in the forefront of SAS development to discuss recent advances and to foster novel ideas and solutions to the increasing challenges of complex structures in modern materials science. Researchers from Austria, France, Germany, Japan, and the U.S.A. presented their advanced projects. Topics covered the latest trends in instrumentation development: from the state-of-the-art laboratory SAXS equipment to the synchrotron-based SAS systems, which use both hard and soft, as well as intermediate energy, X-rays. The research topics included a broad range of structural results for nanocomposite materials, organic electronic materials, and biological complexes.

The session was well attended and the talks were followed by lively discussions indicating a significant interest in modern SAS techniques.

Michal Sabat and Cheng Wang

3.3.1 Evening Session on Diversity and Inclusion

L-R: Catherine Drennan, Krystle McLaughlin, Stephanie Wortel

This session, the first of its kind at ACA, provided a forum to host talks on topics addressing a wide range of diversity and inclusion issues. These included successful strategies for approaches through training, mentoring or research, and for engaging diverse populations through outreach.

Catherine Drennan, MIT and HHMI, opened the well-attended session with an hour-long hybrid talk, *Does Diversity Training Work?* Catherine began with a discussion of the stereotype threat training that her lab developed, which is now used for training TAs in chemistry and biology at MIT and is also in use at other universities for both TA training and in new faculty orientations. Stereotype threat is the perceived risk of confirming a negative stereotype. This potentially debilitating fear has been shown to distract and discourage students, resulting in poor performance, which feeds both the false stereotype and the student's insecurities. Stereotype threat can affect anyone; all are vulnerable. Catherine outlined the successful gains they see from just an hour-long training period, in terms of the expressed ability of trainees now able to confidently identify and reduce stereotype threat to maximize student performance. Then, for the last part of her talk attendees participated in a portion of the actual training. This was an enjoyable and eye-opening experience for many attendees, as participants were encouraged to pair up for discussion and then share their experiences with the group. With this exercise, Catherine hoped to make attendees feel more comfortable in bringing the training back to their own institution and running it. Next, **Stephanie Wortel**, New York Academy of Sciences (NYAS), gave a talk entitled, *Connecting Young Scientists to Students After School to Combat Underrepresentation*. Stephanie detailed the successes of the Afterschool STEM Mentoring Program she directed at NYAS for the past five years that connected elementary and middle school students with professional scientists. She then discussed the generalizability of this program to other cities and the ways professional scientists can reach young community members by leveraging existing community structures. After both talks there was a high level of audience engagement with lively discussion in the Q&A periods.

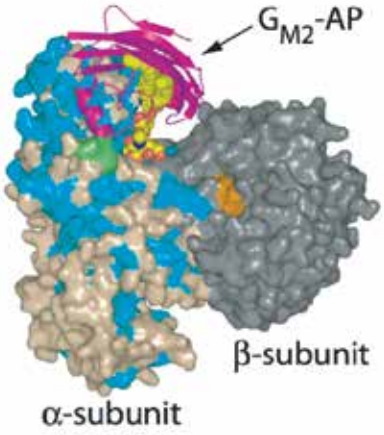
We plan to hold the **Diversity and Inclusion** session again in Denver at ACA 2016. We expect to invite an expanded list of speakers given the interest, significance and impact of the topic for the ACA community. The session is co-sponsored by the BioMac and Young Scientists SIGs.

Krystle McLaughlin

4.4.1: Structural Glycobiology

The session on **Structural Glycobiology** was a geographic world tour, as well as a tour across the breadth of molecules involved in glycobiology.

The first talk by **Brian Marks**, U Manitoba, Winnipeg, Canada, presented some brand new data hot-off-the-press, or not yet actually even in press. Brian has developed and patented a new form of β-hexosaminidase A, an enzyme mutated in some forms of lysosomal storage disease. Hex A normally forms a heterodimer of α and β subunits (see illustration below). Brian set out to make a single polypeptide with the activity of Hex A and the stability of Hex B, thereby making it small enough for use as a gene therapy tool. Remarkably, he has been able to engineer the molecule into a homodimer, HexM, that shows activity as a replacement for Hex A. This has shown indications in animal models that it can rescue the phenotype when either Hex A or B is knocked-out. Attendees at the ACA session were the first to hear about this exciting result!



A model of β-hexosaminidase A and the GM2 activator protein with bound substrate GM2.

Paul Emsley, MRC Laboratory of Molecular Biology, Cambridge, U.K., changed gears completely to discuss issues and potential solutions to the many poor stereochemical structures of N-glycans (and sugar-based molecules in general) in deposited protein structures. Paul has developed a builder/refinement routine within the COOT software for adding common N-glycan structures to electron-density maps in realistic conformations. He was encouraged by the audience to extend this to include, among other things, sugar

ring conformations in saccharide-based inhibitors and substrates.

Our tour then took us back up to Winnipeg for a short talk by **Patryk Zaloba**, from Brian Mark's laboratory, on his structure determination of a family GH73 glycosidase FlgJ from *Salmonella*. The active site of GH73 enzymes is often occluded by a flexible loop, making mechanistic studies difficult. In this variant, the loop was removed, allowing the testing of mechanistic questions.

Following the coffee break, we traveled all the way to Australia for a talk by **Helen Blanchard**, Griffith U, Gold Coast. Helen gave a nice overview of her excellent work characterizing galectins, particularly gal-3. Her structures have led to the design of the first high-affinity, selective gal-3 inhibitors with potential application as anti-leukemic leads. Helen's structures were critical in determining how to build compounds with substituents that mediate the selective recognition of gal-3 over other galectins.

Returning to North America, we finally made it to the U.S.A. with a talk from **Mark Saper**, U Michigan. Mark has used a combination of crystallographic, binding, and computational methods to understand how LpoA can span the periplasmic space of variable width in Gram-negative bacteria, specifically *H. influenzae*. Mark was able to identify a hinge conformational change between the domains of LpoA that gives it the flexibility to accommodate the periplasmic space.

The next speaker returned us to Canada but kept us in the realm of bacteria. **Marcia Chaudet**, U Waterloo, is a graduate student in the lab of David Rose. Marcia has been examining the structures of GH31 enzymes from the gut microbe, *B. thetaiotaomicron*, testing the hypothesis that these enzymes play a role in digesting starch products that are resistant to the action of the human starch digestion system. Marcia described her process of obtaining the structures, despite poor phasing signal, by using a combination of molecular replacement and anomalous scattering.

We ended the session back in the U. S. A. with a talk by **Kittikhun Wangkanont**, a student with Laura Kiessli at U Wisconsin – Madison. He presented the first structures of X-type lectins. Although there are human X-type lectins, it is not known what their normal roles may be, since they bind galactofuranose residues, which are not found in mammals. Kittikhun presented the structure of human intelectin-1 along with some preliminary binding data, results obtained to try to discover its physiological ligand.

The **Structural Glycobiology** session featured not only the geographic breadth of interest in this area worldwide, but also the rising importance and attention being given to the field. Even more importantly, cutting-edge unpublished research was presented from an impressive set of young and established investigators.

Michael James and David Rose

4.1.5: (Bio)Chemistry in the X-ray Beam

(L-R), Sean McSweeney, Yasufumi Umena, Robert Thorne, Nigel Moriarty (at rear), Carrie Wilmot, Garth Simpson, Elspeth Garman. Photo courtesy of Elspeth Garman.

The session, **(Bio)Chemistry in the X-ray Beam**, brought together a number of talks to investigate many aspects of the study of the kinetic processes that may be occurring intentionally or unintentionally in the X-ray beam during a diffraction experiment.

Carrie Wilmot, U Minnesota, provided a concise overview of the experiments necessary in order to understand enzymatic activity through crystallographic measurements. Carrie highlighted the importance of understanding oxidation state during the reaction using specific examples taken from work in her lab. In the session's second presentation **Yasufumi Umena**, Okayama U, Japan, discussed his work undertaken to determine the valence states of the Mn atoms in photosystem-II. Yasufumi demonstrated that high-resolution structures and anomalous dispersion techniques can be used to help understand the water splitting reaction so important to this system. The phenomenological changes caused to the crystalline sample through irradiation by X-rays were discussed by **Robert Thorne**, Cornell U, highlighting in particular the challenges awaiting the intrepid crystallographer undertaking studies at the latest (and future upgraded) generation of synchrotron sources. **Garth Simpson**, Purdue U, then discussed imaging of the electrical field developed through photo-electron escape and showed that it is possible to visualize the local changes to crystalline structure. In the final talk of the session, **Nigel Moriarty**, Lawrence Berkeley Lab, discussed the methods employed to provide appropriate chemical restraints in Phenix that allow for correct modeling of the species present in a crystal structure.

Sean McSweeny and Elspeth Garman

4.2.1: General Interest III

Ilia Guzei, U Wisconsin – Madison, opened the session with the entertaining and inspiring story of the **Wisconsin Crystal-Growing Competition** (see pp. 66-67) that he organized and orchestrated for high-school students in the state of Wisconsin in honor of IYCr. Contacting more than 45 companies, Ilia was able to get commercial sponsors to donate materials. Crystals, artwork, and pictures were submitted for evaluation for several different prizes by a panel of 6-7 chemists and crystallographers. The competition was an immensely successful celebration of IYCr and, should anyone wish to replicate it, the details of the effort are published in an article in *J. Chem. Ed.* Following Ilia, **Amy Sarjeant**, CCDC, undermined the popular notion that crystal structure quality is often inversely related to journal impact factor. Using the CSD to track the top 61 journals reporting crystal structures between 1997 and 2012, Amy demonstrated that there was no correlation between the R factor of reported crystal structures and the impact factor of the journal. With all of the data amassed, Amy found some other interesting trends in the popularity of certain structures/materials over time, revealing that culinary and crystallography fads are not so different.

The rest of the session featured a series of studies highlighting interesting compounds or useful tools, techniques, and tricks in crystallographic analysis. **Paul Forster**, U Nevada, Las Vegas, described how his group's crystallographic studies are guiding their synthetic efforts to produce new and interesting Tc compounds, rapidly expanding our understanding of this surprisingly under-studied element. **Larry Falvello,** U Zaragoza, Spain, followed Paul, describing analyses of samples he's encountered that can only be formed and studied *in situ* by carefully controlling temperature and other experimental factors. **Timothy Ramadhar**, Harvard Medical School, then spoke on the previously hotly contested topic of the crystalline sponge method, in which highly porous framework materials are used to incorporate and thereby 'crystallize' compounds that otherwise cannot be crystallized. Timothy pointed out the strengths and weaknesses of this technique, illustrating them with specific examples of success or failure and emphasizing the importance of having a well-characterized framework material with the right pore sizes for the target molecule. Following Timothy, **John Rose**, U Georgia, reported on the increasing success of the native SAD method due to advances in hardware and software that enable better data collection. **Bryan Chakoumakos**, Oak Ridge National Lab, then described the fascinating microstructure of sturgeon ear bones and how careful powder XRD analyses are providing a new level of understanding about the habitat and growth of these fish. **Adel Mesbah**, Institut de Chimie Séparatif de Marcoule, Bagnols-sur-ceze, France, closed the session with a discussion of synchrotron powder diffraction experiments that led to a new, monoclinic structure for hydrated rhabdophane in which the water molecules could actually be located.

Stacey Smith

4.2.2: Cool Structures

L-R: Allen Oliver, Soorya Kabbekodu, Karina Heffernan, Yulia Sevryugina, Craig Bridges (at rear), Elinor Spencer, Patrick Carroll (at rear), Christopher Durr

The **Cool Structures** session, sponsored by the Small Molecules SIG, commenced with an engaging talk on high-pressure crystallography by **Elinor Spencer**, Virginia Tech. In her presentation Elinor thoroughly described the high-pressure experiment, along with its challenges, and provided the necessary information for the audience to understand the fundamentals of this field of crystallography. Her talk concluded with a discussion on the structural changes in new lanthanide complexes over a range of pressures and how these changes alter the luminescent properties of these lanthanide compounds. Elinor's talk prefaced that of the Small Molecules SIG's **Etter Student Lecturer**, **Karina Heffernan**, Virginia Tech. Karina described a series of rare earth phosphates and how under moderate pressure these materials can transition between several classifications of mineral topologies. The first half of the **Cool Structures** session concluded with **Yulia Sevryugina**, Texas Christian U, presenting a series

of new borate structures and how borate topology is developed.

Following the break, **Sorrya Kabbekodu**, International Centre for Diffraction Data, described the internal structure of the Powder Diffraction File with a focus on how inorganic materials are classified within the database. **Craig Bridges**, Oak Ridge National Lab, presented the mechanism of charge transport in Li-ion batteries. This was a preface for Craig's discussion of modified battery materials being characterized at Oak Ridge that carry a higher charge, with an ultimate view toward the needs of sustainable energy technologies with less reliance on fossil fuels. The final speaker for the session, **Patrick Carroll**, U Pennsylvania, gave a talk on some 'un-cool structures' from his lab. Patrick's 'uncool structures' were four challenging studies undertaken during the past year. Not only did he present these crystallographically problematic structures but he also provided an in-depth analysis as well on how the problem was overcome; of note was the breakdown of a C-centered orthorhombic structure that was ultimately a rotational twin of a primitive monoclinic cell and the successful resolution to that problem. Patrick's talk, along with Elinor's, highlighted the instructional and informative nature that is the hallmark of the **Cool Structures** session.

Christopher Durr and Allen Oliver

4.2.3: Structured Nucleic Acids

The **Structured Nucleic Acids** session featured recent advances in the structure, function, and dynamics of nucleic acids and protein-nucleic acid complexes.

Presented talks included lectures on reverse transcriptase bound to a DNA template (**Sergio Martinez**, Rutgers U), on a transcriptional regulator bound to a cognate DNA promoter (**Shuishu Wang**, Uniformed Services University), and on a Group II intron catalytic RNA harboring an unusual 2',5'-phosphodiester linkage (**Navtej Toor**, U California, San Diego). **Heping Zheng**, U Virginia, presented a new online tool called Mg-RNA Server (***http://www.csgid.org/metalnas***) to assist in the identification/validation of bound magnesium ions in crystal structures, which can be particularly difficult to assign properly.

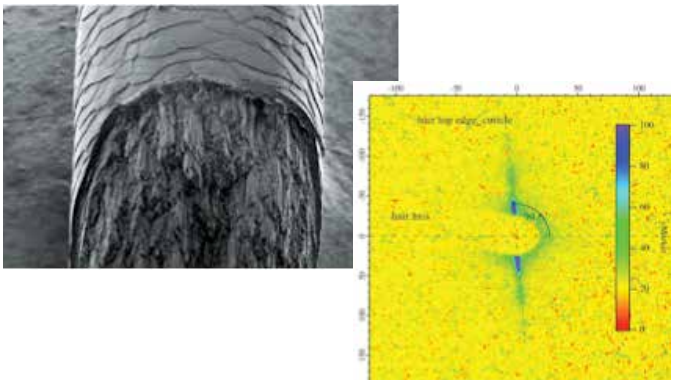
Blaine Mooers, U Oklahoma, presented an interesting case study on challenges that can arise during structure determination of long duplex nucleic acids that harbor intramolecular pseudo-translational symmetry. **Markus Wahl**, Freie Universität Berlin, Germany, presented ongoing work on the structure and function of protein-RNA sub-complexes belonging to a larger complex called the spliceosome, including the structure of an ATP-dependent RNA helicase called Brr2, which is located near to the spliceosome's catalytic core.

Eric Montemayor and Manal Swairjo

4.2.4: Imaging with X-rays and Electrons

Lively discussions on various imaging techniques were presented in the interdisciplinary session, **Imaging with X-rays and Neutrons**. We were fortunate that during the afternoon we heard a report on a new discovery, and one on unusual applications, along with reviews of methods and their applications in forefront research. This session, which was sponsored by the Light Sources SIG, showcased the multiple facets and power of imaging techniques using photons and particles, and the complementarity of synchrotrons and electron microscopes. Embracing a wide range of topics, applications in medical, biological, chemical, physical, materials and engineering sciences were discussed.

Dean Chapman, Canadian Light Source (CLS), discussed the use of medical synchrotron imaging methods and applications, and their impact on society. Dean introduced diffraction enhanced imaging (DEI) and other medical imaging methods being developed at the CLS. He explained that using multiple X-ray energies (usually two) it is possible to differentiate soft from hard tissues, improving and expanding the amount of information that can be extracted from living biological subjects. Reporting on a new discovery, **Vesna Stanic**, Brazilian Synchrotron Light Source, described how she and her collaborator Kenneth Evans-Lutherodt, Brookhaven National Lab, discovered an intermediate structure of hair that had never before been observed, between the cuticle and cortex structures. Combining submicron X-ray diffraction and transmission electron microscopy the team identified the structure as being composed of beta keratin. Usually associated with reptiles and birds, beta keratin adds strength, toughness, and elasticity and provides a supporting explanation on the reasons why humans at different parts of the world have different hair types.



Vesna Stanic reported on the discovery of an intermediate structure of hair, between the cuticle and cortex structures, that had heretofore not been observed. Employing X-ray micro-imaging methods, Vesna used electron microscopy to complement her results.

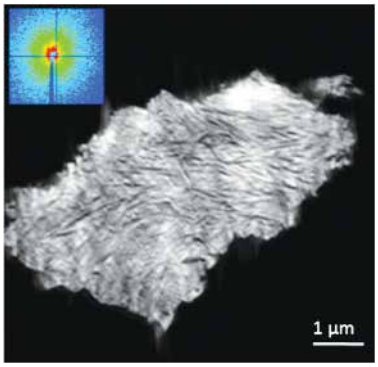
Balaji Raghothamachar, Stony Brook U, reviewed the importance of X-ray diffraction topography in the study of materials. Focusing on crystal growth and characterization of defect structures in crystals Balaji showed several examples correlating electronic/optoelectronic device performance and defect distribution, including defect studies in nanomaterials and protein crystals. Following Balaji's presentation **Guillermo Calero**, U Pittsburgh, discussed the importance of protein crystal quality in the molecular structure determination of macromolecules. Using transmission electron microscopy (TEM), bright field microscopy and ultraviolet fluorescence microscopy, Guillermo introduced a novel application for these well-known techniques, namely, the characterization of the growth process and crystal quality characterization of submicron sized macromolecular crystals. He showed that with TEM it is possible to distinguish nanocrystals from granular precipitates commonly observed in crystallization trials. Not only does TEM allow the direct visualization of crystalline lattices, but electron diffraction

Turn to p. 50

4.2.4: Imaging with X-rays and Electrons, ctd.

patterns also permit one to determine different crystal forms and in turn identify those forms that potentially will yield higher order X-ray diffraction and therefore are of higher crystalline quality.

Following the break **Andrei Fluerasu**, Brookhaven National Lab, introduced the audience to the X-ray photon correlation spectroscopy (XPCS) method. In contrast to crystalline matter, liquids, glasses, colloids, etc., do not show long-range structural order. Using coherent X-rays to probe colloidal particles Andrei showed that it is possible to determine the arrangement of these particles from the diffraction pattern, the so-called speckle pattern. A change of the speckle pattern with time in turn reveals the dynamic behavior of the sample. Andrei described some recent results using XPCS on the dynamics of dense –'crowded' – colloidal suspensions near the colloidal glass transition. He further showed preliminary data demonstrating a path towards measuring complex dynamics in biological systems and biological hybrid materials. **Mariana Verezhak**, U Joseph Fourier, winner of the **Etter Student Lecturer Award**, Materials SIG, showed the first 3D reconstruction of human dentin samples visualized with a voxel size of 28 nm using coherent X-ray diffraction imaging (CXDI). The CXDI technique is based on measuring the Fraunhofer speckle pattern of an object, using a highly coherent synchrotron beam, and subsequent application of a phase-retrieval algorithm for image reconstruction. Mariana used bone and dentin samples as models for heterogeneous composite materials. The 3D dentin nanoporosity is believed to have a biological role in cell communication and mechanosensing. Although the achieved resolution is still not high enough to visualize individual crystals in bone-like tissues, it is one of the best if not the highest spatial resolutions achieved to date by X-ray imaging methods. Rounding out an afternoon of discoveries and reviews, **Chris Jacobsen**, Argonne National Lab, presented the current status of soft X-ray cryo-microscopy to image cells and tissues using ionizing radiation with maximum preservation of structure and chemistry. Comparing the capabilities and roles of X-ray versus electron microscopy as determined by basic interactions, Chris argued that electrons excel for high-resolution imaging of samples thinner than a micrometer, while X-rays offer a path to image thicker samples such as whole eukaryotic cells and thin tissue samples. He also highlighted the role of cryo sample preparation methods, along with the combination of fluorescence studies with ptychography (a coherent diffraction imaging method), for combined studies of biological structure and function to obtain thousand-fold increases in sensitivity for elemental and spectroscopic imaging compared to electron microscopes.



Winner of the Etter Student Lecturer Award, Mariana Verezhak, showed a 3D reconstruction of human dentin samples visualized with voxel size of 28 nm, the highest attainable resolution reported so far.

Vivian Stojanoff and Dean Chapman

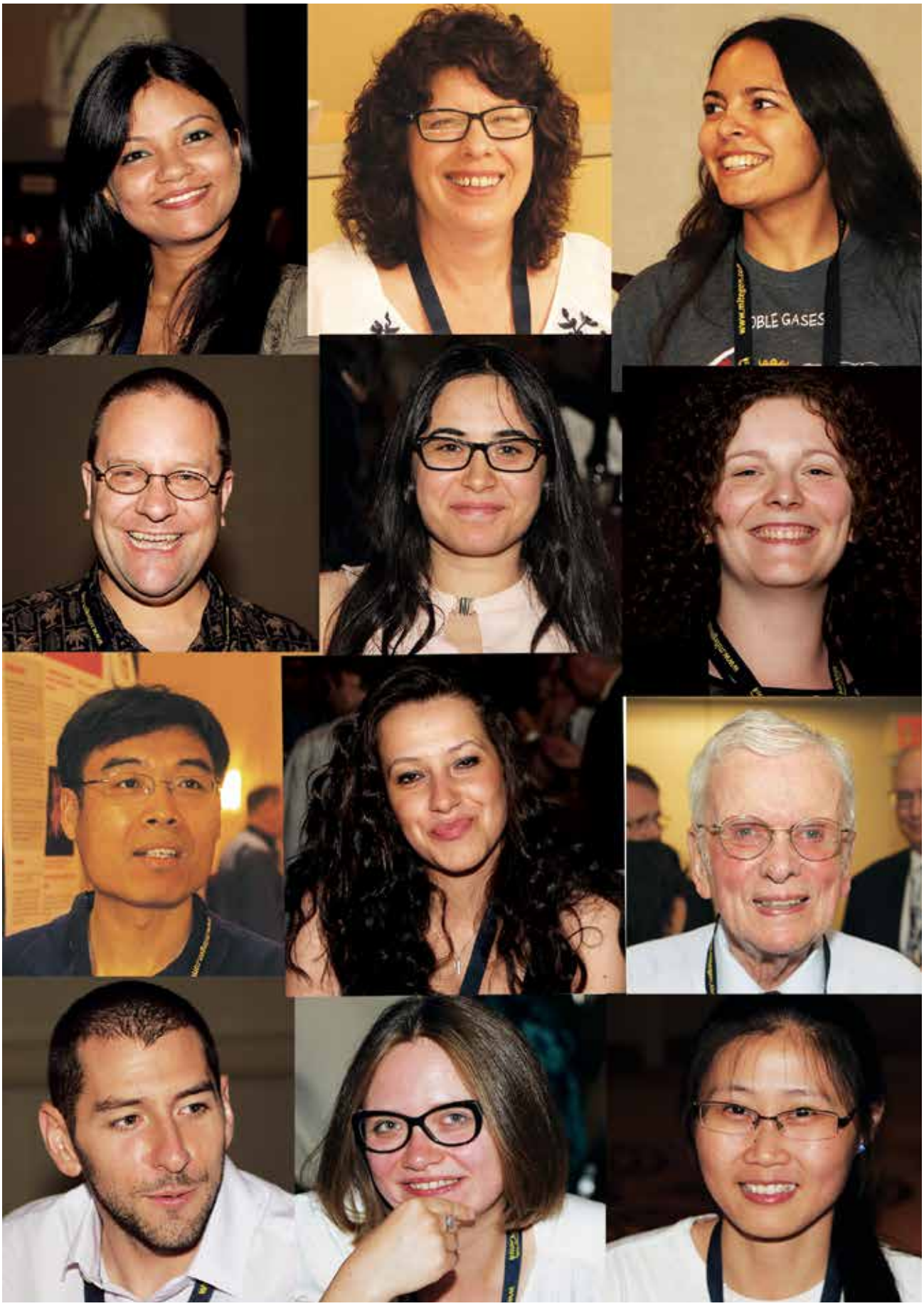
4.2.5: Play it Cool? Ambient and Cryogenic Approaches

Topics in the session, **Play it Cool? Ambient and Cryogenic Approaches**, concerned both the basic physics of the temperature response of macromolecular crystals and macromolecules, and some practical aspects of X-ray data collection at both ambient and cryogenic temperature.

Rob Thorne, Cornell U, started things off with a general overview of crystal cooling, including some discussion of how cooling damages crystals (even if crystalline ice is not formed). Rob showed recent work using a simple and effective model to explain the mechanism of ice prevention by standard cryoprotective agents. He continued his talk with additional discussion of the effects of cooling rates on ice formation and crystal damage, and finished with some discussion of the prospects for collecting data between ambient and cryogenic temperatures. **Takashi Kumasaka**, Spring-8, Japan, followed Rob and showed a novel technique of encasing crystals in a hydrogel for data collection by soaking them in a hydrophilic glue (polyvinyl alcohol) for a few minutes prior to data collection. This approach allows for robust ambient temperature data collection (when used with a humidity controller) as well as cryo data collection without an additional cryoprotection step. Takashi showed impressive results from a variety of crystals. **Doug Juers**, Whitman College, showed an approach using a flow of humid air over the crystal-viewing microscope that limits deleterious effects from dehydration during crystal handling, cryosoaking, and cryomounting. This approach was used to demonstrate the dependence of low temperature unit-cell volumes and crystal order on the thermal contraction of the cryosolvent. Doug also showed a new approach for cryoprotection using vapor diffusion to deliver volatile alcohols to loop-mounted crystals.

After a short break, **Ana Gonzalez**, SSRL, compared radiation damage at ambient and low temperature (100 K) in crystals of thaumatin, lysozyme, and cyclophilin A. In each case, several data sets were collected at increasing levels of radiation dose. At cryogenic temperature, greater doses yielded greater conformational variability. This however was not the case at room temperature. The conclusion is that elevated conformational heterogeneity in room temperature crystal structures (relative to low temperature) is not a result of radiation damage. **Danny Axford**, Diamond Light Source, U.K., discussed data collection on beamline I24 at Diamond at both cryogenic and ambient temperature. Danny showed remarkable successes using *in situ* diffraction on virus crystals, which are notoriously challenging targets for cryo-cooling. He also discussed recent work using the *in situ* approach on membrane protein crystals, including novel sample mounting platforms. **Daniel Keedy**, U California, San Francisco, finished the session by describing multi-temperature experiments on the diabetes therapeutic target PTP1B (a phospho-tyrosine protein phosphatase). Data sets were collected at multiple temperatures between 200 K and ambient temperature. The relative population of two conformations of an important loop was found to depend on temperature, and the detailed Rube Goldbergesque impact of this loop conformation on a distant ligand-binding site was explored.

Doug Juers



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ACA Summer Course in Chemical Crystallography 2015

ACA Summer Course 2015, L-R: fourth row – D. Decato, G. Tansman, G. Sheldrick, D. Duchamp, J. Sears, A. Lopez, A. Oliver, O. Lier, S. Adilov, L. Daniels; third row – T. Hubin, N. Gerasimchuk, T. Luo, K. Lee, R. Smith, T. King, G. Yang, D. Zhang, Z. Wei, C. Stern; second row – R. Papoular, J. Yan, B. Massman, A. Blake, L. DePue, B. Noll, L. Hatherly, O. Phillips, N. Henderson, A. Sarjeant; first row – P. Mueller, N. Valdez, D. Gerlach, H.-L. Huang, V. Young, J. Glusker, L. Stevens, L. Dawe

The fourth year of the ACA Summer Course in Chemical Crystallography co-hosted by Northwestern University and the University of Notre Dame commenced on June 21, with a welcome reception for the 24 attendees and 10 commencing faculty held in the Institute for Technology at Northwestern. Attendees from across the globe, including China, England, Kazakhstan and Peru, and domestic participants, both academic and industrial, were on the course roster. Many of the faculty have been involved with the course over the current and former incarnations of the program and are well versed in the demands and rigors of the course. The ten-day course followed a similar format to that of previous years with the mornings given over to lectures on the theory of the experiment and the afternoons and early evenings covering hands-on workshops. Workshop material covered included interpretation of the *International Tables*, Symmetry and Space Group analysis, and practical work on sample preparation for both single-crystal and powder-diffraction experiments. Later on this practical work included hands-on use of the prevailing software in the field, once again for both SCXRD and PXRD.

Among the highlights of the lecture series were a pair of plenary lectures, one presented by Jenny Glusker and the other by George Sheldrick; it was a real treat for attendees and faculty at the course to hear both of these speakers. George led off with a presentation discussing the features of SHELXT and the premise behind the algorithm. Jenny presented her talk covering the history of women in crystallography; it's always great to hear where we came from and how far we have come as a field in such a short time.

The course is an intense, ten-day 'boot camp', especially for the first several days; the lectures start at 8:45 AM, and there are practical components through until 8:00 PM in the evening. Despite the intensity of the opening days (*see Deidre Gerlach's summary on the next page*) there is a vigor from both the attendees and the instructors that continues to motivate everyone through the program. Some of the pressure is alleviated once structural modeling on the computers commences. During these time periods attendees have the opportunity to collar a faculty member and work on specific problems. Since there is a wide range of experience from novice crystallographers to advanced practitioners who have collected multiple datasets, and sometimes are in charge of their departmental facility, the questions cover all aspects of crystallography. These questions would come at almost any time or given opportunity; breakfast was a popular time for students to engage the faculty with problems, prior to the course starting formally for the day.

The lecture material of the first several days is primarily single crystal in nature. However, the theory is identical for any form of X-ray diffraction. Two days are given over to powder diffraction and its applications. These two days always enlighten students that there is a use for this experiment of which they were unaware. This often results in a number of students obtaining some data on otherwise unusable samples; this year was no exception with several powder diffractograms being recorded on samples that were unable to be recorded as single crystals.

The Sunday of the course is an 'open day.' Despite this name it has become a tradition that faculty will be present on campus, and many students take advantage of this and come for dedicated one-on-one instruction. It is perhaps one of the most interactive days, despite being an unscheduled day in terms of the program. The last days of the course cover topics such as twinning, disorder, database use and, perhaps most critically, structure finalization.

Photos reproduced with kind permission from Peter Müller.

The final day is possibly the most rewarding for the faculty. It is a chance for them to have a break, and the students each present a short talk on something that they have worked on, discovered, understood or otherwise gained insight into during the course. Unusually for these talks, this year commenced with one of the faculty, Jim Kaduk, giving a talk on PXRD structures for which he had had the opportunity to collect data during the course. All of the attendees gave interesting and insightful presentations. It is always a delight to see the fruits of newly gained knowledge during these talks, especially when a challenging problem has been overcome and the attendee now knows how to tackle these problems in the future or that the science behind our field is not as mystifying and arcane as it originally might have seemed. Many of the international attendees express their thanks with photos from their homelands.

We would like to thank our sponsors: American Crystallographic Association, The National Academies of Sciences through the U.S. National Committee for Crystallography, Bruker AXS, Rigaku, Agilent, the International Centre for Diffraction Data, the Pittsburgh Diffraction Society, MiTeGen, OLEXSys, the Cambridge Crystallographic Data Centre, Hampton Research, Mosaic Distribution, the University of Notre Dame and Northwestern University, for their continued support of the course. The faculty have our gratitude for their donation of time, energy, enthusiasm and knowledge to this course. Finally, our thanks go out to the attendees, without whom we would not have the course.

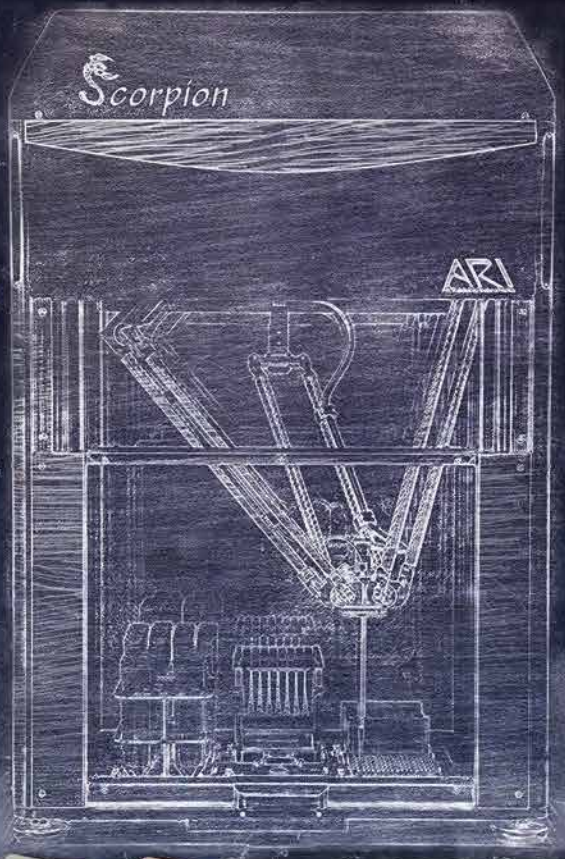
Allen Oliver, Amy Sarjeant and Charlotte Stern

Chicago's subway/el system is very easy to navigate between the airport and Northwestern University. Goodrich Hall does not have air conditioning. Allen Oliver is from New Zealand and not from Australia – get it straight! An iris crystal shape is a sign of bundled needle crystals and not single crystalline. Cooling the crystal during diffraction reduces the amount of background on the CCD camera. Room temperature data collection is acceptable, but will likely have larger thermal disorder and ellipsoids. Jahn-Teller distorted complexes are more susceptible to thermal distortion. Synchrotrons can tune the wavelength of the radiation source. X-rays in the source are generated by applying a high voltage that shoots electrons at the source metal which results in the emission of x-rays at a particular wavelength for that metal. The seven crystal systems are triclinic, monoclinic, orthorhombic, tetragonal, hexagonal or trigonal, rhombohedral, and cubic. These are often defined by cell length and angle equivalence or non-equivalence, but are incorrectly defined as such. The Laue symmetry is the symmetry of the shape of the polyhedron that forms the unit cell and there are twelve. There are fourteen Bravais lattices that are defined by adding symmetry of primitive, face-centering, body centering and full face to the Laue classes. The three most common space groups are triclinic, monoclinic, and orthorhombic. The name Lauren is very common. Seven crystal systems with thirty-two point groups with Bravais lattices yields two hundred and thirty unique space groups. Thirty-five percent of all crystals reported are in P21/c, nineteen percent are in P-1, nine percent are in P212121, seven percent are in C2/c, five and a half percent are in P21, and about four percent are in Pbca. An open circle on a symmetry diagram represents an inversion center, an iris is a two-fold rotation axis, a hurricane is a screw axis perpendicular to the plane shown, a thick line is a mirror, and an arrow at the corner is a glide plane but are dashed lines when perpendicular. The University of Indiana is in Indiana, Pennsylvania and no one knows about it except that Charles Lake does excellent crystallography. Rocks don't need to be cooled to have a diffraction pattern collected on them. The seven crystal systems are defined by their symmetry, not by angles and bond length equivalence or non-equivalence. A triclinic crystal system has one-fold symmetry, monoclinic has two-fold symmetry, trigonal has three-fold symmetry, tetragonal has four-fold symmetry, hexagonal has six-fold symmetry, orthorhombic has three perpendicular two-fold axes, and cubic has four three-fold axes. A proper rotation is just a rotation whereas an improper rotation is a rotation with an inversion. Improper rotations get the symbol of the number with a bar overhead. A two-fold improper rotation is simplified to a mirror plane alone, m; and a six-fold improper results in 3/m such that there is a three-fold rotation and a mirror. The translation operations give the fourteen Bravais lattices. Translation is defined as unit cell translation, centering operations, screw axis, and glide planes. I'm not so good at seeing three dimensions on two dimensional representations. Bruker's D2 Phaser is really easy to operate. Even if a sample has no crystallinity useful information can be found from the powder diffraction. MiTeGen has really kick ass crystal mounting pins and they are super easy to use. The dot vector version of Bragg's law, or Laue Transmission, is a better representation of the constructive interference of diffraction. The phases are more important to model than the intensities. Dave Duchamp somehow made the problem of phases click with my mind as it is the wavefunctions used to model the constructive or deconstructive interference and the phasing dictates the start of that wave being more sine or cosine character. The molybdenum K-alpha wavelength is 0.71Å, copper K-alpha is about 1.54 Å, and chromium K-alpha is about 2.29 Å. The maximum diffraction angle is 90°. Where x-rays are used to get a diffraction pattern from the electron density, neutron diffraction gives a diffraction from nucleus positions. Because the model must use sine and cosine functions to model, the phases are very important to model they are a fraction of the interaction of the models. Poor phases means less accuracy. Systematic absences are a result of only translational symmetry that result in deconstructive interference. The International Tables have all the symmetry information needed for each space group including a listing of special positions and observed reflections which define the systematic absences. Crystallography is about a hundred years old. Patterson's method for treating the phasing problem revolutionized the way crystal structures could be solved. ShelXT ignores systematic absences and uses Laue group instead. The phasing is solved first using Patterson's method then the space group is determined. George Sheldrick claims that he only wrote XPREP to show that a program could not be used to determine the space group. Lindo Patterson used opera to get him the connection he needed. The use of a heavy atom in a crystal that is diffracting will enhance all of the signals and cause simpler math for the Patterson's method. Two truths about electron density are used to solve with direct methods: positivity – such that all electron density is positive everywhere, and atomicity – such that all atoms are discrete. The value for E, the normalized structure factor, can indicate a centro- or non-centrosymmetric space group. Random error is good, systematic errors are bad, but too much random error can skew the goof value. Constraints are rigid and should be used sparingly; restraints apply general ranges of values in which atoms can refine within. Extinction corrections can be applied to fix low angle data that is not matching the calculated intensities. The Flack number is calculated to help determine the handedness of the space group. OLEX2 is pretty use friendly and uses a lot of the same commands found in XP. A lower CFOM, figure of merit for the Bravais lattice indicates higher symmetry group is suggested. The .ins file uses the command cards TREF for direct methods and PATT for Patterson's method. Solving with XT is intrinsic phasing which is still direct phasing, but now with more black magic. OLEX2 can write a PDB file using the WPDB card which has spatial coordinates that can be used for other programs like computational software. Also, can generate the file needed for a three-dimensional printer. A micro-source doesn't require the use of cooling water and is even better for small crystals. A monochromator absorbs the extra radiation and puts out a single sharp wavelength x-ray. Although CCD detectors are still very common, CMOS and hybrid pixel array detectors are more advanced.. High pressure peripherals are used for materials crystals, and electrical current peripherals can be used to run current through the crystal as diffraction occurs.

Reproduced with kind permission from Deidra Gerlach – this was just the first three days of the course …

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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What's New on the ACA History Website

We publish the full-length Living History memoirs on the ACA History website, including all the photographs and references. Webmaster Patti Potter has just put up the memoirs by Edgar Meyer, John Helliwell, and Ned Seeman. See ***http://www.amercrystalassn.org/history_people_list***. The video of John's Patterson Award presentation "Synchrotron radiation macromolecular crystallography: instrumentation, methods and applications" (***https://www.youtube.com/watch?v=SkXWUpfYKVo***) is also up on YouTube and linked to the website.

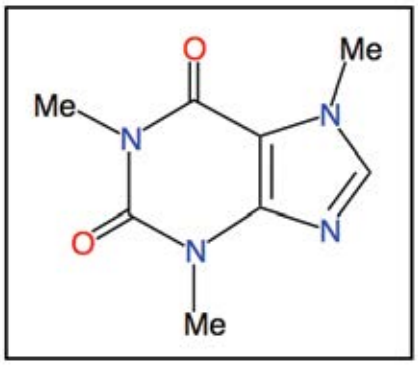
In addition to video of the award presentations, we also publish movies of historical talks, such as the ones by Sue Byram "Evolution of Small Molecule Instrumentation in North America" (***https://www.youtube.com/watch?v=fhFxBZ0RoaA&feature=youtu.be***) and Donald Caspar "Origins of Structural Biology and Trials and Errors in its History: an idiosyncratic view"(***https://www.youtube.com/watch?v=fp6EtPMNzB0&feature=youtu.be***). The latest in this series is Jenny Glusker's talk about Dorothy Hodgkin from the 2014 Albuquerque meeting. If you missed the talk, you can go to "Early Crystallographic Investigations by Nobel Laureate Dorothy Hodgkin" (***https://www.youtube.com/watch?v=7e5WiSGMoTo&feature=youtu.be***) on the ACA History website.

Here are two photos from Jenny's description of Dorothy's life. The first shows Dorothy's research group in 1954; Dorothy is second from left in the first row and Jenny is fourth from the left in the back row. The second photo (thanks to the Hodgkin family) features Dorothy and her husband Thomas at the Nobel Prize celebration in 1964.

Virginia Pett

Spotlight on Stamps – The World's Most Popular Drug

Caffeine (1,3,7-trimethylxanthine) is the world's most widely consumed psychoactive drug even though, unlike several closely-related substances, its use is legal and unregulated in most countries. As a well-known central nervous system stimulant, it has been estimated that close to 90% of adults in America ingest caffeine daily in the form of coffee, tea, cocoa products, or carbonated drinks. Its consumption in moderate quantities (i.e., less than 500 mg of caffeine or 3-4 cups of coffee per day) is generally considered safe by the U.S. Food and Drug Administration. However, an alarming trend in the United States is the increasing number of adolescents who consume the so-called energy drinks, which typically contain high doses of caffeine, on a regular basis.



The stamp illustrated in this note belongs to a set of five issued in Portugal last year to celebrate the International Year of Crystallography (2014) and to recognize some of the fields that have contributed to and benefitted from the development of X- ray crystallography, including geology, physics, mathematics, and structural biology. In turn, the chemistry stamp features the molecular structure of caffeine with the nitrogen atoms of the heterocyclic rings colored light blue and the oxygen atoms of the two carbonyl groups shown in vermilion. Interestingly, the Cambridge Structural Database, which is the principal repository of crystallographic data for organic and organometallic compounds, contains more than 160 structural determinations of caffeine co-crystallized with other molecules. A careful analysis of all these structures will certainly require a lot of patience and, of course, a good supply of coffee to drink!

Daniel Rabinovich

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Frank Fronczek

Puzzle Corner

In this issue are the solutions to the previous DISORDERED and Crystal Connections puzzles, new puzzles of both types, and mention of those who successfully solved the previous ones. As always, I will be pleased to see your solutions (***ffroncz@lsu.edu***) and your ideas for future puzzles.

Previous Crystal Connections (#3) – All are types of maps:

1) First letter of a 2-letter 1982 movie title – *E* (*from the movie E.T.*)

2) Sum of a number and the negative of another - *difference*

3) Joseph *Fourier*, credited with discovery of the greenhouse effect (*yes, the same Fourier*)

4) Topographic line of equi-elevation - *contour*

5) Beth *Patterson*, Louisiana Celtic bouzouki musician (*A bouzouki is a Greek stringed instrument similar to the mandolin*.)

The first to provide the correct solution was **Greg McCandless** (UT Dallas), and **Dan Frankel** (Bruker) was first with the DISORDERED solution. Here is the new Crystal Connections:

Crystal Connections #4

What do the answers to these clues have in common?

1) On the whole, I'd rather be in _____

2) Surname of the last husband of Martha Dandridge Custis

3) Packenham's last fight: Battle of _____

4) The song "Razzle Dazzle" is from this Broadway musical

5) "Breaking Bad" setting

6) _____ Lulu: 1963 Jan and Dean hit song

Send me those answers and comments!

*Frank Fronczek – **ffroncz@lsu.edu***

DISORDERED

Reorder these words to bring the solution into focus.

PRIZEOLA	POLARIZE
JEBTVOICE	OBJECTIVE
DEMOZO	ZOOMED
LESSEN	LENSES
NEKHIRT	THINKER

When the microscope produced only fuzzy images of crystals, the optics repairman said

Answer: HE'D LOOK INTO IT

DISORDERED

Make the model words fit the observed letters

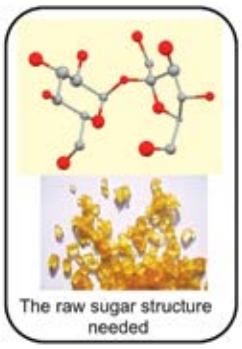
SUCRETOF

CAMERINO

SCHRIEF

SOBERI

DETOXERS



The raw sugar structure needed

Answer:

We would like to thank Bruker and ACA for their part in sponsoring this year's YSSIG mixer at the City Tap House. The venue was only a five-minute walk from the Sheraton, and this was a popular event! Everyone had a fun time with delicious appetizers and drinks, and our Amazon gift card raffle. It was great to see our senior ACA members interacting with younger members. We are now looking for a venue for next year's mixer, so if you have any suggestions let us know!

None of these events would be possible without funding from our many generous sponsors, including Laboratory Product Sales (LPS), SPS, MiTeGen, Bruker, and of course ACA! And did we mention that ACA granted all Etter Student Award winners a free registration for the Denver meeting? It was great seeing old friends and meeting new ones! Please come back next year!

Yulia Sevryugina & Kimberly Stanek

YSSIG in Philadelphia

YSSIG events at the Philadelphia meeting were well attended, and we have gotten a lot of interest from some of our younger members to get involved with sessions next year. Here are some of our highlights from Philadelphia.

The YSSIG chaired and co-chaired many sessions at this year's meeting, including the *Etter Early Career Symposium*, *Application of SANS/SAXS to Structural Biology*, *Molecular Machines*, and a pair of *Hot Structures* sessions. For the first time this year, YSSIG offered a professional development workshop on *Communicating Your Science*. The workshop was taught by the engagement and science communications manager of the ACS, Darcy Gentleman; NIH program director, Joseph Gindhart; chair of the Department of Health Policy and Public Health, University of the Sciences, Amalia Issa; principal medical writer, Katherine Sippel; and a consulting professional, Celeste MacElrevey. YSSIG also held a *Career Odyssey Panel* with representatives holding positions in industry, academia, government, and consulting. Thank you to all the speakers who volunteered their advice at these sessions!

We saw increased attendance from undergraduates in YSSIG, thanks in part to our continuation of the *Undergraduate Symposium* hosted by Krystle McLaughlin and sponsored by the Society of Physics Students (SPS). This symposium, now in its second year, included an encouraging lecture by Bill Duax on his life in crystallography, a reception, and the poster competition for undergraduate students that awarded a cash and MiTeGen products prize to Ren Wiscons from Oberlin College. We would like to encourage undergraduate students to attend the ACA annual meetings! **Important – your travel expenses can be covered by travel awards now offered by the Society of Physics Students!** Please monitor the ACA website for further information. And, of course, YSSIG will be welcoming you in Denver with our reception and a poster prize!

The YSSIG was also involved this year in an inaugural *Evening Session on Diversity and Inclusion*, where Catherine Drennan (MIT), Stephanie Wortel (NYAS), and Dione Rossiter (AAAS) talked about engaging diverse populations through outreach using crystallography. Krystle McLaughlin will continue leading this session in Denver.

Scenes from 2015 YSSIG mixer at City Tap House

Engineering Crystallography: From Molecule to Crystal to Functional Form

The 48th Course of the International School of Crystallography, *Engineering Crystallography: From Molecule to Crystal to Functional Form*, took place in Erice during the first two weeks in June, in a period of unusually sunny and extraordinarily warm weather. Participants from 33 countries gathered for this edition of the School. The directors of the course, Kevin Roberts (U Leeds), Robert Docherty (Pfizer) and Rui Tamura (U Kyoto), with the support of Gerard Coquerel (U Rouen) and Christer Aakeroy (Kansas State U) focused on the scientific content of the Course, centered around the preparation of new materials through prediction and control of the molecular assemblies. The Local Organizers, Paola Spadon (U Padua), Annalisa Guerri (U Florence) and Giovanna Scapin (Merck), led the 'Orange Scarves Team' during the whole course ensuring that everything ran smoothly. Erin Davis, Fred Boyle and Fabio Nicoli provided the IT support for the workshops and for all the audio/video and network necessities.

The opening talk of the Course, given by Robert Docherty, presented the translation of molecule to crystal to product in the pharmaceutical sector. Kevin Roberts presented two talks, on *Crystallization Route Map* and *Crystal Morphology*, while Christer Aakeroy presented a lecture on supramolecular assembly and solid-form architecture. This was followed by a talk during which the link between the crystal structure and mechanical properties of organic materials was highlighted (C. Malla-Reddy, Indian Institute of Science). Joop ter Hoorst (U Delft) explained the importance of supersaturation as the driving force for nucleation and growth. The importance and influence of interfaces during the crystal-growth process was elegantly captured by Michael Ward (New York U). The definition of molecular chirality and the importance of the resolution of chiral molecules were introduced to the participants in a series of connected lectures on the first, second and fourth days (Reiko Kuroda, U Tokyo, Rui Tamura and Gerard Coquerel). The theme of stability was presented, first focusing on chemical reactivity and crystal defects (William Jones, U Cambridge) and then describing the physical stability of polymorphs and solvates (Ulrich Griesser, U Innsbruck). As the school proceeded, 'molecule to crystal' modeling techniques were described in detail by Robert Hammond (U Leeds), and solid-state computational modeling, including crystal-structure prediction, was reviewed (Aurora Cruz-Cabeza, Roche CH). Neil Feeder (CCDC) extended the discussion by further reviewing the information available in the Cambridge Structural Database (CSD) and discussing the impact of solid-state informatics on solid-state structure design. On day five, two talks from leading exponents in the field introduced crystallization-process modeling concepts (Marco Mazzotti, ETH) and crystallization-process control (Zoltan Nagy, Purdue U). Allan Myerson (MIT) gave a lecture on different crystallization processes for production, such as evaporation and cooling, while Christopher Price (GlaxoSmithKline, U.K.) introduced the technique of comparing and contrasting batch and continuous processing. The use of Discrete and Finite Element Modeling (DEM/FEM) to allow the connection between the particles formed in primary manufacturing and their possible impact on secondary processing (flow, mixing) were described by Charlie Wu (U Surrey). Ana Kwokal (GlaxoSmithKline, U.K.) elucidated the work on solution and solid-state characterization. Jerry Heng (Imperial College) targeted solid-state and surface characterization. Software tutorials on Mercury by the CCDC, on Visual Habit from Leeds University, and on the Crystal 16 crystallization workflow (Avantium) were run twice during the week. These were very popular sessions with a high level of engagement and enthusiasm from the participants. The final afternoon was dedicated to a lively interactive panel discussion where students could ask seven panelists – Meir Lahav (Weizmann Institute of Science), Joel Bernstein (New York U), C. Malla Reddy, Ulrich Griesser, Christopher Price, Neil Feeder and Kevin Roberts – questions on all aspects of the course (see photo immediately below). To facilitate the discussion,

students were asked to submit questions in the days preceding the panel discussion so that broad themes could be identified and used to jump-start the conversation.

Participants presented more than 70 posters; each poster session (scheduled for the late afternoon) had a preview during lunch, in order to give the poster presenters the opportunity to visit other posters in their session. To promote the interaction of the students with the lecturers, six fifteen-minute oral presentations by young participants, selected from the poster abstracts, were also included in the program. Awards for the best posters (one for each session) were given to Stuart Kennedy (Durham U) and Ran Drori (New York U). In addition, the Lodovico Prize, recognizing the best student in the lecture hall and in the social activities, was awarded to Elena Meirzadeh (Weizmann Institute of Science) with a special mention to Marlena Gryl (Jagiellonian U) (see photo below).

The Orange Team organized a series of events to ensure that all participants felt the Sicilian atmosphere: a dinner with Sicilian dishes; a local folk group singing and dancing traditional regional songs; and a 'dinner tasting,' to let the participants appreciate the typical Italian cuisine and culture. On the first day of the school, a presentation given by Martin Schmidt (U Frankfurt) provided a brief overview of the history of the town of Erice. Two excursions during the course (one to the Phoenician island of Motia and the other to the ancient cities of Selinunte and Segesta) also allowed the participants to appreciate the cultural heritage of this part of Italy dating back to 1200 BC.

The course was generously supported by IUCr, ECA, OPCW, CCDC, PANalytical, DECTRIS, AbbVie and Merck.

Christer Aakeroy, Gerard Coquerel, Robert Docherty, Kevin Roberts, and Rui Tamura

Updates from 2014-2015 AIP Science & Technology Fellows

It is hard to believe that this is my fourth and final installment as an AIP Congressional Science Fellow! My time in Senator Franken's office flew by, and it has been truly a life-changing experience. In just 12 short months, I learned an incredible amount, gained a new appreciation for the role of science (and scientists) within the legislative branch of the federal government, and made many lifelong friends.

Most of my time this summer was spent on the Senate Energy and Natural Resources (ENR) Committee's markup of the broad energy bill, which I described in the summer issue of *ACA RefleXions*. This was certainly the most memorable and rewarding experience of my fellowship year, especially because I was able to take the lead in my office for many parts of the process. In particular, I was responsible for the discussions and negotiations regarding the incorporation of Senator Franken's energy priorities into the energy bill, which was designed to receive broad bipartisan support. After weeks of meetings and phone calls, I was extremely proud that a number of his top priorities were incorporated, such as federal funding for energy-storage research, a technical assistance program for identifying beneficial energy-storage projects, and enhanced federal support for energy-development projects on Tribal lands.

However, a number of the Senator's priorities could not be included in the base bill, and these had to be offered as amendments at the ENR Committee markup. My primary responsibility during this process was to provide Senator Franken with supporting information and materials for the amendments he decided to offer. He is very data-driven so this was a great opportunity for me to apply my data collection, processing, and analysis skills in order to provide him with the most convincing and up-to-date arguments. Senator Franken then used this information to fight for some of his energy priorities, such as a national energy efficiency standard that would reduce our energy use and carbon emissions nationwide and help consumers save money on their energy bills. He also did a great job of highlighting the importance of energy-benchmarking programs that would allow the owners of multi-tenant buildings to identify those buildings that would benefit most from energy-efficiency upgrades. Ultimately these provisions were not adopted, but it was an honor to help my boss fight for energy policies that are good for the environment, the economy, and the people of the United States.

The ENR Committee markup required many long days and late nights in the office, and it was exciting to be involved in this process at the ground level. But for me the most rewarding aspects of the markup were the behind-the-scenes activities, which served as excellent professional development opportunities. For example, negotiating is a skill with which I had very little practice prior to the fellowship; physics research is quite absolute, and the numbers involved often result in a single 'final answer.' By contrast, negotiations in Congress are rooted largely in empathy and compromise, neither of which is emphasized in the training one receives within a graduate physics program. And while my work in energy policy certainly required consideration of the relevant numbers – energy savings, costs, profits, and emissions, for example – it quickly became apparent that decisions are more likely to be made based on the underlying politics. I found the first-hand experience of negotiating during the markup to be extremely valuable, and I am confident that this will be a helpful new skill as I continue down my career path.

Finally, these negotiations also provided me with a great opportunity to get to know the incredible Senate staffers who work on energy issues. It was fascinating to witness first-hand the very different approaches taken by certain offices, either due to different politics, constituencies, or philosophies about the role of the federal government. And while I did not always see eye-to-eye with my colleagues, there is no doubt in my mind that we all shared the same goal of advancing sound energy policy that would benefit the American public. I have great respect for those who are dedicating their careers to this goal, and I am grateful that I had the opportunity to work with them over the past year. As for me, now that my AIP Fellowship has ended, I am heading over to the U.S. Department of Energy to work as a AAAS Fellow in the Office of Energy Policy and Systems Analysis, Office of Climate, Environment, and Energy Efficiency. I am excited for this new adventure, and I hope that I will be able to continue to work with the colleagues and friends I have made in the Senate!

Caitlin Murphy

Calm.

Well, relatively speaking. It's been over six months since I entered the U.S. Department of State as the American Institute of Physics State Department fellow. I've gone through a handful of distinct stages dealing with the job: excitement, firehose, and knife juggling. These stages still coexist, but now somehow it all feels calm. Everybody is moving all the time, but what before appeared to be chaos is now much more

predictable. Events are still surprising, but the reactions to these events, and the coordination among the actors involved, are now discernible. What initially appeared as a random flailing of limbs has turned into a dance.

This dance is not a slow dance. Things are easier now that I have a fuller understanding of the processes involved, in particular what needs to be done in certain situations and how long it will take. At the heart of this dance lies the process known as 'clearance.'

The U.S. Department of State is a large entity. Along with USAID, the budget request for fiscal year 2016 was $50.3 billion. This supports not only staff members in Washington, D.C., but also the largest diplomatic corps in the world, which allows the U.S. to maintain direct engagement with 190 countries. These overseas staff report back valuable information on local conditions not only to Department of State officials but also to many other U.S. federal agencies. The risk of such a large organization is that the left hand may not always know what the right hand is doing. When external powers scrutinize every word said or printed, it's important that such an organization coordinate its messaging. Thus enters the clearance process.

Clearance is one of those things that seemed to take a lot more time to do a few months ago, largely because I didn't really understand the process. It's really just asking other people to take a look at something you've written (or you've had sent to you) and getting their comments, in order to make sure that what you're saying about a subject matches what they are saying. In the academic world, this can require a good amount of effort. I proofread a manuscript a couple of weeks ago, which took five hours of my Saturday. Here in the Department, the materials one looks at are generally just a few pages long. In addition to that, sometimes only one or two sentences will actually be about your topic, a brief mention of hydropower in a larger document about Peru's development strategy, for example. 'Clearance' consists of finding the sentence that directly touches on your issues ('equities,' in the local language) and making sure you're happy with the wording. It often only takes a matter of minutes.

The upside about understanding more about the process is that I can plan and organize my schedule much more effectively. My to-do list every morning is generally long, and previously when an email appeared that asked me to do something it would knock my whole schedule out of whack. Now I'm able to look at the item (called a 'tasker') and determine how much time it's going to take to reasonable accuracy. Even for items that have a very short turn-around time ('short-fuse taskers'), I look at my schedule and think, "I can fit this in right before my meeting at 2PM." Then I forget about it and return to what I was originally working on until 1:45PM rolls around, or until I find myself with a little free time before then.

The dance continues. Some days I falter and step on someone's foot, or find myself out of sync with everything else that's going on, but these days are fewer and farther between. The next step of the process is to learn how to accomplish something strategic in this environment. When tasks are generally broken down into sections only minutes long (it's rare to find 30 minutes of uninterrupted time), how does one think long-term and accomplish something that will last? Since AIP and the Department of State have decided to extend my contract by a year, I have 18 more months to figure this out. Should be enough time, right?

Disclaimer: The views expressed in this article are those of the author and do not necessarily reflect the views of the U.S. Department of State or the U.S. Government.

Matthew McGrath

Celebrating 50 Years of the Cambridge Structural Database

The beginning of July in Cambridge saw crystallographers from around the world gathering to celebrate the first fifty years of the Cambridge Structural Database. From the opening lecture by Olga Kennard, the Founder and first Director of the Cambridge Crystallographic Data Centre, to the closing session, when the current Executive Director, Colin Groom, turned his crystal ball to the next fifty years, attendees were taken on the journey from Olga's vision for one of the first scientific databases to the creation of a vast curated resource of immense value to scientific research. With over ¾ million curated crystal structures, the CSD is now used by researchers and educators worldwide to answer questions in structural chemistry, drug discovery, materials science, formulations, and much more.

The symposium program celebrated the community achievement that is the CSD with presentations from CCDC staff past and present, and our colleagues in industry and academia. Sessions explored current applications in molecular recognition and design, solid form informatics, and structural chemistry. You can access the program, summaries of the symposium sessions, and the CSD50 newsletter at ***http://www.ccdc.cam.ac.uk/csd50/***.

Editor's Note: This summary is reproduced from the September 2015 issue of *Crystallography News*, a publication of the British Crystallographic Association (***http://www.crystallography.org.uk/crystallography-news/***). See *Crystallography News* for a full account of the symposium proceedings.

CSD50 attendees gather in the garden of Downing College Cambridge

50 years of the CSD in a snapshot

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Stephen Harrison Receives the 2015 Welch Award in Chemistry

Stephen Harrison

ACA member Stephen Harrison, Professor of Biological Chemistry and of Molecular Pharmacology and of Pediatrics at Harvard Medical School and Boston Children's Hospital and investigator in the Howard Hughes Medical Institute, has won the 2015 Welch Award in Chemistry for his "outstanding contributions to the X-ray crystallography of viruses and protein nucleic acid complexes." The Houston-based Welch Foundation is one of the largest private funding bodies in the U.S.A. for basic chemistry research. He received the award at the 2015 Welch Conference on Chemical Research, "Next Generation Medicine," held in Houston, TX, on October 26-27.

Stephen carried out his undergraduate studies in chemistry and physics and received his graduate degree in biophysics at Harvard University, where he has been part of the faculty since 1971. Within the athenaeum he has served several academic appointments, with stints as visiting scientist and visiting professor in the U.K. and Germany. In 1984 he was awarded the Ledlie Prize from Harvard University, the first of a long list of recognitions for his extraordinary contributions to science. Among the others, he received the Louisa Gross Horwitz Prize (with Don Wiley and Michael Rossmann) in 1990, the ICN International Prize in Virology in 1998, and the Gregori Aminoff Prize in Crystallography in 2006. He is a member of the National Academy of Sciences, associate member of the European Molecular Biology Organization and foreign member of The Royal Society, London.

His main research topics are viruses, and their interaction with host cells, and eukaryotic cell division, which he investigates using mainly crystallography and cryo-EM techniques. He started working on the structural aspects of viral particles in the 1970s, and in a seminal work published in Nature in 1978, he and his associates reported the structure of the tomato bushy stunt virus, which paved the way to high-resolution studies of more challenging human pathogens. In recent years, he has been investigating the structural details of the uptake mechanisms adopted by enveloped and non-enveloped viruses to invade the host cells. In particular he has focused on dengue and influenza viruses, representative of the enveloped virus category, and on rotavirus, belonging to the non-envelope viral family and one of the major causes of infectious gastroenteritis in infants. While dengue and influenza viruses use fusion proteins to meld their envelope with the host cell membrane, thus allowing transfer of the viral genetic content inside the host cytoplasm, rotavirus forces its way into the host cell by means of several surface proteins that disrupt the cell membrane.

In parallel to this work, Stephen has also been researching immunity development against influenza and HIV viruses, in collaboration with several other groups in the U.S.A., with the long-term goal of using the information derived from these studies to design better vaccines. Finally, he has his mind set on the 3D structure determination of the entire kinetochore, a protein complex that connects the chromosomes to the microtubules of the mitotic spindle and that plays a key role in eukaryotic cell division.

2015 Barrett Award to Brian Toby

Brian Toby (R) receiving his Barrett Award from Jim Kaduk

ACA member Brian Toby received the Barrett Award at the Denver X-ray Conference (DXC) held in Colorado in August 2015. The biennial award, which consists of a monetary prize and a dedicated plaque, was created in 1986 by the DXC Advisory Committee to honor Charles Barrett, a pioneer in the use of X-ray crystallography to characterize metals and alloys at the atomic level.

Brian Toby is Senior Physicist and Group Leader at Argonne National Lab's Advanced Photon Source, where his main interests are to understand the structure-properties relationship of different types of materials, and to develop new software for diffraction data analysis. In collaboration with Robert Van Dreele, he built GSAS-II, a very flexible open source software that can be used for the analysis of diffraction patterns deriving from a wide variety of samples, ranging from materials to macromolecules, in the form of single crystals or powders.

Brian first encountered crystallography while studying chemistry as an undergraduate at Rutgers. He then moved to Caltech, to obtain a Ph.D. in physical chemistry in 1986, specializing in surface science. Subsequently, he worked in different environments, spending time in industry, in academia and in the government sector, before arriving at Argonne in 2005. In the years 2009-2011 and 2012-2014, respectively, he was Vice Chair and Chair of the U.S. National Committee for Crystallography of the National Research Council; in 2005 he won the bronze medal from the U.S. Department of Commerce for 'Contributions to Powder Diffraction Software.' Brian has been a fellow of the International Centre for Diffraction Data since 2004.

Michael James Receives the 2015 NRC Research Press Senior Investigator Award

Michael James

The Canadian Society for Molecular Biosciences has awarded Michael James the 2015 NRC Research Press Senior Investigator Award. The award recognizes "a record of outstanding achievement in research in one or more of the fields of biochemistry, molecular or cellular biology undertaken in Canada by a Canadian scientist (a Canadian citizen or a landed immigrant)." Michael received his Ph.D. in 1966 at Oxford University, under the mentorship of Dorothy Hodgkin. He has been Fellow of the Royal Society, London, since 1989 and Fellow of the Royal Society of Canada since 1985; currently he is Distinguished University Professor Emeritus in the Department of Biochemistry of the University of Alberta in Edmonton, Canada. He is also the Canadian Representative on the ACA Council, and the recipient of the 2009 ACA Buerger Award.

Michael has over 47 years of experience in protein science and X-ray crystallography; one of his main research interests is the structural and functional study of enzymes linked to carbohydrate hydrolysis. In particular, he is interested in proteins involved in lysosomal storage diseases. These are a family of nearly 50 different genetic metabolic disorders, which arise from the mutation of one or more of the enzymes involved in the digestion of macromolecules in the lysosomes. For example, mucopolysaccharidose I (MPS-I) is a rare autosomal recessive disease caused by the deficiency of α-L-iduronidase, the enzyme responsible for breaking down glycosaminoglycans in cells. Michael and his group have determined the crystal structure of α-L-iduronidase alone and in the presence of inhibitors, shedding light into the mechanism of action of the enzyme and putting into context the misfolding mutations that occur in some MPS-I patients. His lab is also interested in the structural genomics of *Mycobacterium tuberculosis*, in the biochemical aspects of protein phosphatases and in the functional study of enzymes encoded by RNA viruses, such as hepatitis C virus, rhinovirus 2, poliovirus and rabbit hemorrhagic disease virus.

ICDD Fellow Awards

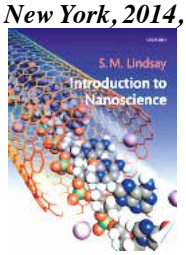
Distinguished Fellow Award to John Faber. The International Centre for Diffraction Data (ICDD) has awarded the 2015 Distinguished Fellow Award to John Faber of Faber Consulting, Inc. John joined the ICDD in 1997; he acted as a Principal Scientist until 2007 and directed the ICDD's educational programs for many years. Upon retirement in 2008, he served on the Board of Directors as a Director-at-Large until 2012. During his time at ICDD he contributed to introducing new databases built upon the relational database technology and to developing new software for powder diffraction pattern recognition, digitization and analysis. Currently John is the Faculty Chairman for ICDD's Rietveld Analysis course. For the last three years, he has been designing software for neutron scattering powder diffraction analysis based on the PDF-4 database.

Fellow Award to Bob He. The ICDD also awarded ACA member Bob He the ICDD Fellow Award. Bob is a material scientist, and currently the Director of Innovation and Business Development XRD at Bruker AXS. He has been working on X-ray diffractometers and methods development since 1986, and earned his Ph.D. in materials science from Virginia Tech in 1992. A pioneer of two-dimensional X-ray diffraction, he is now making an effort to expand the use of 2D detector technology in the pharmaceutical field. He has rarely missed an ICDD Pharmaceutical Powder X-ray Diffraction Symposium, always delivering highly appreciated lectures, seminars and workshops on 2D crystallography. He has published over 30 papers and a textbook on the subject, and has been awarded 16 U.S. patents and two R&D 100 awards for his work on X-ray instrument development. From 2011 to 2014 he has been a teaching Adjunct Professor at the Department of Metallurgical and Materials Engineering, Indian Institute of Technology at Kharagpur.

Chiara Pastore

Book Reviews

Introduction to Nanoscience: S. M. Lindsay, Oxford University Press, New York, 2014, 472 pp., ISBN-13: 978-0199544219.



I received this book a couple of years ago, and it has been sitting on my shelf waiting for me to review it since. As the title suggests, this is a book covering the fundamentals of nanoscience. It is a textbook and, as such, covers just about every topic I studied as an undergraduate student in chemistry: organic chemistry, physical chemistry, quantum mechanics, solid-state physics, instrumentation, thermodynamics, statistical mechanics, and so on, albeit in an order much different than I learned in school. Lindsay's work was published in 2010 and, while current then, is missing some of the new materials developed since. Keep in mind that this is an introduction, so the basics are timeless.

I would suggest the reader start with Appendix B, a transcript of the 1959 lecture by Richard Feynman to the AIP meeting titled, "There's Plenty of Room at the Bottom." This lecture may be considered to be the point of inception of nanoscience, even though many of the tools and techniques were already coming into existence by the time of Feynman's lecture.

Chapter 1, 'What is Nanoscience?' covers the basics of nanoscience including an analysis of the aforementioned Feynman lecture and how many of the predictions he got right (and not quite right). This chapter is set off from the rest of the book as an introduction providing historical context.

Part 1 consists of chapters 2 and 3, and exposes the reader to the tools he or she will need to understand the topics discussed in Part 2.

Chapter 2 reviews quantum mechanics and covers the basics of this field. Chapter 3 follows with a discussion about statistical mechanics and thermodynamics.

Part 2 looks at the tools needed to explore the nanoworld. Chapter 4 reviews instrumentation and covers scanning tunneling, atomic force and electron microscopy, fluorescence techniques, and tools for physical manipulation of tiny objects.

Chapter 5 reviews the processes of top-down construction of materials as is done in the semiconductor industry. Chapter 6 covers the bottom-up production of materials starting with organic chemistry and biochemistry and ending with a discussion about DNA manipulation.

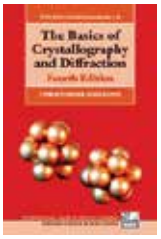
Part 3 consists of four chapters that look at the applications of nanoscience. This section includes chapters on electrons in nanostructures, molecular electronics, and properties of nanostructures, ending with a chapter on molecular biology.

There is a plethora of appendices covering minute (pun intended) details for topics covered in the main text. The book also came with a CD containing movies and animated GIFs that demonstrate things like Brownian motion, DNA tethering, etc. One of the movies has a typo that I found somewhat humorous. As a student my advisor taught me, 'Anyone who spells asymmetric with two esses is an a??.' I leave it you to find where the misspelling is.

Joseph Ferrara

The Book Review Section continues on p. 66.

The Basics of Crystallography and Diffraction, 4th Ed.: Christopher Hammond, Oxford University Press, Oxford, 2015, 528 pp., ISBN-13: 978-0199546459.



I came across this book at a Royal Microscopy Society meeting and asked Oxford to send me a copy for review. The title is very descriptive; you must remember that there was crystallography long before diffraction by crystals was observed. This is a textbook for material scientists and geologists, although many crystallographers would find it a useful reference book. One feature of the book I really liked was the attention paid to history. There is a plethora of background information in the text, and the short biographic vignettes in Appendix 3 are very informative.

This is a fourth edition. Not having read any of the first three editions I cannot comment on the improvements. The author suggests there are minor tweaks in this edition with some additional advanced material. Each chapter has a series of exercises with answers provided at the back of the book. The book is well referenced throughout with a Further Reading section after the answer key.

The author begins with classic crystallography,constructing atomic arrangements in the simple patterns, hexagonal closest packing, hcp, and cubic closest packing, ccp, and then building unit cells from them. Next various examples from nature are presented.

In Chapter 2 the author studies lattices in two dimensions, developing patterns and explaining symmetry elements and the plane groups. There is a discussion about border patterns and textiles, and a concluding section on non-periodic patterns in preparation for a subsequent discussion of quasiperiodic crystals.

Chapter 3 and 4 extend the discussion in Chapter 2 to three dimensions with the introduction of the Bravais lattice, three-dimensional symmetry, the space groups and quasiperiodic crystals. Chapter 5 discusses indexing lattice directions (zone indices) and planes (Miller indices). The cubic, hexagonal and trigonal systems are discussed at length. In Chapter 6 the reciprocal lattice is introduced as well as the relationship between the direct and reciprocal lattices.

Up to this point there is no real discussion about diffraction. In Chapter 7 the author introduces the reader to the diffraction of light using optical principles. This chapter also presents the theory behind the microscope and telescope as well as the concept of resolving power for both instruments.

Chapter 8 introduces the original X-ray diffraction experiments by von Laue, the Braggs and Ewald. Chapter 9 analyzes the principles of X-ray diffraction in detail with discussion about the instrumentation and experimental setup. Chapter 10 covers the subject of diffraction by polycrystalline materials. Chapter 11 moves from X-ray diffraction to electron diffraction and ends with a discussion on image formation in transmission electron microscopes.

The next three chapters cover more advanced material. Chapter 12 introduces the concept of the stereographic projection and its construction and use. Chapter 13 covers Fourier methods with some discussion about structure solution methods from the basic trial and error method to charge flipping. I consider it a weakness as there is no discussion about structure refinement here. Chapter 14 covers tensors from rank 2 to 4 and their applications to materials. I thought this topic was very well explained.

Appendix I provides a list of some software and modeling tools. Software is so ethereal, so I know it would be hard to make the list comprehensive. There are better, more current lists at association websites. Appendix II covers polyhedra. Appendices IV and V cover mathematical relationships and tools useful for crystallography. Appendix VI treats systematic absences and double diffraction while Appendix VII provides a brief introduction to group theory.

Joseph Ferrara

2015 Wisconsin Crystal-Growing Competition

The 2nd crystal-growing competition among Wisconsin high school students ages 14-18 was successfully conducted this year by the UW-Madison Molecular Structure Laboratory. The contest, which perfectly aligns with the Wisconsin Idea, inspired participation of over 550 students and teachers from 25 schools from across the state and one school from Moscow, Russia.

The main goal of the contest was to grow large blue crystals of cupric sulfate pentahydrate. The crystals were evaluated for size and quality by a committee comprised of six Ph.D. chemists and one chemistry graduate student. The high school students submitted 44 crystals that had won their local contests. New for this year was a contest-inspired art competition for which 11 submissions of drawings and mixed media arrived. Additional contest goals were to motivate students to learn about solution chemistry, compound solubility, purification, crystallization, and optical microscopy. 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. All winners were recognized with certificates, books, and cash prizes. The best crystals and drawings are on semi-permanent display in the UW-Madison Chemistry Department.

To promote the contest we set up a booth at the Wisconsin Society of Science Teachers Conference in March 2015 to inform the public about the crystal-growing contest, crystallography, and education at the Chemistry Department. A web site (***http://xray.chem.wisc.edu/WICGC_2015.html***) provided the information necessary to register for the competition, to learn about crystals, and to learn the details of the crystal growing procedure. Links to the related national and international events were provided.

All participants of this important scientific outreach activity were invited to tour the UW-Madison campus, Chemistry Department, and the Molecular Structure Laboratory. They were also invited to the award ceremony that featured several high-profile speakers. Assistant chair Mark Ediger described the significant role of the chemistry department on campus, and John Moore presented a lecture with demonstration experiments to illustrate what it is like to be an undergraduate student

in this department. A guest speaker from University of North Carolina at Charlotte, Dan Rabinovich, spoke about crystals and crystallography on postage stamps. Paula Piccoli described the contest and its significance, and then I awarded the prizes in my role as the contest organizer. Over 70 students, teachers, and parents attended the award ceremony.

I would like to share with you three letters from the participating students, teachers, and leaders of the science clubs.

...This is way cooler than I thought...

Thank you so much again for organizing this event. I think the crystal growing competition is a good opportunity to introduce students to work in the laboratory. Aqueous solutions of copper sulfate are pretty safe to work with and the crystallization conditions allow enough permutations to provide a challenge to the students to find appropriate conditions for growing seed crystals and competition crystals. The students were intrigued by the intense color of the solution alone and literally blown away by the beauty and size of the crystals. We luckily had enough material that they even ventured into growing little crystal gardens. The students had fun, learned to work accurately and cleanly and follow instructions. They learned from their mistakes making adjustments to improve results. They learned to relate results to crystallization conditions and modify conditions to improve results.

My favorite quote: "This is way cooler than I thought!" All of them were looking forward going into the 2016 competition with so much more experience.

Dr. Michael Ruf, coach of a student team, Verona, Wisconsin

I'd also like to thank you for again hosting the Crystal Growing Competition. I also organize a major academic competition and I know how time-consuming it can be, but it is also very rewarding. I want you to know that all of my students gave this competition two thumbs up and they very much enjoyed their visit to UW. Several students commented that they would have liked to stay overnight and take more tours. I am hoping that this competition continues to be an annual event and you continue to have the awards before summer as it easier to get the kids there.

Tim Cox, Berlin High School Chemistry, Wisconsin

I just wanted to tell you that I had a lot of fun doing the Crystal Growing Contest. It was a highly rewarding experience because I was able to create my own experiment within the experiment. It was hands-on and watching the crystals grow under different conditions was very interesting. In my opinion, any chance to learn and have fun while doing one is an opportunity that should not be passed up.

Thank you for organizing this.

Abby Schuett, high school student from Fond du Lac, Wisconsin

It is with great pleasure that I thank the sponsors of the 2015 State-wide WI Crystal-Growing Contest: Agilent Technologies, American Chemical Society, American Crystallographic Association, Bruker AXS, Crystallographic Resources, Hans Reich Chemistry Research Fund, Hestia Labs, International Union of Crystallography, UW-Madison Chemistry Department, and Zurex Pharma. Without their support, the contest would not have been feasible. The sponsors have been acknowledged throughout the contest on the web site and contest-related materials such the Contest Handbook, T-shirts, and posters. The sponsors were acknowledged at the national meeting of the American Crystallographic Association in Philadelphia in August 2015.

Ilia Guzei

Judges evaluate crystals and artwork submissions

Map showing the locations of participating schools in Wisconsin. Ten schools out of 25 participated in the contest for the second time.

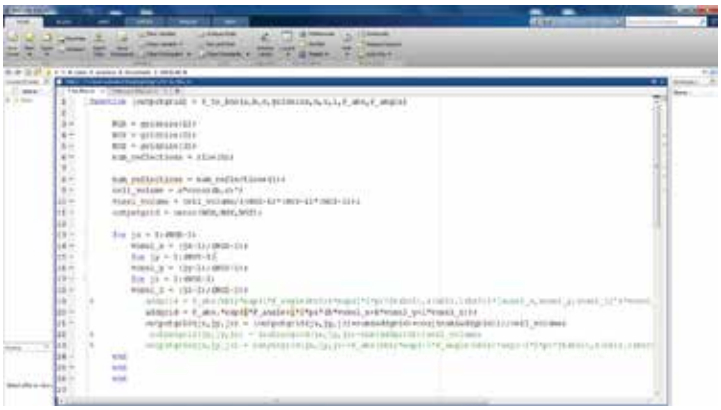
Summary of winning entries

Net RefleXions

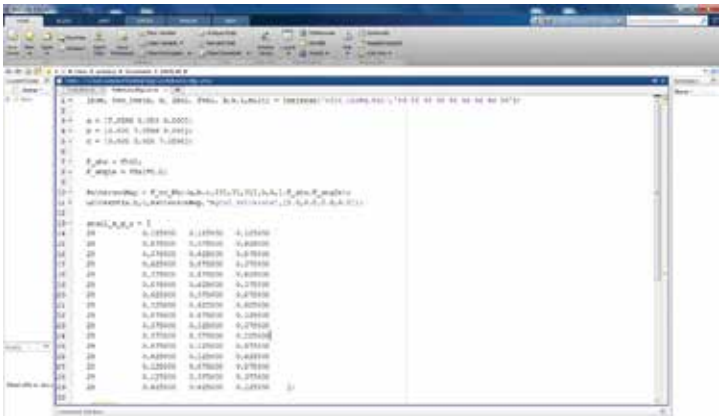
It's that time of the year again. Classes are back in session and all the buildings are once again filled with the excitement of a new school year. So unsurprisingly, when I was asked to contribute to this column, my thoughts quickly turned to software for teaching crystallography. And so I hope to highlight some of the teaching tools that I've found useful (from the perspective of a student) as well as carrying on the tradition in this column of writing about new technologies important for every modern crystallographer. If you have any suggestions for websites or programs that should be shared with the world, feel free to email me at ***avinokur@wisc.edu***

Confession time: as a young crystallographer I find, for the most part, little need to learn how to write, read or manipulate code. Previous generations of crystallographers have designed powerful programs for solving and refining structures, and many of these programs come with attractive GUI options. But as wonderful and convenient as these programs are, I remember as a beginner finding the whole process of solving and refining crystal structures as a black box. How does the Patterson method work? What about charge flipping? How am I really refining the parameters? On occasion I braved the more technical papers to try to understand the theory behind the black boxes, but (most likely because I lacked the necessary mathematical background) the plethora of equations left me with more questions than answers. Of course after several years of solving crystal structures these methods became very familiar to me, but nevertheless I could never shake off the feeling that there was still something behind the curtain unseen.

This past year, though, I got a chance to peek behind this curtain. I sat in on a graduate crystallography course at University of Wisconsin – Madison, taught for the first time by my advisor, Daniel Fredrickson, and he introduced an unexpected teaching tool, MATLAB. This software was available through MathWorks and, in the case of my home institution, there already was a site license available for all the students. I've encountered similar programs previously, Mathematica for example, but usually in a context of problem sets for quantum mechanics and calculus; so I found it was rather unconventional to use MATLAB in a crystallography course.



But MATLAB quickly transformed before my eyes from wavefunction generator and plotter of complex polynomials into a real live structure-solving software. In combination with covering the theory behind the Patterson method, charge flipping, and least-squares refinement, Fredrickson also distributed code that allowed students to go from reflection data to a solved structure using MATLAB to carry out the calculations and VESTA to visualize the outputs. In the screenshot shown at the bottom of the preceding column, you can see one of the pages of the code for the program that employed the Patterson method. The language proved simple enough that even someone as uninitiated in coding as myself could still follow the code. In the case of the Patterson method, students first inputted the reflection data and then ran a program to generate a Patterson map. After examining the Patterson map in VESTA, they manually inputted potential coordinates of the heaviest atoms, exported a new file (see the screen shot shown below for an example of the modified input file), and recalculated the electron-density map using the new input file. Students repeated the steps until they successfully accounted for all of the electron density.



To me, the beauty of using MATLAB as a teaching tool was its absolute bare-bones transparency. Students were free to play around with the code and see how changing different variables affected their output. This was especially valuable in the case of charge flipping, where the appropriate positive threshold was critical for the solution to converge. Some students, who had more coding prowess, went a step further and started improving the initial code so that the programs ran faster and more efficiently. So overall, it was my impression that MATLAB brought solving and refining methods from the realm of the mathematical and abstract to something more concrete with which students could really interact. And so I encourage you, dear readers, to try it out for yourselves and see if students in your institutions will also enjoy peeking behind the curtain.

Anastasiya Vinokur

Collaboration between the CCDC and IUCr – Making it Easier to Deposit High Quality Data into the CSD

We are pleased to announce the launch of a major enhancement to our data deposition service. Crystallographic data deposition is now even faster and easier with the integration of the IUCr's checkCIF/PLATON service into the process for depositing data into the Cambridge Structural Database (CSD). Researchers can check the integrity of their data during the deposition process rather than having to deposit and validate data separately.

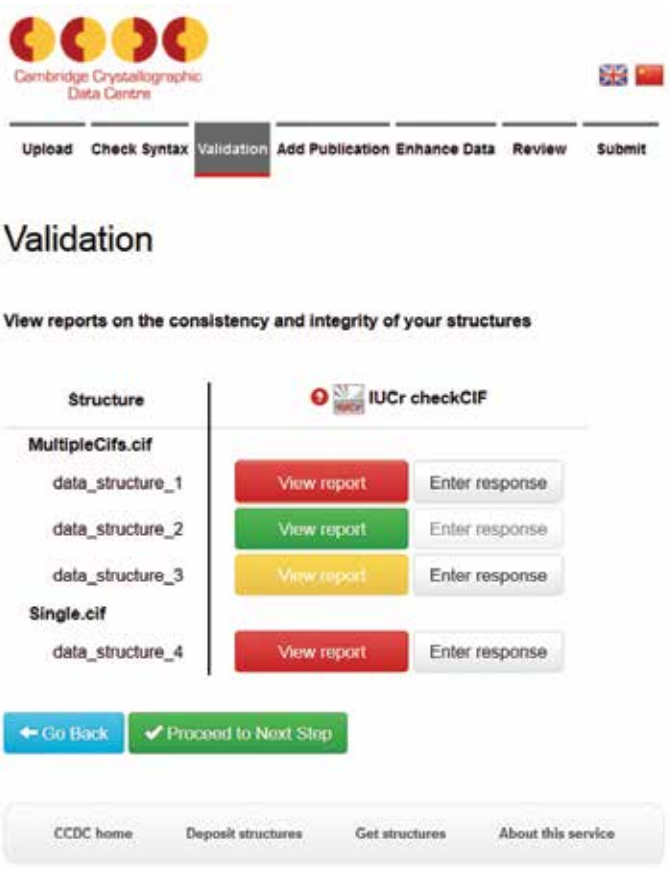
Depositors to the CSD can be confident in the integrity of their data with immediate access to both the edited CIF file and the embedded validation report, and crystallographic reviewers will be able to read the checkCIF report alongside the deposited data to aid peer review of submitted papers.

The integration of checkCIF/PLATON into the CSD deposition process is just one of the CCDC's recent enhancements to give crystallographers an efficient way to deposit high quality small molecule data as part of their regular workflows. We plan to extend this further in the coming months by exposing more CCDC functionality during deposition.

You can read more about this development at ***http://www.ccdc.cam.ac.uk/NewsandEvents/News/Pages/NewsItem.aspx?newsid=40*** and access our deposition service via ***https://www.ccdc.cam.ac.uk/deposit***.

Suzanna Ward

Manager – Cambridge Structural Database, Cambridge Crystallographic Data Centre (CCDC; www.ccdc.cam.ac.uk)



Depositors can now check their data during deposition with the integration of checkCIF/PLATON service into the CSD-deposition process.

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ACA DENVER

Friday, July 22 - Tuesday, July 26, 2016

Sheraton Denver Downtown

Travel Grant Application Deadline: March 31, 2016
Abstract Deadline: March 31, 2016
Advance Registration Deadline: May 31, 2016
Hotel Reservation Deadline: June 28, 2016

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Fankuchen Award honoring Elspeth Garman
Bau Neutron Diffraction Award honoring Benno Schoenborn
Margaret C. Etter Early Career Award honoring Jason Benedict

SESSIONS

In Situ and In Operando Methods
Magnetic Entanglement and Complex Magnetic Materials
Crystallography in Solid-State Chemistry
Cryo Electron Microscopy
Structure-Based Drug Design
Molecular Machines

Meeting logo designed by John Aspinall

Transactions Symposium – Structural Dynamics

Organizers: **Jason Benedict** (University at Buffalo; *jbb6@buffalo.edu*) and **Arwen Pearson** (Universität Hamburg, Germany**;** ***arwen.pearson@cfel.de***)

This transactions symposium will focus on the rapidly growing area of structural dynamics of both chemical and biological systems, as well as solid materials. This resurgence has been driven both by developments in X-ray sources as well as by new approaches for sample delivery, data collection, and processing.

The speakers will present recent work on both equilibrium and non-equilibrium dynamics involving time-scales from seconds to femtoseconds. As well as scientific highlights, the symposium will also include case studies and cutting edge advances in methodology.

As this symposium will produce papers for a special issue of *Structural Dynamics* we will make a particular effort to recruit speakers willing to present work that has not yet been published elsewhere, as well as encouraging a subset of speakers to submit review articles that summarize advances in their sub-field (i.e., structural biology, chemistry, and materials).

General Meeting Information

Obtaining a VISA: Advanced planning by foreign travelers is critical. 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).***

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: FREE WI-FI is included in the sleeping rooms, so bring your laptops and stay connected to home and office. The room rates at the Sheraton are competitive with other properties in the vicinity. We are able to offer these rates by committing to fill a certain number of rooms. By staying in the conference hotel you will help us meet this commitment, which also brings with it free meeting space that helps keep registration fees affordable.

All of our contracts include a number of lower cost rooms available to students. Room sharing can make them even more reasonable – use the ***Room Sharing*** feature under accommodations on the meeting web site.

Financial Support: Travel support will be available for young scientists. Applications should be made by the abstract deadline – March 31, 2016.

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.

DECEMBER 2015

5-8 **13th Conference of the Asian Crystallographic Association AsCA2015.** Kolkata, India.
http://www.asca2015.org

6-10 **4th Nano Today Conference. Nano Today 2015.** Dubai, U.A.E.
www.nanotoday-conference.com.

FEBRUARY 2016

27-Mar 2 **Biophysical Society. 60th Annual Meeting.** Los Angeles, CA.
https://www.biophysics.org/2016meeting/

MARCH 2016

28-Apr 1 **MRS Spring Meeting & Exhibit.** Phoenix, AZ.
http://www.mrs.org/spring2016/

APRIL 2016

4-7 **BCA Spring Meeting.** University of Nottingham, U.K.
http://bca2016.crystallography.org.uk

MAY 2016

27-Jun 5 **49th Erice Course - High-Pressure Crystallography:** ***Status Artis*** **and Emerging Opportunities**. Erice, Italy.
http://crystalerice.org/2016/

JULY 2016

10-14 8th **American Conference on Neutron Scattering**. Long Beach, CA.
http://www.mrs.org/acns-2016/

22-26 **ACA 2016 Annual Meeting**. Denver, CO,
Program Chairs: Amy Sarjeant & Edward Snell.
www.AmerCrystalAssn.org

AUGUST 2016

28-Sep 1 **30th European Crystallographic Meeting. ECM20**. Basel, Switzerland.
http://ecm30.ecanews.org/ecm2016/home.html

DECEMBER 2016

4-7 **14th Conference of the Asian Crystallographic Association. AsCA2016.** Hanoi, Vietnam
http://www.asca2016.org

MAY 2017

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

AUGUST 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

NOTE: New schedule for ACA 2016 Annual Meeting: The meeting will begin on ***Friday, July 22***. The ***workshops*** will be scheduled for all-day on Friday with the ***opening reception*** on Friday evening.The ***exhibit show*** will open Friday evening and end after the Monday poster session. ***Poster sessions*** will run Saturday – Monday, and ***lecture sessions*** will run Saturday – Tuesday. The ***awards banquet*** will take place Tuesday evening, and ***session planning for 2017*** will be on Wednesday morning.

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