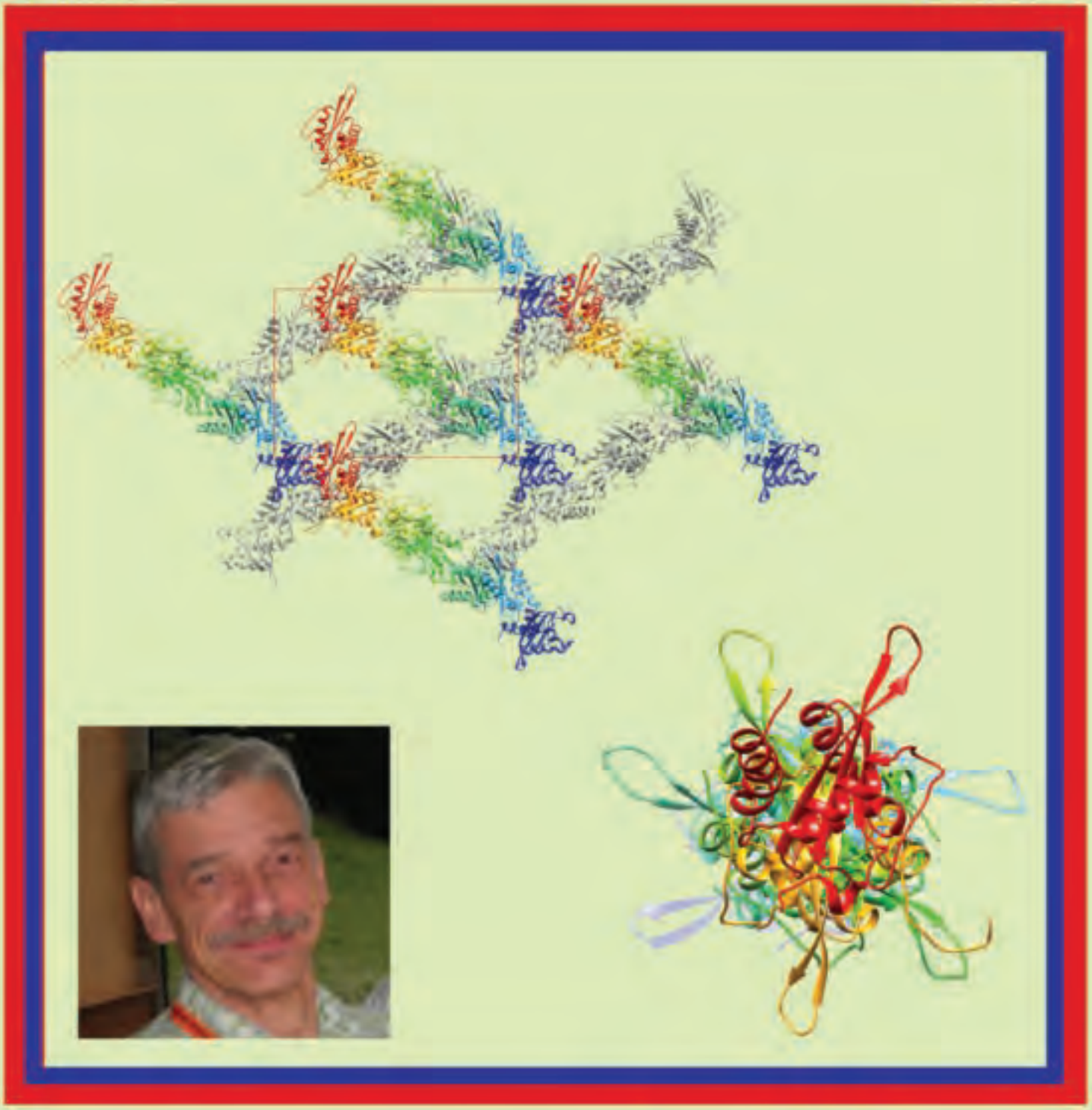
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 3

Fall 2017



Annual ACA Meeting in New Orleans Revisited

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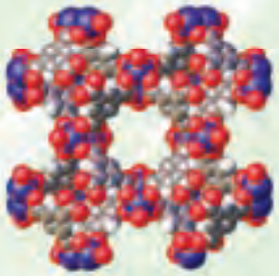
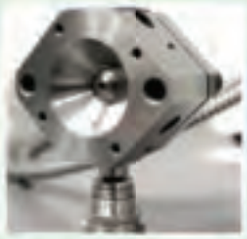


MOFs

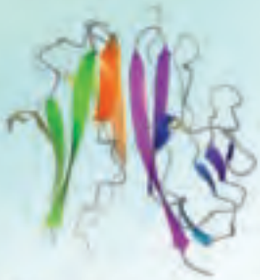
Incommensurates



High Pressure

Charge Density

In situ



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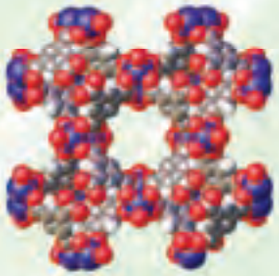

MOFs

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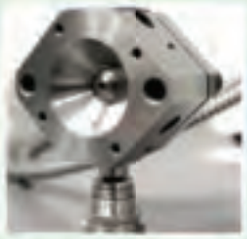

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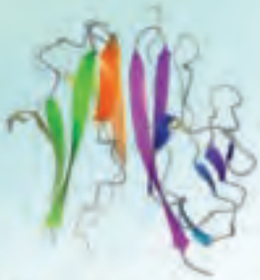

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Sir James Fraser Stoddart
Special Opening Plenary Lecturer in New Orleans

What's on the Cover. The image is from Zbigniew Dauter, who received the 2017 Patterson Award at the ACA Annual Meeting in New Orleans. See p. 10.

Contributions to ***ACA RefleXions*** may be sent to either of the *Editors*:

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President's Column


Amy Sarjeant

Dear Colleagues,

With our annual meeting long past, I'm sure many of us have been able to exhale a little and enjoy a lazy day or two of summer. I've always liked the peaceful time on campus in the summer: more parking, shorter lines for coffee, and the quiet industry of students focused on research. But, like most of you, my life is never peaceful for long. Soon after New Orleans, I headed off adventuring in the realm of structural chemistry.

Shortly after returning from the ACA meeting, I was off again to the **Midwest Organic Solid State Chemistry Symposium**, or MOSSCS for short, at Kansas State University. This informal, student-focused meeting has its roots at the University of Illinois, starting out there in 1988 as a retirement celebration for David Curtin. At this year's Symposium I thoroughly enjoyed the presentations of the students, who were passionate about their research. The informal atmosphere led to a lot of great discussions, both scientific and not, among all the attendees. I came away truly inspired by the science, and pleased to note that many of the organizers and attendees – both past and present – are active members of the ACA community.

After a few days at home to re-pack my bags, I headed out again, this time to the **ACA Summer Course in Chemical Crystallography,** held at Northwestern University. It was a delight to be back on campus and to see how the X-ray Crystallography facility has changed in the two years since my departure. But of course the real pleasure was in helping the class of 26 attendees who came for an intense week of chemical crystallography. I'm eternally grateful to my co-organizers Allen Oliver, Charlotte Stern and Christos Malliakas for keeping the show on the road, to all the instructors who volunteer their time and expertise to make this such an informative and rewarding experience for the students, and to all our sponsors whose donations keep the course running. We send around a survey to the participants every year, and it's a joy to read the comments that come back. Especially ones like this, "The course was an incredible experience that I will carry with me for the rest of my life. Course material and instructors were phenomenal. I'm very thankful for this opportunity." However, the best part of the summer school comes years afterwards when I see alumni presenting their work at ACA meetings.

After the ACA Summer Course, I've had about a month off from traveling leading up to the **IUCr Congress** in Hyderabad, India. As of this writing (mid-August) the IUCr has yet to happen, but the enthusiasm for crystallography is clearly building in advance of this much-anticipated event. I hope I will be seeing many of you there!

But enough about me. What about you? What do crystallographers and structural scientists get up to in the summer? Folks at the APS have been busy hosting a symposium on drug discovery in recognition of 25 years of pharmaceutical research at the synchrotron, as well as the **CCP4 Workshop** and the **National School on Neutron and X-ray Scattering**. I know several of my colleagues hightailed it up to Canada to attend the 100th meeting of the **Canadian Society for Chemistry** (CSC) just after our annual meeting. Jim Britten ran his **Chemical Crystallography Workshop** and Louise Dawe hosted the **4th Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec** (CEMWOQ-4, for short) in the lead-up to the CSC meeting. Once again, two long-standing ACA members spreading the word about crystallography to the broader community of structural scientists!

In addition to spreading the word of crystallography like a scientific Johnny Appleseed, members of Council are still hard at work on the business of ACA. We met briefly in Buffalo over the summer to work through several issues we're facing with our transition. We're pleased to say that both our CFO and CEO, Rao and Bill, will be staying on board for the next few years. We've been investigating website and membership database options. Thanks to all the donations to the website fund, we should be able to see some real improvements on our site. We continue to work with AIP to make sure we get the most out of our relationship with them (see the article beginning on p. 53 for more details).

I hope your summer has been relaxing and productive and that you are ready to tackle the newest challenges of structural science this Fall.

Amy Sarjeant

RefleXions from Canada


Tomislav Friščić

As I write this, we have just returned from the **24th Congress & General Assembly of the IUCr** that took place August 21-28 in Hyderabad, India. It has been a busy and event-packed meeting for everyone, and the Canadian delegates have been no exception. Two Canadians were keynote speakers at the meeting: **David Bryce**, U Ottawa, one of the pioneers of the emergent area of NMR Crystallography, a topic that he addressed in his lecture *Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables*; and **Farideh Jalilehvand**, U Calgary, who is an expert in speciation of sulfur and metal species in biologically-relevant environments, a topic that she presented in her lecture *X-ray absorption spectroscopy and chemical speciation: from archaeology to biology*. At the IUCr Congress, Farideh also co-chaired a workshop dedicated to **X-Ray Absorption Spectroscopy for the Crystallographer**.

It therefore appears particularly suitable to highlight these eminent speakers in this, and in coming editions of ***RefleXions from Canada***. Here I start with David Bryce, currently Full Professor and University Research Chair in Nuclear Magnetic Resonance at the University of Ottawa, and the Chair of the Department of Chemistry and Biomolecular Sciences. He earned his B. Sc. (Hons) in Chemistry in 1998 from Queen's University (Kingston, Ontario), followed by a Ph.D. in 2002 from Dalhousie University, where he worked with Rod Wasylishen. Following postdoctoral work with Ad Bax at the Laboratory of Chemical Physics at NIH, David took up a faculty position in his home

Fig. 1: (left) David Bryce and Yijue Xu discuss the results of some mechanochemical milling experiments; (right) L-R: Cesar Leroy, Patrick Szell, and David Bryce get ready for some NMR crystallography.

city of Ottawa in 2005. His current research interests include solid-state NMR spectroscopy of low-frequency quadrupolar nuclei, NMR studies of materials, NMR crystallography, halogen bonding, mechanochemistry, and quantum chemical interpretation of NMR interaction tensors. His group (Fig. 1, above) has authored NMR software products downloaded >500 times in 25 countries.

The Bryce group are pioneers and promoters of NMR Crystallography, an emergent field that employs NMR spectroscopy data to refine or solve crystal structures. While this hot area of research has strongly focused on the interpretation of ^{1}H chemical shifts, the Bryce group have provided novel contributions and advances by recognizing that the majority of the elements in materials are quadrupolar, and that special experimental and analytical methods are required to use their NMR spectra to their full potential. The group's initial proof-of-principle work focused on simple systems, wherein unambiguous results were achievable (*Phys. Chem. Chem. Phys.* **2009**, *11*, 7120-7122). They followed on by developing a more sophisticated experimental and computational protocol in which structural models of solids can be refined jointly against experimental quadrupolar couplings and a DFT-optimized energy term – as described in examples of their work in *J. Phys. Chem. C* **2012**, *116*, 19472-19482, and *CrystEngComm* **2013**, *15*, 8727-8738. There is particular interest in the use of this methodology for understanding and characterization of pharmaceutical materials, such as polymorphs, and solvates, and this has also been addressed in the group's publications, including *J. Pharm. Sci.* **2012**, *101*, 2930-2940 and *Can. J. Chem.* **2014**, *92*, 9-15. Beyond NMR crystallography, the Bryce group have been active in a wide range of topics, notably for making major, internationally-noticed contributions in utilizing NMR spectroscopy for understanding supramolecular chemistry in the solid state, particularly for studying the behavior of halogen bonds – an area in which they have provided a series of articles describing pioneering studies of the halogen bond with multinuclear solid-state NMR spectroscopy. Historically, NMR spectroscopy of solids has played a key role in the understanding of *hydrogen* bonding, and the Bryce group are now making in-roads in its use in the hot area of *halogen* bonding. In that context, they have reported the first measurement of spin-spin (J) coupling within a halogen bond, and have established a novel reporter on the strength and geometry of these bonds – you can check these out in their paper: *CrystEngComm* **2014**, *16*, 7285-7297. In *J. Am. Chem. Soc.* **2014**, *136*, 6929-6942 they reported how NMR is characteristic of halogen bonds in solids, and utilized DFT approaches to interpret spectroscopic data, revealing a unified NMR description of halogen bonds and hydrogen bonds. These pioneering early steps towards NMR understanding of halogen bonding have led David to join the IUPAC commission on *Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements*.

Besides David and Farideh, there have been a number of Canadian contributions at the IUCr congress in Hyderabad. Louise Dawe tells me that there have been a total of two Keynote Lectures, nine Conference Lectures and twelve Poster Presentations. On top of all these, Canadian contributors have co-chaired four Microsymposia: **Patrick Mercier**, National Research Council Canada, co-chaired the microsymposium **Minerals/gems in Industrial Applications**; **Natalie Strynadka**, U British Columbia, co-chaired the microsymposium **Mechanisms of Bacterial Resistance**; **Louise Dawe**, Wilfrid Laurier U, co-chaired the microsymposium **New Approaches in Crystallographic Teaching**; and **Hanna Dabkowska**, McMaster U, co-chaired the microsymposium on **Crystallography for Space Sciences**.

A list of all these contributions can be found (with cool pictures!) in the carefully assembled and maintained Twitter stream of the Canadian National Committee for Crystallography (CNCC), with the Twitter handle:**@CNC_Crystals**.

For me it was a particular pleasure to contribute a little bit towards the functioning of the IUCr, as a member of the Canadian

Turn to p. 4

Delegation (Figs. 2a,b, below), chaired by Louise Dawe, and including also Pawel Grochulski, Canadian Light Source, and Patrick Mercier. For us it was especially delightful to see Hanna Dabkowska elected (Fig. 2c, below) as the Vice-President of the IUCr – Congratulations Hanna!

Fig. 2 - Canadian Delegates at the 24th IUCr Congress: (a) L-R: Pawel Grochulski, Louise Dawe, Tomislav Friščić, McGill U; (b) L-R: Pawel, Louise, and Patrick Mercier; (c) Hanna Dabkowska (right) moments after being elected IUCr Vice-President.

The representatives of the CNCC also had the opportunity to meet all Canadian contributors to the IUCr Congress during a casual get together at the local Le Cafe. The get together gave us all a fantastic opportunity to meet and chat over a cup of coffee, and to acknowledge the student recipients of the Larry Calvert Travel Awards administered by the CNCC: **Naheda Sahtout** and **Thirumalai Ulaganathan**, U Saskatchewan, and **Jenna Skieneh**, Western U (Fig. 3, below).

Fig. 3: (left) Canadian participants of the 24th IUCr Congress having a good time over a coffee at Le Cafe; (right) Chair of the Canadian Delegation Louise Dawe congratulating the Larry Calvert Travel Award winner Jenna Skieneh.

Again, if you wish to know more about our Canadian National Committee for Crystallography and its activities, a lot of information can be found on the exciting and frequently updated webpage that has been put up and is constantly improved by Louise Dawe: ***http://xtallography.ca/***.

Fig. 4. Logo of the upcoming 2018 Annual ACA Meeting in Toronto from: http://www.amercrystalassn.org/2018-meeting-homepage.

I would like to conclude this brief update from Canadian crystallographers by alerting you to the coming 2018 ACA Annual Meeting (Fig. 4, left) that will be taking place in Toronto, Ontario – with Gerald Audette and Tiffany Kinnibrugh as Program Chairs, as well as Louise Dawe and David Rose as Poster Chairs. For more information, see pp. 58-59.

Hopefully you will all be able to join us in Toronto in July 2018!

So much for now – as always, if you would like me to address or highlight any special topics or events, or if there are activities that I have missed covering, or if you simply want to share stories of Canadian crystallographers, please share them with me by e-mail (***tomislav.friscic@mcgill.ca***), and I will do my best to include them in a forthcoming column.

Best regards from increasingly cold Montreal in October!

Tomislav Friščić

From the Editor's Desk

This issue features reports from the ACA's Annual Meeting in New Orleans. Connie Rajnak has put together the cover and ***What's on the Cover*** (see p. 10) featuring our 2017 Patterson Award winner, Zbigniew Dauter.

Our coverage of the Annual Meeting depends upon the efforts of many people. These include the session organizers and poster prize judges, who have drafted reports. We owe a special thanks to our *ACA RefleXions* Photographer Peter Müller and to Richard Bromund for their fabulous photos, along with our student volunteers responsible for the session group photos coordinated by Vicky Doan-Nguyen, Chelsy Chesterman and Anastasiya Vinokur with assistance from Kristina Vitale.

Our gold open-access journal, *Structural Dynamics*, published jointly by ACA with AIP Publishing, continues to grow and thrive. Majed Chergui, our *Structural Dynamics* Editor-in-Chief, was pleased to have the opportunity to meet many of you in New Orleans.

For additional information on *Structural Dynamics*, see pp. 7-9. ACA members can take advantage of a special discounted rate when publishing their work in our journal!

In this, my final ***From the Editor's Desk***, I want to say how much I've enjoyed serving as your Co-Editor these past four years. We are indeed fortunate that Ed Stevens will be taking over my Co-Editor duties beginning with our Spring 2018 issue. Welcome aboard, Ed! In closing, I would like to thank everyone, including Marcia Colquhoun and the team in Buffalo, and especially my Co-Editor Judy Flippen-Anderson, for all of their invaluable help!

Tom Koetzle

ACA History Project News

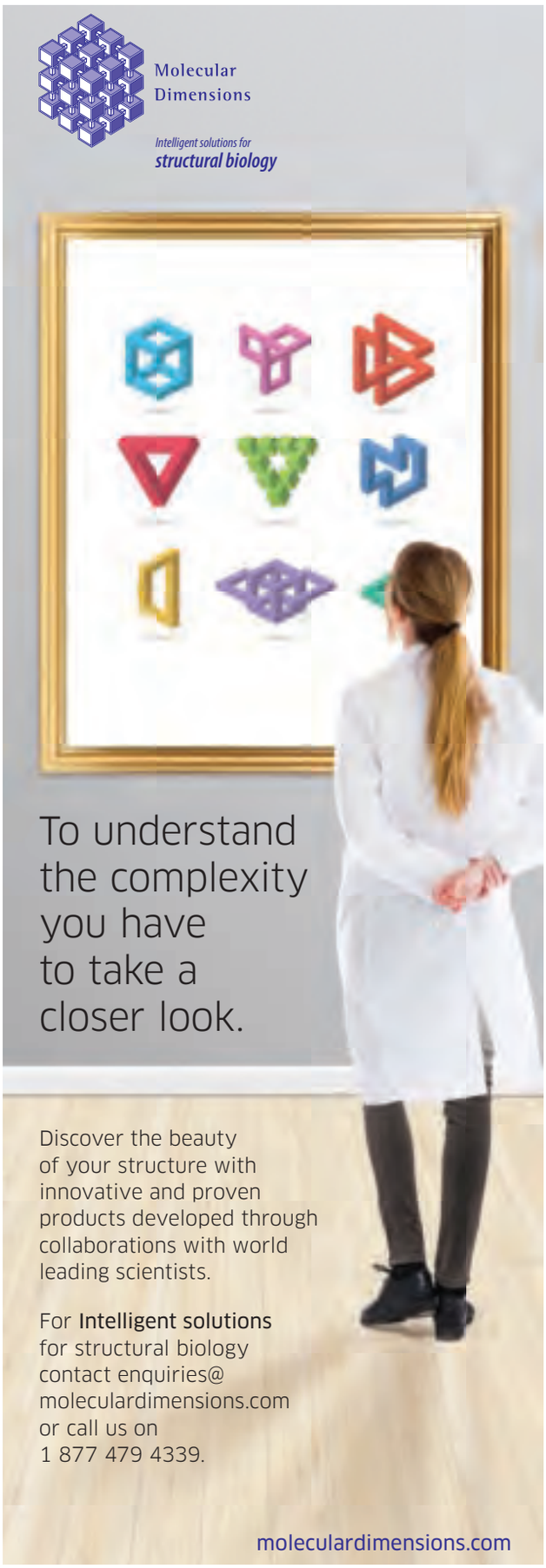
As of August 25, the ACA History webpages have had **207,447** unique visitors in 2017! The average visitor came to the site 1.5 times, and while they were at the site they viewed 2.4 different pages. Clearly, the public is interested in the history of 20th century crystallography as told through memoirs and biographies, ACA award lecture videos, and articles describing the significance of structural science.

In keeping with our aim to encourage more interest in ACA History pages, Webmaster Vanessa Reitz has revamped the ACA History Home page with an appealing, graphic interface. We'd like to hear your reactions to the new design: ***http://www.amercrystalassn.org/history_home***.

Winnie Wong-Ng's full-length Living History autobiography is now online. It describes Winnie's odyssey from China and Hong Kong to the U.S. and Canada, then finally to the National Institute of Standards and Technology (NIST), where the broad scope of her research illustrates the wide variety of questions that can be answered by X-ray diffraction.

Also online now is the video of Elspeth Garman's Fankuchen Award lecture, in which she gives some humorous anecdotes from her "Travels in Protein Crystallography" as well as how she determined the radiation dose maximum for protein crystals. See Elspeth's page for links to her other videos, "From chocolate to drug discovery – what crystallography has done for the world" and "Crystallography one century AD (After Dorothy)."

Virginia Pett
pett@wooster.edu



Net RefleXions

Anastasiya Vinokur

I don't know about you, dear reader, but in the opinion of this young crystallographer, the 2017 ACA meeting in New Orleans was a real blast. It especially was a treat to attend so many sessions that addressed one of the central questions for crystallography (and science in general): that is, how to effectively communicate our work. As reaching the public with good, sound science and engaging a new generation of researchers becomes even more of a hot topic, from a sampling of multiple talks from this meeting on online resources to enhance laboratory modules, effective tweeting, and the values of online tutorials, it is very clear that the web plays an integral role in our pursuits of outreach.

But although there has been a lot of discussion with regard to the content of our websites and tutorials, there was one dimension of web design that we did not address in New Orleans. An all-important aspect of user experience: accessibility. Most of us most likely have never considered how our color choices or font sizes might affect a user with color blindness (which affects 8% of men and 0.6% of women, according to *Wikipedia*) or how a hearing-impaired member of the public can engage with our crystal growing videos. These are the questions that, as responsible web designers, whether amateur or professional, we should ask ourselves so that our websites are not only aesthetically pleasing but also functional.

For example, to reach users with a wider range of seeing abilities, we can insure that our contrast between font and background is at least 7 to 1 and use additional cues besides colors to communicate information such as links for further content. Leaving breadcrumbs (showing the user their progress through the website) could help mentally-challenged site visitors more effectively navigate through our tutorials, and including transcripts of the spoken portions of our videos or providing closed captioning will enhance our reach to users with auditory disabilities.

It may seem like a lot to consider, but luckily there are many resources from tutorials to blog posts to shorthand lists that are available to help improve accessibility of online content. A great starting point on your quest for greater accessibility is the website for Web Accessibility Initiative (***https://www.w3.org/WAI/intro/accessibility.php***), which provides not only solid advice on web design but also includes user experiences that help drive the point about how vital seemingly small design decisions are in narrowing or expanding our web traffic.

Armed with this knowledge, I wish you all the best of luck as you put together new amazing web content. Sadly, this will be my last installment of ***Net Reflexions***. I hope you have enjoyed the column as much as I enjoyed writing it for you, dear reader. It has been a real honor.

Anastasiya Vinokur

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TRANSACTIONS FROM THE
66th Annual Meeting of the American Crystallographic Association (ACA)

"Spanning time scales from seconds to femtoseconds, the rapidly growing field of structural dynamics explores both equilibrium and non-equilibrium processes in chemical, biological, and condensed matter systems. Advances in X-ray sources and detectors as well as new approaches for sample delivery, data collection, and processing continue to drive exciting discoveries in atomic and electronic motion in systems large and small."

The current issue of *Structural Dynamics* is a special topic issue with a selection of invited papers representing a rich diversity of research that was presented in July 2016 during the 66th Annual Meeting of the American Crystallographic Association in Denver, CO.

PREFACE

INVITED ARTICLES

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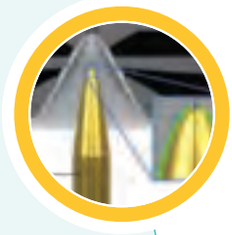


A Tribute to Ahmed H. Zewail

Ahmed Zewail had a profound impact on the scientific community and his legacy will continue to feed and benefit future generations for years to come. His support on the *Structural Dynamics* editorial board was invaluable and the community came together to build a Special Topic issue in honor of his contributions to ultrafast Structural Dynamics. We are grateful for the consideration and engagement of all who contributed. The articles shown below are a sample of the papers published in the Special Topic: Ultrafast Structural Dynamics — A Tribute to Ahmed H. Zewail.

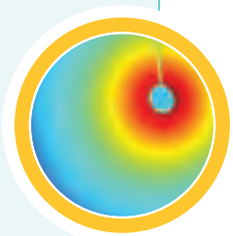
PERSPECTIVES

Perspective: Structure and ultrafast dynamics of biomolecular hydration shells
Damien Laage, Thomas Elsaesser, and James T. Hynes
Structural Dynamics **4**, 044018 (2017)
DOI: 10.1063/1.4981019

Perspective: A toolbox for protein structure determination in physiological environment through oriented, 2D ordered, site specific immobilization
M. Altissimo, M. Kiskinova, R. Mincigrucci, L. Vaccari, C. Guarnaccia, *et al.*
Structural Dynamics **4**, 044017 (2017)
DOI: 10.1063/1.4981224

ARTICLES

A general method for baseline-removal in ultrafast electron powder diffraction data using the dual-tree complex wavelet transform
Laurent P. René de Cotret and Bradley J. Siwick
Structural Dynamics **4**, 044004 (2017)
DOI: 10.1063/1.4972518



Shaped cathodes for the production of ultra-short multi-electron pulses
Ariel Alcides Petruk, Kostyantyn Pichugin, and Germán Sciainia
Structural Dynamics **4**, 044005 (2017)
DOI: 10.1063/1.4974779

Pulse length of ultracold electron bunches extracted from a laser cooled gas
J. G. H. Franssen, T. L. I. Frankort, E. J. D. Vredenbregt, and O. J. Luiten
Structural Dynamics **4**, 044010 (2017)
DOI: 10.1063/1.4978996

Beating Darwin-Bragg losses in lab-based ultrafast x-ray experiments
Wilfred K. Fullagar, Jens Uhlig, Ujjwal Mandal, Dharmalingam Kurunthu, Amal El Nahhas, *et al.*
Structural Dynamics **4**, 044011 (2017)
DOI: 10.1063/1.4978742

SVD-aided pseudo principal-component analysis: A new method to speed up and improve determination of the optimum kinetic model from time-resolved data
Key Young Oang, Cheolhee Yang, Srinivasan Muniyappan, Jeongho Kim, and Hyotcherl Ihee
Structural Dynamics **4**, 044013 (2017)
DOI: 10.1063/1.4979854

Compression of high-density 0.16 pC electron bunches through high field gradients for ultrafast single shot electron diffraction: The Compact RF Gun
Hazem Daoud, Klaus Floettmann, and R. J. Dwayne Miller
Structural Dynamics **4**, 044016 (2017)
DOI: 10.1063/1.4979970

High current table-top setup for femtosecond gas electron diffraction
Omid Zandi, Kyle J. Wilkin, Yanwei Xiong, and Martin Centurion
Structural Dynamics **4**, 044022 (2017)
DOI: 10.1063/1.4983225

Ultrafast electron microscopy integrated with a direct electron detection camera
Young Min Lee, Young Jae Kim, Ye-Jin Kim, and Oh-Hoon Kwon
Structural Dynamics **4**, 044023 (2017)
DOI: 10.1063/1.4983226

Nanotip-based photoelectron microgun for ultrafast LEED
Gero Storeck, Simon Vogelgesang, Murat Sivis, Sascha Schäfer, and Claus Ropers
Structural Dynamics **4**, 044024 (2017)
DOI: 10.1063/1.4982947

Double-shot MeV electron diffraction and microscopy
P. Musumeci, D. Cesar, and J. Maxson
Structural Dynamics **4**, 044025 (2017)
DOI: 10.1063/1.4983390

Improving temporal resolution of ultrafast electron diffraction by eliminating arrival time jitter induced by radiofrequency bunch compression cavities
J. G. H. Franssen and O. J. Luiten
Structural Dynamics **4**, 044026 (2017)
DOI: 10.1063/1.4984104

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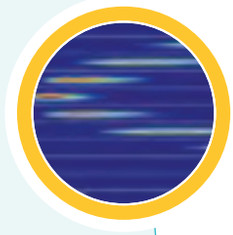
Design and implementation of an optimal laser pulse front tilting scheme for ultrafast electron diffraction in reflection geometry with high temporal resolution
Francesco Pennacchio, Giovanni M. Vanacore, Giulia F. Mancini, Malte Oppermann, Rajeswari Jayaraman, *et al.*
Structural Dynamics **4**, 044032 (2017)
DOI: 10.1063/1.4991483

Localized holes and delocalized electrons in photoexcited inorganic perovskites: Watching each atomic actor by picosecond X-ray absorption spectroscopy
Fabio G. Santomauro, Jakob Grilj, Lars Mewes, Georgian Nedelcu, Sergii Yakunin, *et al.*
Structural Dynamics **4**, 044002 (2017)
DOI: 10.1063/1.4971999

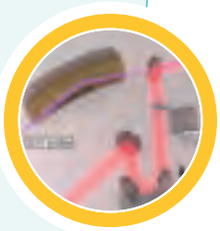


Optically induced lattice deformations, electronic structure changes, and enhanced superconductivity in $YBa_2Cu_3O_{6.48}$
R. Mankowsky, M. Fechner, M. Först, A. von Hoegen, J. Porras, *et al.*
Structural Dynamics **4**, 044007 (2017)
DOI: 10.1063/1.4977672

Dynamic diffraction effects and coherent breathing oscillations in ultrafast electron diffraction in layered 1*T*-TaSeTe
Linlin Wei, Shuaishuai Sun, Cong Guo, Zhongwen Li, Kai Sun, *et al.*
Structural Dynamics **4**, 044012 (2017)
DOI: 10.1063/1.4979643

Defect-mediated phonon dynamics in TaS_2 and WSe_2
Daniel R. Cremons, Dayne A. Plemmons, and David J. Flannigan
Structural Dynamics **4**, 044019 (2017)
DOI: 10.1063/1.4982817

Stacking order dynamics in the quasi-two-dimensional dichalcogenide 1*T*-TaS_2 probed with MeV ultrafast electron diffraction
L. Le Guyader, T. Chase, A. H. Reid, R. K. Li, *et al.*
Structural Dynamics **4**, 044020 (2017)
DOI: 10.1063/1.4982918



Modeling nonequilibrium dynamics of phase transitions at the nanoscale: Application to spin-crossover
Sang Tae Park and Renske M. van der Veen
Structural Dynamics **4**, 044028 (2017)
DOI: 10.1063/1.4985058

Ultrafast carrier thermalization and trapping in silicon-germanium alloy probed by extreme ultraviolet transient absorption spectroscopy
Michael Zürch, Hung-Tzu Chang, Peter M. Kraus, Scott K. Cushing, *et al.*
Structural Dynamics **4**, 044029 (2017)
DOI: 10.1063/1.4985056

Femtosecond time-resolved X-ray absorption spectroscopy of anatase TiO_2 nanoparticles using XFEL
Yuki Obara, Hironori Ito, Terumasa Ito, Naoya Kurahashi, *et al.*
Structural Dynamics **4**, 044033 (2017)
DOI: 10.1063/1.4989862

Distortion dependent intersystem crossing: A femtosecond time-resolved photoelectron spectroscopy study of benzene, toluene, and p-xylene
Anne B. Stephansen and Theis I. Sølling
Structural Dynamics **4**, 044008 (2017)
DOI: 10.1063/1.4977735

Angle-resolved photoemission spectroscopy of liquid water at 29.5eV
Junichi Nishitani, Christopher W. West and Toshinori Suzuki
Structural Dynamics **4**, 044014 (2017)
DOI: 10.1063/1.4979857

Molecular couplings and energy exchange between DNA and water mapped by femtosecond infrared spectroscopy of backbone vibrations
Yingliang Liu, Biswajit Guchhait, Torsten Siebert, Benjamin P. Fingerhut, *et al.*
Structural Dynamics **4**, 044015 (2017)
DOI: 10.1063/1.4980075

Picosecond sulfur K-edge X-ray absorption spectroscopy with applications to excited state proton transfer
Benjamin E. Van Kuiken, Matthew R. Ross, Matthew L. Strader, Amy A. Cordones, *et al.*
Structural Dynamics **4**, 044021 (2017)
DOI: 10.1063/1.4983157

Ligand manipulation of charge transfer excited state relaxation and spin crossover in $[Fe(2,2'\text{-bipyridine})_2(CN)_2]$
Kasper S. Kjær, Wenkai Zhang, Roberto Alonso-Mori, Uwe Bergmann, *et al.*
Structural Dynamics **4**, 044030 (2017)
DOI: 10.1063/1.4985017

Ultrafast kinetics of linkage isomerism in $Na_2[Fe(CN)_5NO]$ aqueous solution revealed by time-resolved photoelectron spectroscopy
Azhr A. Raheem, Martin Wilke, Mario Borgwardt, Nicholas Engel, *et al.*
Structural Dynamics **4**, 044031 (2017)
DOI: 10.1063/1.4990567

Molecule-specific interactions of diatomic adsorbates at metal-liquid interfaces
Jan Philip Kraack, Andres Kaech and Peter Hamm
Structural Dynamics **4**, 044009 (2017)
DOI: 10.1063/1.4978894

Structural enzymology using X-ray free electron lasers
Christopher Kupitz, Jose L. Olmos, Mark Holl, Lee Tremblay, *et al.*
Structural Dynamics **4**, 044003 (2017)
DOI: 10.1063/1.4972069

A comparison of the innate flexibilities of six chains in F_1-ATPase with identical secondary and tertiary folds; 3 active enzymes and 3 structural proteins
Monique M. Tirion
Structural Dynamics **4**, 044001 (2017)
DOI: 10.1063/1.4967226

Outrunning damage: Electrons vs X-rays—timescales and mechanisms
John C. H. Spence
Structural Dynamics **4**, 044027 (2017)
DOI: 10.1063/1.4984606

Photoinduced molecular chirality probed by ultrafast resonant X-ray spectroscopy
Jérémy R. Rouxel, Markus Kowalewski and Shaul Mukamel
Structural Dynamics **4**, 044006 (2017)
DOI: 10.1063/1.4974260

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Zbigniew Dauter, Senior Investigator at the Macromolecular Crystallography Laboratory and Head of the Synchrotron Radiation Research Section at the National Cancer Institute, received the **2017 Patterson Award** and presented his lecture: *The Patterson Award for a lucky crystallographer* at the annual meeting of the ACA in New Orleans.

The cover image depicts the crystal structure of a fungal CAP protein[1], solved in the laboratory of Oluwatoyin Asojo (Baylor College of Medicine) with the use of selenourea, the novel anomalously scattering reagent introduced by Zhipu Luo, a member of the Dauter lab (see below). In this structure, seven protein molecules pack according to an unusual non-crystallographic 7_5 screw axis.

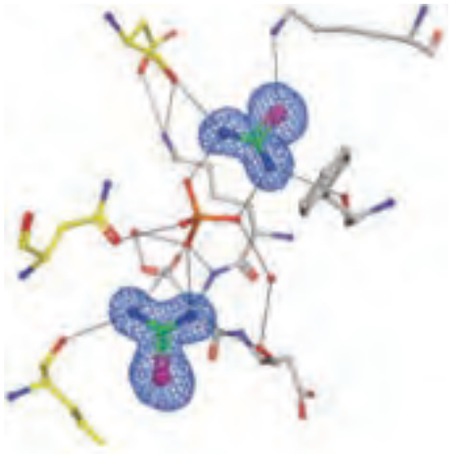
Dauter's research group (a part of the Macromolecular Crystallography Laboratory of NCI) is located at the synchrotron site of Argonne National Laboratory and specializes in biostructural research based on the unique properties of synchrotron radiation. Its high intensity makes it possible to record very high resolution diffraction data, and its wavelength tunability allows recording anomalous diffraction signals of various scatterers used for phasing novel crystal structures of macromolecules. The previously established "quick cryo-soaking of halides" approach[2] has been responsible for a number of crystal structures not amenable for other types of derivatization.

Recently, Zhipu Luo, a member of the lab, introduced a new practical and effective reagent, selenourea[3], which can be soaked for a short time into native crystals of proteins or nucleic acids, providing a significant anomalous signal of selenium atoms. The chemical properties of selenourea molecules differ from other derivatization reagents, as selenoureas can serve both as donors and acceptors of hydrogen bonds formed with polar groups of macromolecules. Selenourea is an effective and easy to use reagent with a potential to gain popularity in the crystallographic practice.

[1] Baroni, RM, Luo, Z, et al., Asojo, OA (2017). Crystal structure of MpPR-1i, a CAP protein from *Moniliophtora perniciosa*, the fungus that causes Witches' Broom Disease in Cacao. *Sci. Rep.*, in press.

[2] Dauter, Z, Dauter, M, Rajashankar, KR (2000). Novel approach to phasing proteins: derivatization by short cryo-soaking with halides. *Acta Cryst.* **D56**, 232-237.

[3] Luo, Z (2016). Selenourea: a convenient phasing vehicle for macromolecular X-ray crystal structures. *Sci. Rep.* **6**, 37123.



At right: The anomalous difference peaks (red), and

at left: The 2Fo-Fc map (blue) of selenourea molecules bound at the surface of a protein.

Contributors to this Issue

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Pauling Poster Prizes

The Pauling Poster Prize was established by the ACA and is supported by member contributions to honor Linus Pauling, a pioneer in American structural research and a very supportive member of ACA for many years. At each annual meeting up to seven of the best trainee (*postdoctoral*, *graduate* or *undergraduate*) poster presentations receive Pauling awards. Some of the awards consist of a certificate, a $250 prize, and a copy of a Linus Pauling book. Up to three **ACA Pauling Poster Prizes** honor Linus Pauling's contributions to science and U.S. crystallography; the **Herman R. Branson Pauling Poster Prize** recognizes the contributions of Herman Russell Branson, one of the first African American physicists to make crystallography the focus of his research. The **Muttaiya Sundaralingam Pauling Poster Prize** recognizes the ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids done by Muttaiya Sundaralingam and his colleagues. The **Louis Delbaere Pauling Poster Prize** in honor of Louis Delbaere, former Canadian President of the ACA, and sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, is given to the highest ranked *graduate* or *undergraduate* poster from a Canadian laboratory. Finally, the **IUCr Pauling Poster Prize** is sponsored by the International Union of Crystallography and is given to a *graduate* or *undergraduate* poster selected by the committee. The winner of the IUCr Pauling Prize receives complimentary online access to all IUCr journals for one year or a complimentary volume of *International Tables* or other IUCr publication, a copy of *The Little Dictionary of Crystallographic Terms* and an IUCr-2017 polo shirt.

In New Orleans, eligible posters and presenters were evaluated for the Pauling Prize by a panel of 14 judges. Trainees were judged both on the work presented on their posters and on their general knowledge of the subject and crystallography. All posters and presenters were found to be of very high quality, which made the task of determining the best posters very difficult. Following are the winners of the 2017 Pauling Poster Prize, as well as one honorable mention. Photos are shown of winners who were able to attend the conference banquet and accept their awards in person. The majority of the awardees are also shown with their prize-winning posters.

The committee to review posters for the Louis Delbaere Pauling Poster Prize, consisting of Mariusz Jaskólski and Lisa Keefe, reluctantly concluded that there were not enough eligible contenders for a serious competition, and that no presentation qualified for the distinction. The 2017 Delbaere Prize was not awarded.

New Orleans Posters Chair Bruce Noll announcing the Poster Prize presentations at the Awards Banquet

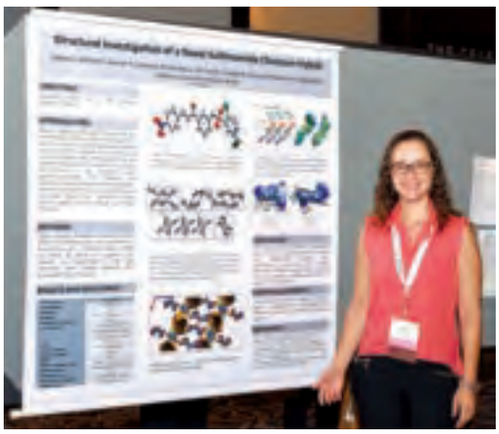
The ACA Pauling Poster Prizes (*presented by Gerald Audette*)

Brinda Selvaraj, Oak Ridge National Laboratory, poster **11-Su**: *Investigation of the Bacteriochlorin rings and its environment in Fenna-Matthews-Olsen antenna complex revealed by neutron and ultra-high resolution X-ray crystallography*.

Brinda Selvaraj, at left, with Gerald Audette

Lidiane Michelini, Universidade Federal de Goiás, Brazil, poster **17-Su**: *Structural investigation of a novel sulfonamide chalcone hybrid*.

L-R: Amy Sarjeant, Lidiane Michelini, Gerald Audette



Lidiane Michelini with her prize-winning poster

Herman R. Branson Pauling Poster Prize (*presented by Allyson Fry-Petit*)

The Branson Pauling Poster Prize was given to **Fiyinfoluwa Adesioye** of the Centre for Microbial Ecology and Genomics in the Genomics Research Institute at U Pretoria, RSA. Her poster **131-Su** was titled, *The crystal structure of a novel Carbohydrate Esterase 7 family esterase from a hot desert metagenome*. The presentation highlighted Fiyin's important work on solving the structure of a novel CE7 acetyl xylan esterase, NaM1. In addition to the structure solution her work encompassed the encoding of

Turn to p. 12

the esterase, chemical synthesis of the gene, cloning, expression, purification, crystallization, and thermal analysis. This research provides an interesting piece in the puzzle of understanding substrate specificities and thermolability in deacetylases.

Fiyinfoluwa Adesioye, at left, accepting the 2017 Herman R. Branson Pauling Poster Prize, presented by Allyson Fry-Petit

Fiyinfoluwa Adesioye with her prize-winning poster

Honorable Mention – **Kartik Manne**, U Alabama at Birmingham, poster **5-Su**: *Structural biology of proteins responsible for biofilm regulation and dispersion*.

L-R: Kartik Manne, Amy Sarjeant, Allyson Fry-Petit

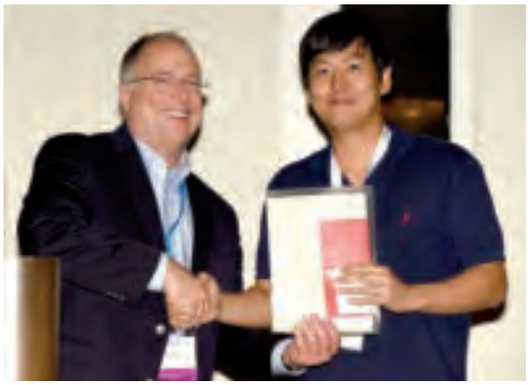
Muttaiya Sundaralingam Pauling Poster Prize (*presented by Christopher Colbert*)

Ashley Campbell, U Missouri, poster **29-Su**: *Trapping conformational states of the SidA ornithine hydroxylase in crystallo*.

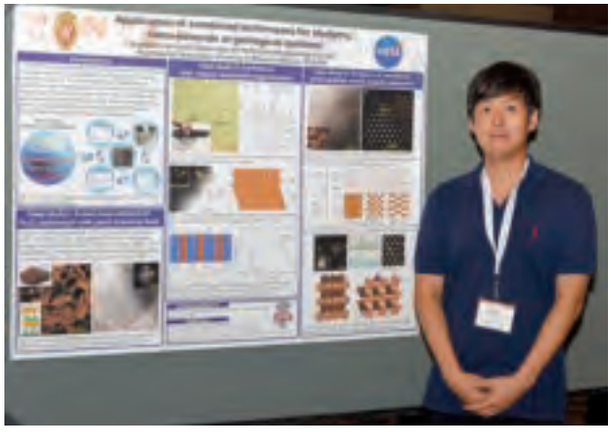
Ashley Campbell, at right, with Christopher Colbert

IUCr Pauling Poster Prize (*presented by Bruce Noll for Frank Fronczek*)

Seungyeol Lee, U Wisconsin – Madison, poster **23-Su**: *Application of combined techniques for studying nano-minerals in geological systems*.



Seungyeol Lee, at right, with Bruce Noll



Seungyeol Lee with his prize-winning poster

Gerald Audette

Structural Dynamics Poster Prize

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

The winner of the Structural Dynamics Poster Prize at ACA 2017 was **Nicholas Keul** from Athens, Georgia for his poster **40-Sa**: *The role of intrinsic disorder in human uridine diphosphate glucose dehydrogenase*.

Nicholas Keul, at right, with John Helliwell

Nicholas Keul with his prize-winning poster

Nicholas is in the fourth year of his graduate program of research at U Georgia. Building on open and closed form crystal structure knowledge of the enzyme he combined mutagenesis and biophysical characterization methods to show that a disordered functionally important tail of the polypeptide acted as what he vividly called a "Brownian motion antenna."

The various candidate posters were of a very high quality. The Editor-in-Chief of *Structural Dynamics* Majed Chergui was very impressed by these and by the winning poster especially.

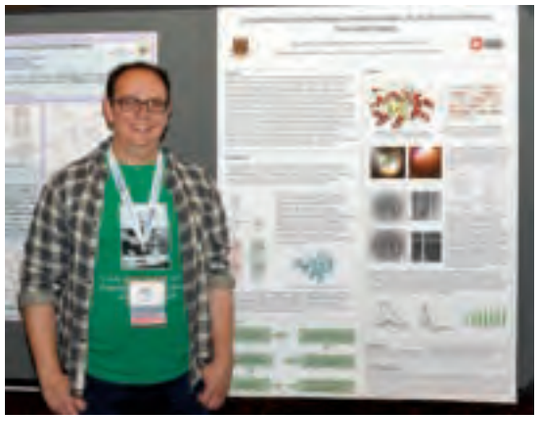
John Helliwell

RCSB Protein Data Bank Poster Prize

The **RCSB (Research Collaboratory for Structural Bioinformatics) Protein Data Bank Poster Prize** recognizes a student, *graduate* or *undergraduate*, poster presentation involving macromolecular crystallography. The award consists of two educational books, and the winner is acknowledged in the RCSB web site and newsletter. This year there were six entrants to be judged by a committee consisting of Marian Szebenyi, Jan Abendroth, and Greg Hura.

The winner was **Miguel Torres** (with co-authors Mehran Dastmalchi, Peter Facchini, and Kenneth Ng), a graduate student at U. Calgary, Canada, for his poster **110-Su,** *Crystallization and preliminary structural studies of an aldo-keto reductase from opium poppy***.** Miguel clearly has a talent for making good posters, as he won the same award at the Denver meeting (the judges had no idea!).

Miguel Torres, at right, with Marian Szebenyi



Miguel Torres with his prize-winning poster

The judges also recognized **Makayla Anderson** (and co-authors David Roberts and Jacqueline Roberts), of DePauw U, with an Honorable Mention for their poster **113-Su**, *Unique crystal structures of an SmtB/ArsR transcriptional factor from Methanosarcina acetivorans*. The project described in the poster represents dedicated work by a succession of undergraduate students, of whom Makayla is the latest.

Marian Szebenyi

L-R: Marian Szebenyi, Makayla Anderson, Bruce Noll (at rear)

CrystEngComm Poster Prize

CrystEngComm, published by the Royal Society of Chemistry, is aimed at the materials, chemistry, crystallographic, and crystal engineering communities and is committed to, "covering all aspects of crystal engineering – the design, including synthesis of crystals and crystal growth, synthesis and evaluation of solid-state materials with desired properties." The RSC sponsors the **CrystEngComm Prize** for, "the best student, graduate or undergraduate, poster presentation in the area of crystal engineering/supramolecular chemistry." This year's judging committee for the *CrystEngComm* Poster Prize was Christine Beavers and Tony Hu.

The 2017 winner of the CrystEngComm Prize is **Raúl Castañeda**, New Mexico Highlands U. Raúl's poster **13-Sa**: *Co-crystals of dithieno[3,2-a:2',3'-c]phenazine derivatives and trimeric perfluoro-ortho-phenylene mercury* described his work with a series of co-crystals. His goal was to determine the structural ramifications of functionalizing one component

Raúl Castañeda, at right, with Christine Beavers

Raúl Castañeda with his prize-winning poster

with various halogens or substituting a pyridyl ring in place of a phenyl. Starting with dithienophenazine (DTPhz) and trimeric perfluoro-ortho-phenylene mercury (TPPM), he did not observe any co-crystallization. He was able to observe two distinct 1:1 co-crystal structure types, once the DTPhz was functionalized with halogens, and intriguingly, a non-centrosymmetric structure resulted when the halogen was fluorine. The pyridyl substituted DTPhz did co-crystallize with TPPM, but this structure also incorporated a water molecule. As Raúl stated in his abstract, the focus of this study was to understand how, "small changes in substituents [can] give a variety of packing motifs and interactions." The judging committee for the poster prize felt that Raúl's poster was well presented and fit nicely within the scope of *CrystEngComm*. We congratulate Raúl for his achievement!

Christine Beavers

Taylor & Francis Biomolecular Crystallography Poster Prize

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

The 2017 prize was awarded to **Sharrol Bachas** from Adrian Ferré-D'Amaré's lab at National Heart, Lung, and Blood Institute, NIH, Bethesda for his poster **112-Sa**: *Induced fit in the specific recognition of transition metal ions by a gene-regulatory RNA*. Sharrol presented a crystallographic analysis of alternative metal ion recognition by yybP-ykoY riboswitches. Proper data collection strategy, and challenging and rigorous structure determination

Sharrol Bachas, at right, with Przemyslaw Porebski

Sharrol Bachas with his prize-winning poster

and refinement allowed him to observe a flexible binding site that adopts variable coordination schemes with different metal ions. Sharrol demonstrated that the analogous mechanism is employed by gene-regulatory proteins functioning in the same pathway as the yybP-ykoY riboswitches.

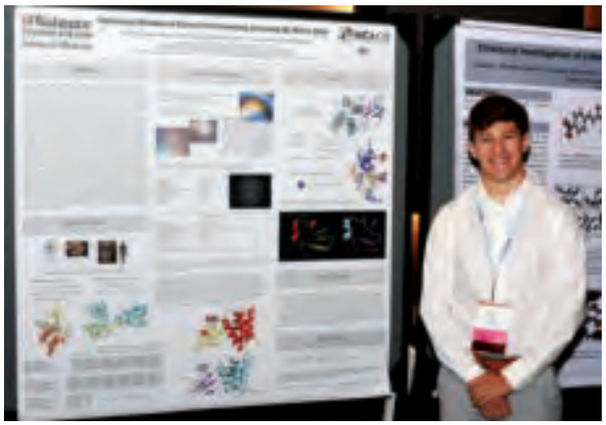
Przemyslaw Porebski

MiTeGen - Society of Physics Students Undergraduate Poster Prize

The **Undergraduate Poster Prize**, co-sponsored by the AIP Society of Physics Students (SPS) and MiTeGen, was established in 2014 to recognize the best undergraduate poster presentation at ACA. The recipient of this award receives a $250 cash prize, generously donated by MiTeGen and SPS, along with a gift card for crystallographic supplies though MiTeGen.

This year's winner was **Garrett Ginell** from Cornell College for the excellent presentation of his research on poster **129-Su**: *Structural studies of Ebola viral homolog encoded by Microbats*.

Garrett Ginell, at left, with Krystle McLaughlin



Garrett Ginell with his prize-winning poster

Structural Dynamics Editor-in-Chief Majed Chergui, at left, with George Phillips at the Structural Dynamics booth.

Editor's note: Photos in the **Poster Prizes in New Orleans** section are by Peter Müller.

The judges also would like to give honorable mention to another presenter, **Makayla Anderson**, DePauw U, for poster **113-Su**: *Unique crystal structures of an SmtB/ArsR transcriptional factor from Methanosarcina acetivorans*. Makayla also received honorable mention in the **RCSB Protein Data Bank Poster Prize** competition, see p. 13. The judges for the 2017 Undergraduate Poster Prize were Krystle McLaughlin and SPS Director Brad Conrad.

We hope that this prize continues to inspire and encourage young undergraduate researchers in the field of crystallography.

Krystle McLaughlin

Oxford Cryosystems Low Temperature Poster Prize

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

This year's winner of the Oxford Prize was **Carlos Pinheiro**, Universidade Federal de Minas Gerais, Brazil, for his poster **19-Sa**: *Hard X-ray-induced valence tautomeric interconversion in cobalt-o-dioxolene complexes*.

Carlos Pinheiro, at left, with Bruce Noll

2017 Poster Prize Winners, L-R: back row – Sharroll Bachas, Miguel Torres, Posters Chair Bruce Noll, Raúl Castañeda; front row – Garrett Ginell, Fiyinfoluwa Adesioye, Lidiane Michelini, Seungyeol Lee. Not shown – Ashley Campbell, Nicholas Keul, Carlos Pinheiro, Brinda Selvaraj.

The ACA's **67th Annual Meeting** kicked off in New Orleans on Friday, May 26, 2017 with four full-day workshops: a **CSD Workshop – Communication and Innovation**, along with workshops on **CrysAlisPro and Olex2: From Raw Data to Publication**, **Introduction to PHENIX for Beginning and Advanced Crystallographers**, and **Research Data Management**. The latter workshop continued into early evening with a technical sub-session on high-performance computing and networking issues. A **First Time Attendee and Student Meeting Orientation** was held Friday evening. This was followed by a **Special Plenary Lecture** by **Sir James Fraser Stoddart**, 2016 Nobel Laureate in Chemistry. The **Opening Reception Exhibit Show**, generously hosted by the exhibitors, capped off the evening. Reports from the **Workshops** and from this year's **Travel Award Winners** will be featured in our winter issue of *ACA RefleXions*. Watch also for upcoming coverage of Fraser Stoddart's lecture, including Tomislav Friščić's interview with Sir Fraser.

The **Patterson Award** for 2017 was presented to **Zbigniew Dauter**. **Helen Berman** received the **David Rognlie Award**, **Christine Dunham** received the **Margaret C. Etter Early Career Award**, and **James O'Brien** was honored with ACA's **Elizabeth Wood Science Writing Award**. Dauter's Patterson award-winning work is featured on our cover (see also ***What's on the Cover*** on p. 10). The **ACA Transactions Symposium**, *Going beyond PX with cryo electron microscopy, tomography, and diffraction*, was chaired by **Stephen Burley** and **Michael Rossmann**.

The meeting wrapped up Tuesday evening with ACA's annual **Awards Banquet**. The evening's program chaired by ACA President, **Amy Sarjeant**, included the presentation of the **ACA Fellows – Class of 2017**: **Marilyn Olmstead** and **Brian Toby**. The ACA honored this year's 11 **Poster Award Winners** along with two students selected to receive honorable mention from among the exceptional array of posters presented at the meeting (see pp. 11-15 for news on the ***Poster Prizes in New Orleans***). This year's awards banquet program featured a fascinating talk by our Wood award-winner James O'Brien, who regaled us with his *Tales of famous mad hatters* spanning five centuries. To cap off the evening, we were treated to entertainment by New Orleans band, Dr. Jazz.

Yulia Sevryugina and **Ilia Guzei** were **Program Chairs** for the meeting; **Bruce Noll** was **Posters Chair**; **Chelsy Chesterman**, **Vicky Doan-Ngyen** and **Anastasiya Vinokur** coordinated the **Session Photos** with assistance from ACA's **Kristina Vitale**; and **Richard Bromund** and **Virginia Pett**, ACA's **Videography Team**, recorded the award lectures and the Stoddart interview. AIP Publishing's **Robert Finnegan** did his usual great job with the **Exhibit Show**.

Bill Duax, at left, and Tom Terwilliger at the opening reception exhibit show Friday evening

L-R: Wesley Vaz, Lidiane Michelini, and Carlos Pinheiro discussing a point during the Monday evening poster session

James O'Brien, a/k/a The Mad Hatter, delivering his talk at the awards banquet

Sir Fraser Stoddart delivering his opening plenary lecture

Brian McMahon and Virginia Pett

Anthony Solis and Jessica Hoy of AIP Publishing

Photos by Richard Bromund or Peter Müller. New Orleans meeting logo design: Kandis Elliot

Wood Award Winner James O'Brien Entertains New Orleans ACA Awards Banquet Crowd with Tales of Famous Mad Hatters

ACA President Amy Sarjeant presenting James O'Brien with the 2017 Elizabeth Wood Science Writing Award. Photo by Peter Müller.

Attendees of the 2017 ACA **Awards Banquet** in New Orleans got a real treat. Forgoing a more general talk about ways to present science in an accessible manner, this year's **Wood Award** recipient, **James O'Brien**, Missouri State U, gave a stellar example of such an effort when he gave a talk on the fascinating, colorful history of the "Famous Mad Hatters."

O'Brien has been part of the Missouri State Chemistry faculty for 35 years. He has won multiple awards for his teaching and research and was named Distinguished Professor in 2002. Beyond the academic arena, O'Brien is no stranger in sparking interest in science among non-scientists. He uses his passion for history and literature to reach a wider audience. An avid Sherlockian, in 2013 O'Brien published *The Scientific Sherlock Holmes*, where he explored the chemistry, forensic science, and botany utilized by everyone's favorite detective to solve various crimes.

For the ACA, O'Brien presented his lecture on the historical victims of mercury poisoning. From Thomas P. "Boston" Corbett, who killed John Wilkes Booth, to the first tsaritsa Anastasia Romanovna, to even Sir Isaac Newton, the presented list of victims of mercury poisoning was truly illustrious. O'Brien delivered an engaging account of the various forms of mercury and its early medical uses (mainly to cure syphilis) and industrial purposes (for hat making), as well as the common symptoms of mercury poisoning, all entwined with the personal histories of famous men and women. It was truly an artful blend of history, chemistry and medicine.

From O'Brien's talk, not only did we learn to appreciate the medical advances of the 21st century and workplace safety regulations, but also how our hobbies and passions can make us better ambassadors for science!

Anastasiya Vinokur

Scenes from the Awards Banquet

Christopher Colbert and Erica Saphire. Photo by Richard Bromund.

Krystle McLaughlin. Photo by Peter Müller.

Luo Yoyo, center, dancing with Anna Gardberg, at left, and Sangita Sinha, at right. Photo by Richard Bromund.

L-R: top row – Jeffrey Lovelace; Ed Stevens; Hanna Dabkowska and Marvin Hackert; second row – Irina Kriksunov and Jeney Wierman; Tomislav Friščić; third row – Bill Duax and Sue Byram; James Holton and Ana Gonzalez; bottom row –Stephan Ginell, Garrett Ginell and Lisa Keefe; Carl Schwalbe. Photos by Richard Bromund or Peter Müller.

Their ACA Family Turned Out in Force to Celebrate with Jeanette Krause and Allen Oliver on Sunday Afternoon in Storyville Hall at the Hyatt. The Newlyweds Continued Celebrating throughout the Week.

Photos by Richard Bromund or Peter Müller.

Zbigniew Dauter Receives 2017 ACA Patterson Award

Amy Sarjeant presenting the Patterson Award for 2017 to Zbigniew Dauter. Photo by Peter Müller.

Describing himself in his lecture title as a very lucky crystallographer, **2017 ACA Patterson Award** winner **Zbigniew Dauter**'s immediately humble approach resonated warmly with his highly appreciative audience. Many decades of experience in crystallography formed the time line for his talk and of his incisive contributions to new diffraction methods in crystallography, also then resonating with the Patterson Award descriptor itself. Zbigniew paid tribute to the rigorous science training he had received in Poland where he studied chemistry in the Technical University of Gdansk and received an M.Sc. there in 1971. He undertook a Ph.D. under the supervision of Professor Zofia Kosturkiewicz of the University of Poznan and was awarded his Ph.D. by the Technical University of Gdansk on the crystal structure studies of the antitumor derivatives of acridine.

A chance meeting at an Erice School of Crystallography led to a Post Doc job offer for Zbigniew in 1981 with Michael Woolfson in York University, UK. In 1983 he moved across the campus from Physics to the Chemistry Department to work with Guy and Eleanor Dodson. Overnight use was made of the York computer by Zbigniew and his close colleague Zygmunt Derewenda, also working at York, which they had decided was the most effective for their calculations. This stay in York Chemistry included a memorable meeting with Max Perutz, who described how alligators are able to stay under water for relatively long periods of time, based of course on the 3D structures of hemoglobin. While in York, Zbigniew worked on the cadmium and mercury derivatives of insulin in what he referred to as his favorite space group *R*3.

More luck occurred for Zbigniew with an offer of a job in 1985 at the EMBL Hamburg Outstation where Keith Wilson had recently been appointed Head of Outstation. A key development was the image-plate scanner by Jules Hendrix and Arno Lentfer, also in Hamburg. Zbigniew energetically saw the new opportunities it presented on the beamline for protein crystallography. A stream of new studies at atomic resolution became possible, and new collaborations were joined with George Sheldrick in an exciting phase of Zbigniew's already by now internationally recognized research career.

After nine years and a short period back in York, Alex Wlodawer tempted Zbigniew to the USA to work for the NIH at the NSLS in Brookhaven where he would run X9B. A study provocatively entitled, *Can the anomalous signal of sulfur become a tool for solving protein crystal structures?*, published in *J. Mol. Biol.* (1999) caught the wide interest of the protein crystallography community. Working with his wife Miroslawa their publication on the halide soaking method, either sodium bromide or sodium iodide, published in *Acta Cryst.* (2000), proved to be very effective as a new phasing method, there being several hundred structures in the PDB that have used this method so far alone. The theme of ultra-high resolution, with its important impacts in biological chemistry started in Hamburg, continued with a study of Z-DNA at 0.55 Ângstrom resolution that was published in *Nucleic Acids Res.* in 2011. Other examples described by Zbigniew included a complex case of pseudosymmetry undertaken with Joanna Sliwick and Mariusz Jaskólski and most recently introducing a new phasing compound, seleno urea, in work with Zhipu Luo. In an overview of the sources of satisfaction in his career Zbigniew highlighted the chances there were at synchrotron facilities for him to meet many people.

Zbigniew concluded his talk with a tribute to his wife Miroslawa. There were appreciative tributes from many members of the audience to Zbigniew after his lecture and who also inquired as to his thoughts on several topics. He commented on synchrotron radiation crystallography data collection and processing, remarking that these days it is fast, perhaps only taking minutes, but that people could be less than competent in methods. Zbigniew's sage advice was to take time and not rush. On the excellent training that he had received in Poland he again paid tribute to his Ph.D. supervisor, Professor Zofia Kosturkiewicz, who was also a demanding supervisor. In addition the crystallography schools, such as at Erice, were excellent. There was also a high level of rigorous teaching in the Polish schools in mathematics, physics and chemistry. In a memorable remark for all present Zbigniew affirmed that, "Data collection is a scientific process, not a technicality."

John Helliwell

ACA Honors Helen Berman with Rognlie Award

Helen Berman was the first recipient of the newly established **ACA David Rognlie Award** (see below), recognizing "an exceptional discovery or technical development of particularly high impact in any area of structural science." Indeed, it would be hard to find anybody else who has had higher impact on the structural science of macromolecules than Helen, taking into account her outstanding achievements in the fields of crystallography, nucleic acids, proteins, and their systematics.

Helen was initiated into protein crystallography as a student in the laboratory of Barbara Low, and then graduated from the lab of George Jeffrey in Pittsburgh, working on structures of sugars. There she became, in her own words, "enamored of computing," as applied to various structural problems. After a number of years at the Fox Chase Cancer Center in Philadelphia, Helen moved to Rutgers University as a Professor of Chemistry, where she educated a large number of young structural biologists and recently "actively" retired.

Amy Sarjeant, at left, with Helen Berman holding her Rognlie Award. Photo by Peter Müller.

Helen published several hundred publications on structures of various proteins and nucleic acids, their classification, and biological function. In 1971 she was, together with Walter Hamilton, Tom Koetzle, and a few others, one of the initiators of setting up the Protein Data Bank as a repository for protein structures, at first with only seven atomic models. Eventually, her greatest service to the community was her leadership of the PDB, undoubtedly the most important resource of knowledge in biology, which Helen led through over 15 years, when it grew to contain more than 130,000 entries.

In her award talk, Helen first presented the most important events in the history of the PDB, from its inception, through the formulation of data standards and deposition guidelines for scientific journals, establishment of the wwPDB in three sites (Rutgers, Cambridge, and Osaka), requirement of deposition of experimental data (e.g., structure factors), and provision of a wide variety of practical search and analysis tools for PDB users.

Next, Helen discussed the future challenges that PDB will face in the coming era of integrative biology, where diverse kinds of hybrid information and data from various biostructural techniques, such as crystallography, NMR, electron microscopy, small-angle scattering, or bioinformatics need to be stored and analyzed. Mechanisms for processing and presentation of such integrative entries have to be developed, since these types of hybrid entries are expected to grow in the near future, as very large complexes and molecular machines require application of several methods for comprehensive analysis of their structure and function. Members of the wwPDB and community groups are currently actively discussing the best ways to tackle this and some other problems awaiting the PDB, in order to make sure that it will continue to be the most useful and comprehensive repository for the biomedical community.

In her memoir Helen once said that her dream was, "to understand biology and medicine at the molecular level so that it will be possible to circumvent the errors of our genes." Her achievements, full of "exceptional discovery and technical development," have very substantially advanced the fulfillment of that dream.

Dave Rognlie

The David Rognlie Award is named to honor a much loved longtime member of the American crystallographic community, the founder of Blake Industries that was the sole supplier of Huber equipment in North America; equipment that forms the basis of so many X-ray synchrotron beamlines. Many remember Dave as an ever-present fixture at ACA and other crystallography meetings, charming the visitors to the Blake booth in the exhibition with his warm smile, laughter, and excruciating metal puzzles. Dave grew up in a small northwestern Minnesota village, Climax, pop 250. An outstanding student and athlete, he financed his way through college by working summers as a farm hand and "bussing dishes" along with a four-year scholarship from a regional lumber company, graduating from the University of North Dakota with a degree in electric engineering. Dave cut his teeth with 10 years (to the day) of employment at GE before leaving to found Blake. Why the name Blake Industries? It was the maiden name of the wife of his founding partner, who dropped out before the company got going! Learning business at the knee of his Swedish maternal grandfather, who ran an implement dealership where all transactions were verbal (with phone and electricity rare) along with a handshake, he carried these principles to Blake, where many of us remember Dave personally delivering the equipment and supervising the installation. He continued well beyond retirement age because, he would say, "I just love what I do," meaning coming to meetings and engaging and enabling the enthusiasm and enterprise of scientists old, and especially, young. Dave will be remembered with fondness by all those who knew him. But through the Rognlie Award, he will also be honored so that future generations of crystallographers become acquainted with his name through the title of the award, but more importantly through the citation of the award itself, to the values he believed in and embodied in his life: his generosity of spirit, optimism, selflessness, and unstinting desire to help others to succeed in their endeavors.

Zbigniew Dauter
Simon Billinge

Helen Berman. Photo by Richard Bromund.

Christine Dunham Receives Etter Award

Amy Sarjeant presenting the Etter Award for 2017 to Christine Dunham. Photo by Peter Müller.

The **Etter Early Career Award** for 2017 was presented to **Christine Dunham**, Assistant Professor in the Emory University School of Medicine's Department of Biochemistry. 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.

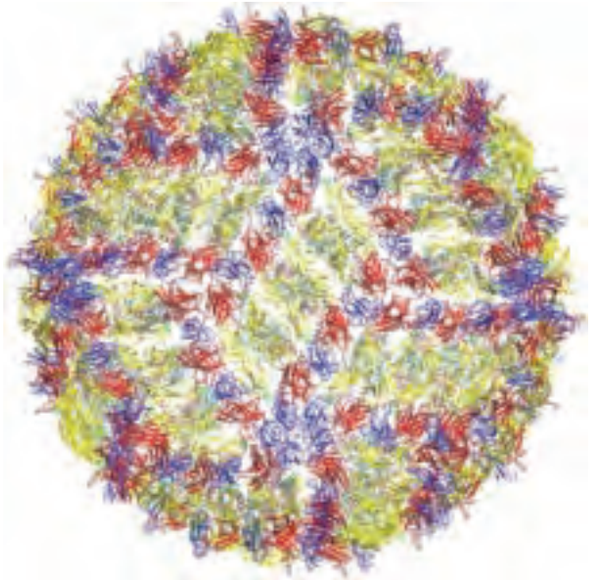
Christine was honored for her impressive work, featured on our spring 2017 cover, which included X-ray crystallography and cryogenic transmission electron microscopy (cryo-EM) to resolve structures of ribosomes and bacterial toxins. In addition to her innovative research, Christine has been dedicated to training and mentoring undergraduate and graduate students to be the next generation of crystallographers. The **Etter Symposium for Young Scientists, Session 4.1.1**, immediately followed Christine's award lecture on Tuesday morning (see p. 41).

Vicky Doan-Nguyen

ACA Transactions Symposium: Going Beyond PX with Cryo Electron Microscopy, Tomography, and Diffraction

This year's **ACA Transaction Symposium** concerned itself with what has become known as the "Resolution Revolution." Structural crystallography of biological substances has been overwhelmed by the growing importance of electron microscopy during the last two or three years. Two factors have contributed to this amazing turn of events. One of these is the sudden development of direct electron counting detectors (DEDs) for use with electron microscopes, and the other is the gradual development of techniques to turn the collection of many thousands of images of a randomly oriented molecule into three-dimensional structure. Each image is a projection of the molecule. Thus if the relative orientation of these images can be determined, then it is not difficult to combine all these images into a three-dimensional structure. However, until recently such structures could not be much better than about 25 Å resolution. Nevertheless that was very useful as most large biological assemblies cannot be crystallized but these "low" resolution electron potential maps could be fitted with the structure of the component molecules determined by X-ray crystallography to give "pseudo atomic resolution" structures of, for instance, viruses and molecular motors that drive bacterial motion. However the advent of the DEDs allowed not only a more accurate response to electrons, but also a very fast read-out that took no more than 1 millisecond – a time shorter than most gravitational or electromagnetic variations. Thus the cryo-EM images could be corrected for motion between successive image records, removing much of the blur that had been typical of most EM observations. As a result in the last two or three years there have been numerous structure determinations, with resolution limits better than 3 Å, of objects whose structure and functional mechanism had heretofore been a mystery.

The meeting opened with **Stephen Burley** (Co-organizer, Rutgers U) giving a short explanation of the events that were changing the biological landscape from the perspective of the RCSB Protein Data Bank. Then **Michael Rossmann** (Co-organizer, Purdue U) followed, describing the structure of Zika virus whose near atomic resolution structure determination



Atomic model of Zika virus. Figure courtesy of Michael Rossmann. Adapted from Sirohi et al., SCIENCE 352: 467 (2016).

had been achieved in about one month. The significance of this structure (see figure above) was not only because Zika virus infections have become a major world health concern, but also because the structure of the homologous structures of other similar flaviviruses (e.g., dengue and West Nile) had been determined previously by a combination of low-resolution electron microscopy and atomic resolution X–ray structures of the component proteins, thus justifying the earlier indirect pseudo atomic methods and demonstrating the far greater speed and simplicity of the new cryo technology.

There followed a variety of examples of the power and versatility of the new cryo-EM technology. **Peijun Zhang**, U Oxford and Diamond Light Source, UK, described the structure of dynamin; **Yuan He**, Northwestern U, and **Seth Darst**, Rockefeller U, showed structures of RNA polymerases; **Hong Zhou**, UCLA, described the structure of a bacteriophage RNA genome; **Shikebi Watanabe**, Johns Hopkins U, showed the structure of neuronal

synapses; and **Wah Chiu**, Baylor College of Medicine, reported on recent high-resolution structure determinations and discussed the importance of validation of both EM image/density map data and structural models derived therefrom.

Most impressive of all for the ACA audience, **Maryam Khoshauer**, MPI, Martinsried, Germany, described a 3.2-Å resolution structure determination of hemoglobin (MW 68KDa). The hemoglobin tetramer is so small that conventional single-particle EM techniques fail to find the orientation of the molecules. However, with the addition of a "phase plate" to increase contrast, this has now been possible. Hemoglobin was one of the first two proteins whose structure had been determined. Thus now there seem to be few limits on where cryo-EM can improve, extend and open new vistas.

In addition there were talks on the new technology. In particular, **Wolfgang Baumeister**, MPI, Martinsried, discussed tomography. Cryo-EM depends on averaging many thousands of presumably identical particles, as is also the case for conventional crystallography. However as biological objects that we wish to study become ever larger, the likelihood of finding a homogenous sample decreases. This is where tomography can take over. Instead of averaging between many randomly oriented particles, in tomography the sample is imaged in a series of known relative orientations. The problem, however, is that the many exposures to electrons will damage the particle. Another consequence of the new EM technology is that many labs are equipping themselves with powerful microscopes. That also makes it possible to use these microscopes for electron diffraction as opposed to imaging. **Tamir Gonen**, HHMI, Janelia Research Campus, gave a talk on how electron diffraction can be used successfully for analyzing very small crystals. Finally, **Elizabeth Villa**, U California San Diego, discussed how specimens can be better prepared for cryo-EM investigations using ion beam milling.

A brief final round-table discussion among the speakers, the leadership of the ACA, and audience members made it clear that structural biology has entered a new era, wherein protein crystallography and nuclear magnetic resonance spectroscopy have found a powerful new partner in cryo-EM.

Symposium speaker registration fees and travel/accommodation expenses were partially reimbursed using contributions from the ACA and four corporate sponsors, including FEI, Jeol USA, Gatan, Inc., and Direct Electron, LLP.

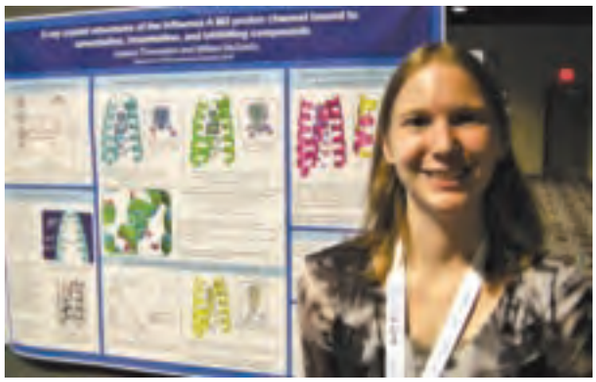
Michael Rossmann
Stephen Burley

Joe Reibenspies, at left, and Richard Staples. Photo by Peter Müller.

General Interest Posters

As usual, I could choose from a wide variety of scientifically stimulating and beautifully presented posters in New Orleans. For this column I have selected four posters that addressed particular interests of mine: drug discovery, drug formulation design, research that extracts the maximum information from crystal structure determinations, and radiation damage. Coming from Hong Kong, Brazil and England as well as the USA, these posters also illustrate the worldwide appeal of this ACA meeting. I had taken notes on a number of additional posters; but in those cases my personal choice was matched by carefully considered evaluation from the poster prize judges, who awarded prizes to these posters. Such posters are included in the section on prize winners, see pp. 11-15.

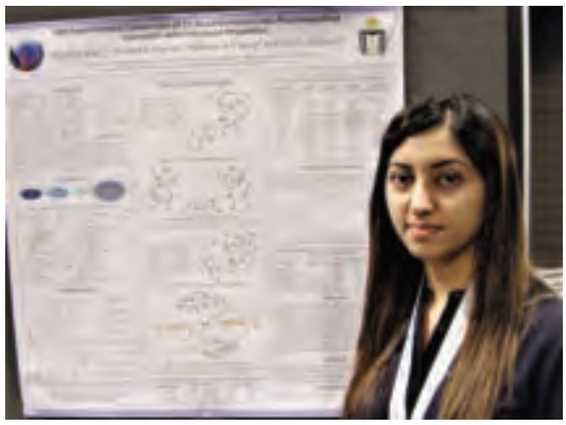
Poster **82-Sa**: *X-ray crystal structures of the influenza A M2 proton channel bound to amantadine, rimantadine, and inhibiting compounds*, presented by **Jessica Thomaston**, U California, San Francisco



The influenza virus continues to be a major cause of illness and a significant cause of death. Once it has obtained access to a host cell by endocytosis, it must unpack its RNA. This process requires an influx of protons via the M2 protein channel. Two drugs from our sparse armamentarium, amantadine and rimantadine, block this channel and abort the infection. Both drugs have an ammonium group attached to an adamantyl cage. Unfortunately, resistance has become widespread in currently circulating viruses. To inform the discovery of new drugs, Jessica has crystallized the protein and determined its structure to much higher resolution than ever before with drugs bound. The extremely difficult task of growing high-quality crystals of this membrane protein was finally accomplished using lipidic cubic phase techniques. Structures of the channel in its $Inward_{closed}$ conformation both with bound rimantadine and with bound amantadine were determined to a resolution of 2.0 Å; the structure of the $Inward_{open}$ channel with bound rimantadine was determined to 2.5 Å. Maps clearly show the orientation of the drugs as well as the positions of ordered water molecules that interact with their ammonium group. Furthermore, the binding mode has been established for a spiroadamantane inhibitor that blocks both the wild-type M2 channel and the heretofore drug-resistant V27A mutant. The binding position of the drug in the wild-type and the V27A channel shifts, but it remains effective. This information helps with the design of drugs to counteract resistance.

Turn to p. 24

Poster **26-Su**: *Mechanochemical conversion of 11-azaartemisinin into pharmaceutical cocrystals with improved solubility*, presented by **Madiha Nisar,** Hong Kong U of Science and Technology (HKUST)

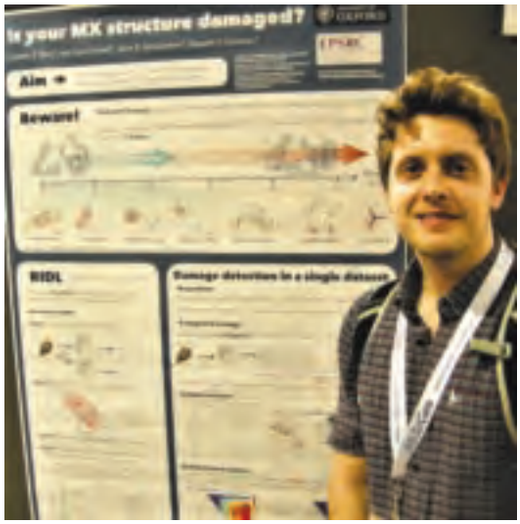


In the ongoing battle against malaria an important advance was the discovery that the natural product artemisinin has antimalarial activity. Subsequently, variants have been synthesized, especially in attempts to improve the bioavailability while retaining or enhancing the activity against *Plasmodium falciparum*, the most dangerous pathogen. While 11-azaartemisinin is effective, it still has poor aqueous solubility. In her poster Madiha reported on cocrystallization experiments by the technique of liquid assisted grinding. Of the 26 coformers tried with 11-azaartemisinin and screened by X-ray powder diffraction, 15 yielded cocrystals, carboxylic acids being particularly effective. The structures of 4 cocrystals subsequently grown from solution were determined, revealing the importance of the introduced nitrogen atom at position 11 in forming a synthon of the type OCNH…OCOH. The cocrystals showed improved solubility and thermal stability. Intriguingly, the cocrystal with another antimalarial drug, mefloquine, gave the highest thermal stability along with much improved solubility.

Poster **38-Su**: *Supramolecular arrangement of two methoxychalcones*, presented by **Hamilton Napolitano**, U Goias, Brazil

Before we discussed his poster, Hamilton and I chatted about his situation in Brazil. His university is located outside of wealthy parts of the country; and therefore his group lacks the resources to produce a blizzard of structure determinations like many groups in the USA or, indeed, Sao Paolo. Instead, this poster, along with two others presented at the ACA meeting by his group members, gave us a helpful lesson in concentrating on a few significant structures and using a variety of techniques to deepen our understanding of them. Chalcone moieties, which are present in many pharmaceutical compounds, have two phenyl rings joined by a prop-2-ene-1-one linker. Two chalcones with constant 4-methoxyphenyl substitution on one phenyl ring but 3,4,5-trimethoxy *versus* 4-ethoxy substitution on the other (MT-TRI *vs*. MT-ETX), were found to differ in degree of planarity and dihedral angles. Intermolecular interactions affecting crystal packing were investigated by Hirshfeld surface analysis, demonstrating the particular importance of C-H…π interactions in MT-ETX. Properties were evaluated by CAM-B3LYP/6-311+G(d) theoretical calculations, which also predicted IR vibrational spectra and enabled the assignment of the normal vibrational modes. Softness and hardness, both obtained from frontier molecular orbitals, showed that MT-TRI is more likely to receive electrons while MT-ETX resists charge transfer.

Poster **125-Su**: *Objective classification of specific radiation damage in macromolecular X-ray crystallography*, presented by **Charles Bury**, U Oxford, UK



Through their publications and by tutoring at crystallography schools Elspeth Garman and her colleagues at Oxford have done much to make us aware of the dangers of radiation damage. Our response to this threat has been rather similar to our response to the threat of burglary: add cryoprotectants and cool to low temperature / install strong doors and windows and keep them locked. Then we settled back and hoped it wouldn't happen to us. However, at 100 K damage can be insidious: specific residues may be widely affected long before diffraction intensities decrease noticeably. Chemical changes include disulfide cleavage, decarboxylation, and methylthiol cleavage. It may become all too easy to misinterpret structure and function around the active site. Charles presented an objective procedure for analysis of a data set to determine whether significant radiation damage has occurred. While $F_{obs}(n) - F_{obs}(1)$ Fourier difference maps based on initial (1) and later (n) data sets have been used in visual searches for signs of damage, interpretation of such noisy maps

can be difficult and may be tainted by preconceived ideas. The RIDL computational method has been developed to quantify specific damage events. Machine-learning algorithms, guided by model protein systems where damage has been well characterized, provide promising ways to identify true damage events. This method can also save beam time: a single dataset is collected, overlapping sub-datasets are defined, and a sliding window can be used to define the boundary between unaffected "early" and damaged "late" data.

Carl Schwalbe

Reception and Symposium for Undergraduate Students

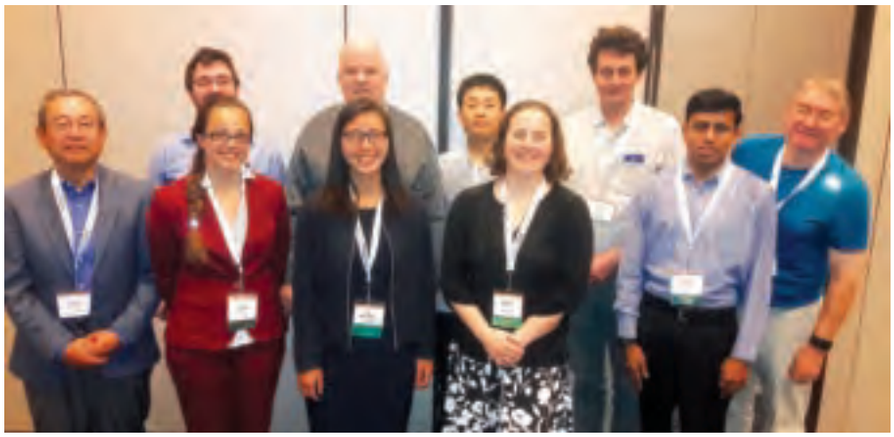
Brad Conrad addressing the group. Dasan Thamattoor is shown seated in the background. Photo by Krystle McLaughlin.

The fourth annual **Undergraduate Student Reception** was held at ACA 2017, in an ongoing collaboration with the Society of Physics Students (SPS), American Institute of Physics. Attendees, mostly undergraduate students, were treated to lunch and then an interactive talk on career pathways and resources for undergraduate students by SPS Director **Brad Conrad**. Brad started off with some interesting employment statistics for students with undergraduate and graduate degrees in the physical sciences, delineating the sectors (i.e., public, private, university, etc.) in which they work. Next he asked the students present to think about where they wanted to be in the next 10 years, and what was their dream job. Students were encouraged to share with their peers, and to also consider the follow-up questions: why and how? What was it about that particular job, at that particular place that made them want it, and how were they going to achieve it? This active examination provided a lot of enthusiastic discussion from the attendees. Resources for undergraduates thinking about different careers were highlighted. Brad also shared a story from his own undergraduate days, which led to the final group activity. One summer, while working as a NIST intern, Brad happened to get into an elevator with Hillary Clinton. Senator Clinton turned to him and said, "So, tell me about what you do here." Brad was caught off guard, and he did not remember saying too much. He told this story as a missed opportunity – if only he'd had an elevator speech prepared! Perhaps it would have led to other opportunities. Attendees were then asked to pair up, create and practice their own elevator speeches – a clear, brief, 30-second summary about research/interests. The reception ended with an open discussion, where many attendees asked questions, as well as gave suggestions for what they would like to see at ACA meetings for students in the future.

Krystle McLaughlin

The audience listening attentively to Brad's talk. Photo by Krystle McLaughlin.

1.1.2: Disorder, Inhomogeniety, and Local Structure in Complex Materials



L-R: Takeshi Egami, Kamila Wiaderek, Martin Donakowski (at rear), Vicky Doan-Nguyen, Thomas Proffen (at rear), Yuanpeng Zhang (at rear), Kate Page, Emil Bozin (at rear), Milinda Abeykoon, Ian Williams (at rear)

Takeshi Egami, Oak Ridge National Laboratory, began the session on **Disorder, Inhomogeneity, and Local Structure in Complex Materials**. He described that in contrast to crystals, many materials – such as glasses, (most) liquids, and many electrochemical materials – exist with their atoms in disordered systems. This can be visualized (see figure below) as ordered, marching soldiers (a 'crystal') versus disordered crowds on the street ('noncrystalline').

Egami introduced PDF, or pair distribution function, to explore disordered systems: PDF examines the entirety of the scattering, not exclusively the Bragg peaks, to produce a histogram of atom-pair distances. He successfully used this methodology to illustrate the structure of the supreme capacitor, disordered hydrous ruthenium oxide ($RuO_2 \cdot xH_2O$). The ruthenia material exists as a nanocomposite of metallic rutile RuO_2 and hydrous water. The water can facilitate proton transfer of the aqueous capacitor while the metallic component is able to facilitate electron transfer.

Vicky Doan-Nguyen, now at The Ohio State U, continued the theme of electrochemical materials with her talk on molybdenum sulfide clusters in a lithium ion battery. With *operando* electrochemical and PDF measurements – coupled with Raman and X-ray photoelectron spectroscopy – she found that the oxidation state of the molybdenum did not change during charge and discharge of the battery. Rather, the sulfide anions of the disordered chalcogenide gel (or 'chalcogel') changed oxidation state and were the redox-active agent in the complex $MoS_{3.4}$ battery electrode.

Emil Bozin, Brookhaven National Laboratory, described how they applied X-ray and neutron PDF techniques to explore dynamic local symmetry breaking in novel materials, emphasizing that this local symmetry breaking is the key for understanding devices from energy conversion to superconductivity. He presented evidence that local, fluctuating broken symmetry states are widespread in functional materials, illustrating this with three examples having implications for photovoltaics, thermoelectrics, and superconductivity.

Kamila Wiaderek, Argonne National Laboratory, presented her work, *Relating ε-$LiVOPO_4$ performance to local environment dynamics and hysteresis*. She used *operando* PDF analysis along with X-ray diffraction to identify potential structural differences between $LiVOPO_4$ synthesized via solid-state and hydrothermal methods, which might affect the diffusion pathways and ultimately limit the cycling efficiency of potential battery applications.

Katharine Page, Oak Ridge National Laboratory, concluded the session by presenting their design for a novel total scattering diffractometer for materials discovery (DISCOVER), proposed for the Spallation Neutron Source (SNS). DISCOVER is expected to be the world's highest resolution dedicated neutron total scattering instrument that will be optimized for studying real materials in their operating environments. Page also explained why the total scattering method holds the key to determine the crystallographic average structure as well as the local structure, often responsible for the physical properties of complex materials.

Milinda Abeykoon
Martin Donakowski

Brandon Mercado, at left, and Mike Takase. Photo by Peter Müller.

Stacey Ortega. Photo by Richard Bromund.

1.1.4: Engaging Undergraduates with Crystallographic Research

This half-day session included an engaging panel of speakers who highlighted the ways in which they are involving undergraduate students in crystallography at their institutions. The talks featured a mixture of topics in both small molecule and protein crystallography. **Tim Royappa**, U West Florida, answered the question of how to teach crystallography without a diffractometer by discussing the incorporation of computational lab modules that use the freely available resources of the Cambridge Structural Database. **Peter Wood**, CCDC, UK, highlighted the benefits of 3D printing to create physical models of molecules for classroom use that are both accurate and inexpensive. **Simon Coles**, U Southampton, UK, discussed ways in which he has embedded real-world aspects in an existing crystallography lab to provide a scaffolded research experience for students. **Rich Matyi**, Florida Polytechnic U, discussed his experience leading a team of undergraduates in the setup and characterization of a new diffractometer system, while **Joe Tanski,** Vassar College, summarized an undergraduate lab module he developed on molecular structure determination, focusing on how students should investigate and describe intermolecular interactions in crystal structures in their reports. **Krystle McLaughlin**, Vassar College, discussed her lab module at Lehigh U that introduces undergraduates to protein crystallography in an effort to excite them about structure. Krystle's series of labs spans crystallization, virtual data collection, model building in Coot, and figure generation with PyMOL. **Bradley Miller**, Bryn Mawr College, wrapped up the session by describing ways in which he incorporates structural biology into the biochemistry classroom, the biochemistry teaching labs and his undergraduate research program.

Joe Tanski
Rachel Powers

1.2.1: Nucleic Acids and Friends

The **Nucleic Acid and Friends** session focused on structures of RNA, DNA, and protein nucleic acid complexes that perform essential tasks in biology. **Hong Li**, Florida State U, presented a tour de force story on how essential snoRNP complexes are formed using a balanced mix of structural and biochemical methods. **Rui Zhao**, U Colorado, Denver, presented her group's exciting new work on a high-resolution cryo-EM structure of the *S. cerevisiae* U1 snRNP spliceosome complex. Alternative splicing allows one gene to code for many proteins, and Rui's talk offered interesting insights into splicing initiation and the choice of performing alternative splicing. **Hideki Aihara**, U Minnesota, presented his group's past and recent work unravelling the complexity and diversity of intrasomes. Hideki highlighted how different viruses use unique combinations of integrases to encase DNA targets. Before the coffee break, **Xinhua Ji**, NIH, took us on his group's decade-long journey examining RNase III enzymes, and how they measure and cut RNA targets using a unique "double ruler" mechanism. **Blaine Mooers**, U Oklahoma, who was in the air flying to the meeting when the session started, heroically arrived just in time to present how local RNA structures and sequence context regulate the fascinating world of RNA editing. Next, the session switched gears to DNA modification and repair. **Alex Drohat**, U Maryland, presented an examination of how epigenetic DNA marks are recognized, decoded, and finally removed. Alex's talk set up **Martin Horvath**, U Utah, who presented a revised mechanism for MutY DNA repair activity. **Fukang Wang**, Zhen lab, Georgia State U, closed the session with a fascinating talk on Se modification of DNA and RNA nucleotides to create a phasing toolbox. Fukang's talk created a lively discussion regarding the versatility of Se-labeled nucleotides and their adaptability to aid the research of the nucleic acids structural biology community.

Aaron Robart

Session 1.2.2: Diffuse Scattering in Complex Oxides

L-R: back row – Daniel Phelan, Richard Welberry, Emil Bozin, Ben Frandsen; front row – Kate Page, Yan Wu, Tedi-Marie Usher, Ying Zhang, Allyson Fry-Petit. Photo by Pavol Juhas.

The session on **Diffuse Scattering in Complex Oxides** featured four invited and four contributed presentations covering a wide range of research utilizing diffuse scattering. The talks highlighted the diversity of experimental techniques related to diffuse scattering as well as the plethora of material systems that can benefit from this type of analysis. On the experimental side, we enjoyed presentations about measuring and modeling single-crystal, three-dimensional diffuse scattering patterns in reciprocal space; real-space based atomic and magnetic pair distribution function (PDF) analysis of powder diffraction data; dynamical pair distribution function (dyPDF) methods using inelastic neutron scattering; and advancements in PDF modeling methods, such as improvements in incorporating particle shape and size into calculated PDFs. The materials investigated included strongly correlated electron systems, relaxor ferroelectrics, magnetoelectrics, magnetic semiconductors, and high-efficiency catalysts. Out of this variety of research emerged a strong common theme: diffuse scattering is rich in information about the local structure of complex materials, which often has direct bearing on their properties and functions. Many thanks to the speakers for their excellent work and engaging presentations!

Ben Frandsen
Kate Page

1.2.4: Important Science from Small Molecules

The **Important Science from Small Molecules** session continued its biennial tradition of bringing together speakers involved in many aspects of chemistry and physics to give presentations involving both theory and experimentation. Speakers came from all levels of academia ranging from second-year graduate students, to post docs, to established professors.

The session began with **Nikolay Gerasimchuk**, Missouri State U, introducing us to recent work from his group on the rich, diverse chemistry of Ag(I) and Tl(I) cyanoximates. Silver cyanoximates were found to display anti-microbial properties while also demonstrating initial promise as battery-less sensors for the detection of UV light. Thallium cyanoximates were shown to form light-insensitive compounds, and demonstrated particularly interesting structural chemistry.

Michael Hall, Texas A&M U, our next speaker, introduced us to the fascinating realm of non-innocent ligands, which were shown to be a particularly intriguing topic for electronic-structure calculations. A range of recently characterized ruthenium and rhenium complexes with non-innocent ligands were described, with selected complexes displaying potential to facilitate the water oxidation of methanol.

Raúl Castañeda, U Ottawa, Canada, followed with an update on his ongoing graduate work focused on using Fe(II) tetrachlorides with pyridinium cations as starting materials for the coordination of imidoyl amines.

Alice Brink, U Free State, Bloemfontein, RSA, wrapped up the first half of the session by providing an excellent overview of the use of rhenium in drug development. Utilizing a new class of ligands, Alice had characterized new Re drug candidates and compared these new compounds to metastable technetium analogues.

The second half of the session started with **Robin Macaluso**, U Texas at Arlington, discussing two Er-Pt-Ga intermetallic compounds that had recently been synthesized by her group via flux synthesis. The two phases were a known modulated structure along with a second new phase, the latter of which was of particular note as magnetic measurements on this new compound displayed geometrical frustration.

Carlos Murillo, Texas A&M U, followed with a presentation focusing on transition-metal complex metal-metal interaction distances, an often-overlooked means of non-covalent assembly, and then detailed the many manifestations of these interactions on structures and properties.

Paul Forster, U Nevada Las Vegas, next introduced us to the mystery that is technetium red, a Tc oxide whose formal oxidation state has remained a bit of a scientific conundrum. Proceeding via a combination of simulation and experimentation, Paul eloquently described the anticipated coordination environment of this unusual phase and finished his talk by highlighting initial experimental results from his group that confirmed theoretical findings.

Gertruida Venter, U Free State, Bloemfontein, RSA, followed with an update on her ongoing work developing new hydroxypyridine-N-oxide (HPNO) ligands and complexation efforts with these ligands and rhodium(I).

Our last speaker of the day was **Jim Donahue**, Tulane U, who reminded us all of the importance of paying attention to the details in crystallography, as he presented two cases of metal-ion misidentification in transition-metal diazadiene chloride complexes. As our previous speakers had detailed the ample ways in which small-molecule structures can provide valuable insights across many disciplines, Jim's talk emphasized the importance of accuracy in small-molecule crystal structures, an important takeaway for all session attendees.

Korey Carter
Alberto Albinati

Training Sessions 2.1.1: Learn Macromolecular Crystallography; Best Practices with Diffraction Images from Known X-ray Structure; and 3.1.4: Apply Macromolecular Crystallography Best Practices to Your Challenging Diffraction Data

***Session 3.1.4** – L-R: Ivan Shabalin, Zbigniew Dauter (at rear), Wladek Minor, Dominika Borek (at rear), Jasmine Young, Maksymilian Chruszcz (at rear), Przemyslaw Porebski, Stephen Burley, Zbyszek Otwinowski (at rear), Paul Emsley. Photo courtesy of Wlakek Minor.*

Both training sessions turned out to be among the most popular and successful sessions of the 2017 meeting. Attendance at both sessions was excellent. The participants could download the content of a bootable USB drive with state-of-the-art software for use during the session. A limited number of USB drives were also distributed during the session 3.1.4. X-ray diffraction data for the session were available from ***http://www.proteindiffraction.org***.

During **Session 2.1.1** five speakers presented different aspects of structure determination and validation. **Janet Smith**, U Michigan, made an introductory presentation. She showed the difficulties related to space-group determination and possible complications that may arise from multi-crystal experiments. **Zbigniew Dauter**, NIH, Chicago, discussed the scientific issues that are behind data collection. **Tom Terwilliger**, Los Alamos National Laboratory, discussed SAD phasing for both easy and challenging cases. **Paul Adams**, Lawrence Berkeley Laboratory, discussed various phasing strategies that should be considered when molecular replacement is used to obtain phases. Finally, **Paul Emsley**, MRC, Cambridge, UK, presented the pitfalls of model building and structure refinement and had a live demonstration of the newest COOT capabilities for building N-linked glycans. Session chairs provided introductions and case studies.

Session 3.1.4 concentrated on a practical approach to structure determination. **Dominika Borek**, UT Southwestern Medical Center, discussed the best practices for data reduction. **Zbyszek Otwinowski**, also of UT Southwestern, presented several difficult cases of space-group determination and methods for troubleshooting such problems. **Maksymilian Chruszcz**, U South Carolina, showed the difficulties of phasing when the data were not collected optimally and demonstrated several cases of crystallization artifacts. **Ivan Shabalin**, U Virginia, showed the complicated cases of refining the structural models, including metal ions, with special focus on refinement and analysis of ADPs. **Przemyslaw Porebski**, also of U Virginia, presented issues related to structure refinement and model building for several difficult cases and applications that simplify model building. Finally **Jasmine Young**, RCSB Protein Data Bank, described the wwPDB OneDep Validation procedure during deposition of macromolecular structures. During the session break Ivan Shabalin carried out live demonstration of structure determination from indexing diffraction images to model refinement.

Stephen Burley
Wladek Minor

2.1.2: Joint Methods for High Rate Data Processing: XFEL and Synchrotron

L-R: Ralf Flaig, Danny Axford, Artem Lyubimov, Aaron Brewster, Nicholas Sauter, James Holton, Herbert Bernstein

Session 2.1.2 on **Joint Methods for High Rate Data Processing: XFEL and Synchrotron** was held the morning of Sunday, May 28. Advances in light sources, detectors, beamline design, sample preparation and crystal delivery enable the generation of diffraction data at unprecedented speeds, with the newest pixel array detectors collecting hundreds of frames per second, and giving terabyte data sets. At the same time, the techniques of serial crystallography, popularized by the femtosecond X-ray pulses found at free-electron lasers, are now being transferred to conventional synchrotron beamlines with notable success, greatly increasing the range of samples available for study. Much of the work reported focused on the data-processing challenges arising from serial crystallography. How will high-rate data be acquired, moved, and stored, and what data analysis pipelines will be needed in order to provide timely scientific feedback to the beamline user? Furthermore, what special treatment is required to merge diffraction data from ensembles of crystals, considering specific problems such as non-isomorphism and the issue of still-shot versus rotation data collection?

The speakers responded to this charge with reports of rapid progress in building the hardware and software infrastructure to collect and process data at very high rates from large numbers of crystals, both at XFELs and at synchrotrons. **Ralf Flaig**, Diamond Light Source, UK, spoke about beamline I04 at Diamond, a fully automated, multiwavelength endstation with multiaxis goniometry, including present efforts to produce a real-time data analysis pipeline. Diamond's **Danny Axford** described their beamline I24, along with the silicon-chip array approach to collecting fixed-target serial crystallography data, both at synchrotrons and XFELs. **Herbert Bernstein**, RIT, spoke on *Synchrotron serial crystallography with multi-stage merging of 1000's of images*, combining a sensitive and accurate cell-based clustering with a reflection-based clustering modified to work with low-completeness datasets. **Artem Lyubimov**, Stanford U, gave details of IOTA, his program to optimize the computational merging of data from large serial crystallography data sets. **Aaron Brewster**, Lawrence Berkeley National Laboratory (LBL), reflected on the integration step itself for still shots, and the importance of devising models that are detailed enough to describe the degrees of freedom in the experiment, and accurate enough to be reproducible. **James Holton**, LBL, examined the question of resolution limit, asking where to cut the data in multi-crystal merging, what limits to use for crystallographic refinement, and controversially, what limits to claim in a publication. **Andreas Foerster**, Dectris, Ltd, was scheduled to speak on *High data rate processing – a puzzle of metadata, compression and software*, but was unable to attend, so Herbert Bernstein presented the slides for him. Nicholas Sauter, LBL, then moderated a discussion on *What gaps remain for serial crystallography?* In particular, still-shot data as presently processed apparently require far higher multiplicity to obtain equivalent maps compared with rotation data, and the optimal algorithms for still-shot data treatment are not yet a settled matter. Much remains to be done as light sources and data collection techniques are upgraded, and there are unique issues for synchrotrons as there are for XFELs, but there is common ground and room for sharing the lessons learned.

Nicholas Sauter
Herbert Bernstein

2.1.3: Porous Materials

L-R: Paul Forster, Len Barbour (at rear), Laura McCormack, Michael Zaworotko (at rear), Peter Wood, John MacDonald (at rear), Wenqian Xu. Photo by ACA Meeting student volunteer.

Porous materials represent an important area of science where crystallography has much to offer, but application of crystallographic techniques can remain far from routine. Many of the most attractive features of metal organic frameworks (MOFs) relate to the behavior of guests inside the pores. While crystallography on the frameworks themselves is not always routine, interpreting the much weaker and more diffuse signal associated with guests within pores may be even more challenging. However, to understand processes such as gas storage and separations and catalysis, this is precisely what must be accomplished.

Michael Zaworotko and his teams at U Southern Florida (1999-2013) and Ireland's U Limerick (2013-present) have been instrumental in the development of MOF chemistry and the closely related field of crystal engineering. His talk entitled *Crystal engineering of hybrid ultramicroporous materials* presented their work in the field. One of their emphases in the field of MOF synthesis has been the preparation of materials with increasingly larger and larger pores extending well into the nanometer scale. While there is certainly scope for utilizing such compounds for molecules too large to fit into conventional crystalline nanoporous materials, such pores are also less useful for many separations processes involving small molecules. A key theme, which he backed up with plenty of examples, is the importance of engineering the right pores for the right behavior.

Next, **Len Barbour**, Stellenbosch U, RSA, provided an excellent complementary talk focusing on the importance of structural flexibility in porous applications. His teams' unique combination of high-quality crystallographic and calorimetric analysis under practical conditions has led to a number of compounds with promise for advanced separations and storage applications. Additional speakers in this morning session included **Travis Mitchell**, U Buffalo, *Development, synthesis, and characterization of dithienylethenes and their incorporation into crystalline solids*, **Laura McCormick**, U St. Andrews, UK, and Lawrence Berkeley National Laboratory, *Nitric oxide and the Kagome lattice*, **John MacDonald**, Worcester Polytechnic Institute, *MOFs as porous hosts for generating singlet oxygen*, and **Peter Wood**, CCDC, UK, *Metal-organics: A rich seam of data for knowledge mining*.

Paul Forster

2.1.4: NMR Crystallography

Session 2.1.4 inaugurated the topic of NMR Crystallography to ACA Annual Meeting Sessions. The session was chaired by Manish Mehta, Oberlin College, and Tomislav Friščić, McGill U, Canada, and involved five speakers who formed a compelling and complementary set, presenting a good cross-section of this growing field. The session was very well attended, with a strong audience of at least 50 throughout all the talks. **Manish Meta** gave the opening remarks on the emerging importance and current state-of-the art in NMR Crystallography. He was followed by **James Harper**, U Central Florida, with his presentation, *Developing accurate crystallography without diffraction*, focusing on the use of theoretical techniques including crystal structure prediction (CSP) and density functional theory (DFT) modeling, for understanding and resolving solid-state crystal structures of organic compounds. An example of James's work is found in *J. Phys. Chem. A*, **2013**, *117*, 5534-5541, focusing on use of solid-state NMR in resolving the dynamics in the disordered crystal structure of methyl α-L-rhamnofuranoside. His lecture was followed by that of **Mihails Arhangelskis**, McGill U. In his lecture entitled *Combined use of solid-state NMR spectroscopy and theoretical modelling as a method of structure determination*, Mihails provided a number of increasingly complex examples of solid-state NMR studies facilitating structural characterization of organic solids. Some of that work can be found in his paper *Chem. Eur. J.* **2016**, *22*, 10065-10073.

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2.1.4: NMR Crystallography, ctd

Following a brief coffee break (during which the audience did not disperse!), the session continued with a presentation of **Kenneth Harris**, Cardiff U, UK, on *"NMR Crystallization": New in situ NMR techniques for time-resolved monitoring of crystallization processes*. In his lecture, Kenneth presented a truly exciting methodology for simultaneous observation of crystallization processes through solution-based and solid-state NMR spectroscopy, in that way providing an extremely and surprisingly clear insight into the processes of nucleation, crystal growth and polymorph selection. More information on the **CLASSIC NMR** pulse sequence that enables these measurements can be found in: *Acta Crystallogr*. **2017**, *C73*, 137-148. One note for non-experts regarding "**CLASSIC**" – the NMR community loves acronyms! A major chemical shift in topic followed, with the lecture *NMR Crystallography in the enzyme active site of tryptophan synthase* by **Leonard Mueller**, U California Riverside. His lecture addressed the world of protein structures, and in particular the active site of the pyridoxal phosphate (PLP)-requiring tryptophan synthase enzyme, where the combined use of X-ray crystallographic and solid-state NMR data, all tied together through theoretical modeling, enabled the identification of the protonation state in a reaction intermediate. More on this use of NMR Crystallography can be found in the recent paper: *J. Am. Chem. Soc.* **2016**, *138*, 15214-15226.

(a) Manish Mehta opening the NMR Crystallography session at the New Orleans 2017 ACA Annual Meeting; (b) James Harper talks on crystallography without diffraction; (c) Mihails Arhangelskis illustrating benefits of solid-state NMR in solid-state structure solution; (d) Kenneth Harris describes the CLASSIC NMR approach to monitoring crystallization in situ; (e) Leonard Mueller discusses understanding protonation in enzyme active sites using NMR Crystallography; (f) Darren Brouwer with his legendary zeolite structure solved by NMR Crystallography.

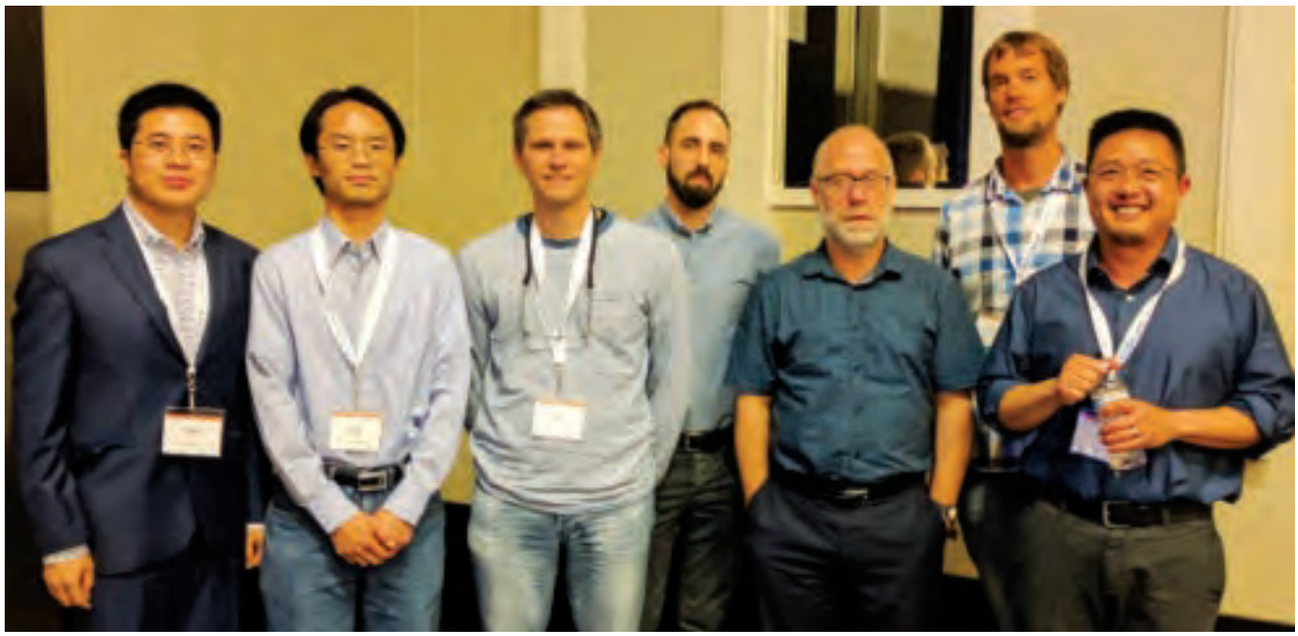
The final talk of the session was by **Darren Brouwer**, Redeemer U, Canada, who gave a clear and compelling illustration of the power of NMR spectroscopy in the solid state for resolution of complex structures. His pioneering work in zeolite structure determination by NMR can be found in: *J. Am. Chem. Soc.* **2005**, *127*, 10365-10366, and more recent work is here: *Acta Crystallogr.* **2017**, *C73*, 184-190. Just like the noted paper from Kenneth Harris, this one has also been published in the special issue of *Acta Crystallographica C*, dedicated to NMR Crystallography and co-edited by David Bryce, University of Ottawa, Canada, and Francis Taulelle, Université de Versailles Saint Quentin en Yvelines, France. The publication of this special issue of *Acta C*, just like this very first NMR Crystallography session at an ACA Annual Meeting, is an excellent demonstration of the acceptance and utility of nuclear magnetic resonance in structural solid-state science and crystallography. This very successful session in New Orleans was aimed to bolster further mixing and discussions of the NMR and crystallography communities, and we believe this was both fun and accomplished in full. Therefore, we would like to invite you to the upcoming **second ever** NMR Crystallography session at the 2018 ACA Annual Meeting in Toronto!

Tomislav Friščić

ACA RefleXions Co-Editor Tom Koetzle (at left) with participants of the first ever NMR Crystallography Session at an ACA Annual Meeting, L-R: Manish Mehta, Mihails Arhangelskis, Darren Brouwer, Kenneth Harris, Tomislav Friščić, James Harper, Leonard Mueller

The not-so-official part of the session took place at the Bombay Club restaurant in the New Orleans French Quarter. Photo courtesy of restaurant staff.

Session 2.2.1: Enzymes of Posttranslational Modification



L-R: Shukun Luo, Danny Huang, Frank Sicheri, Cameron Noland, Roland Dunbrack, Bernhard Lechtenberg, Hua Su. Absent: Carrie Wilmot.

The **Enzymes of Posttranslational Modification** session was dedicated to enzymes (and pseudo-enzymes) that regulate a diverse set of posttranslational modifications including phosphorylation, ubiquitination, lipidation and proteolytic cleavage. The first half of the session firmly focused on kinases. **Frank Sicheri**, U Toronto, Canada, presented work on RNase L. RNase L contains an inactive kinase domain, a pseudokinase, that functions as a regulatory unit to control its RNase activity. Frank explained how the sensory domain of RNase L recognizes the viral second messenger 2-5A in infected cells, while the kinase domain binds ATP. Both events are necessary for RNase L dimerization and activation of its C-terminal RNase domain to degrade viral RNA.

In the second presentation, **Roland Dunbrack**, Fox Chase Cancer Center, explained how it is often worthwhile to take a second look. Roland and his group developed a bioinformatics approach to analyze all possible protein-protein interactions in a crystal structure. He applied his tool to identify novel auto-phosphorylation complexes in published crystal structures. Excitingly, some of these auto-phosphorylation interactions were not identified in the original publications and thus described novel enzyme-substrate complexes.

In the final presentation on kinases, **Hua Su** from Merck presented his work on the identification of a novel inhibitor against the kinase TrkA, a target to treat chronic pain. Unexpectedly, the inhibitor does not bind to the active site, but to an adjacent site that includes a region outside the kinase domain, the juxtamembrane domain.

Following the coffee break, **Shukun Luo**, Columbia U, shared his insights on the structure of the yeast separase/securin complex. Separase is a protease that cleaves the cohesin complex to allow chromosomal segregation during cell division. The inhibitor securin regulates its activity. The structure shows how securin wraps around the whole length of separase to stabilize the complex. Importantly, the structure also reveals securin's mechanism of inhibition by binding and blocking the separase active site.

Cameron Noland, Genentech, discussed his approach to develop much-needed novel antibiotics. His research focused on the structural analysis of the bacterial acyltransferase Lnt, which is required in the last step of lipoprotein biosynthesis and is critical for bacterial infections in a clinical setting. Cameron's work provides novel insights into the catalytic mechanism of this enzyme and lays the foundation for drug development approaches.

Finally, **Danny Huang**, Cancer Research UK Beatson Institute, presented an elegant approach to suppress the p53 transcription factor in cancer. The activity of p53 is controlled by the E3 ubiquitin ligase complex of MDM2/MDMX that targets p53 for proteasomal degradation. Based on a crystal structure of the MDM2/MDMX/E2-ubiquitin complex, Danny's group designed MDM2 mutants that lack E3 ligase activity but retain p53 binding capability. In cells these mutants do not decrease p53 levels but rather reduce expression of p53 target genes, in this way rendering cells hypersensitive to stress. Thus, these mutants point the way to new therapeutic approaches in cancer to inhibit MDM2 E3 ligase activity without affecting its p53 binding ability, which may reduce side effects in healthy cells.

Bernhard Lechtenberg
Carrie Wilmot

2.2.2: Home-Built Software

L-R: Bruce Foxman, Horst Puschmann, Paul Sanschagrin, Paul Boyle, Larry Falvello, Len Barbour, Ken Littrell, Marshall McDonnell, Victor Young. Photo by Brandon Mercado, courtesy of Victor Young.

Considering the ample scope of the software described by the eight speakers in the **Home-Built Software** session, it would appear that the session title encompasses just about all aspects of crystallographic programming. "Home-Built Software" as a topic does cover a large swath of the programming efforts that have taken place to date, since much crystallographic software, from the most extensively used to the most obscure, has been developed by practicing crystallographers, usually in the context of their own laboratories and very often without specific funding for software development.

The session began and ended with talks about well-known and widely used software. **Len Barbour**, Stellenbosch U, RSA, opened the session with a history and description of his program XSeed, a Shelx-PovRay interface written in Pascal beginning in 1984-1985 [*J. Supramol. Chem.* (2001) *1*, 189-191]. The history of XSeed serves as a good example of how a program can develop from a modest beginning to become a powerful tool in the crystallographer's repertoire. Len also described and demonstrated a second program that he has written, a diffractometer simulator that is highly useful in an educational setting. For information on downloading this software, contact Len by e-mail at ***ljb@sun.ac.za***.

The other famous program described in the session is Olex2, the topic of **Horst Puschmann**'s (OlexSys Ltd., UK) closing talk. Unlike essentially all of the other software described in the session, the well known and widely used Olex2 did benefit in its infancy from dedicated funding for software development. One of the key aims of Olex2 is to bridge the gap between difficult concepts and usability. A vast store of information regarding Olex2 can be found at the OlexSys web site, ***http://www.olexsys.org/Software***.

The recently released Python application-programming interface to the Cambridge Structural Database was the subject of a talk by **Paul Sanschagrin**, CCDC. This API permits the home programmer, using Python, to prepare what amounts to extensions of the functionality of the CSD. While there may be something of a learning curve for its use, the potential added value and flexibility that this API adds to the utility of the database make it well worth exploring seriously. More information: ***https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd-python-api/***.

Home-built software has a critical role to play at large facilities. At neutron sources such as SNS and HFIR at Oak Ridge National Laboratory, as described by speakers **Marshall McDonnell** and **Ken Littrell**, the custom-made instruments and the need for flexibility imposed by the diversity of user projects make it essential that customizable but stable, purpose-built software be available. Marshall talked about ADDIE, for processing TOF data for PDF analysis. Ken described in some detail the procedures that he has written, both at IPNS and at Oak Ridge. The software, dedicated to processing SANS data, is largely developed within Igor Pro (a commercial product from Wavemetrics). These modular, extensible procedures have contributed significantly to the user program, figuring in some 90% of the 350+ publications to date from the CG2 and CG3 instruments.

The home lab can benefit in at least two principal ways from the development of home-built software. As described by **Paul Boyle**, U Western Ontario, Canada, the need for efficiency and some degree of quality control and standardization in a productive structure-determination laboratory calls for the use of custom software to achieve desirable results, such as the standardization of file-name structures, the insertion of local information and experimental data into the CIF produced by a refinement program, and the archiving of results in final form in a sustainable and easily utilized manner. Paul described how some readily available tools from the Linux world can aid greatly in automating tasks. The web site of the Chemistry X-ray facility at UWO (***http://xray.chem.uwo.ca/***) has more information on Paul's software.

Larry Falvello, U Zaragoza, Spain, used a programming example involving the analysis of displacement parameters to illustrate some general principles involved in deciding whether to undertake a specific programing project and how to carry it out without going off course. Following Larry's talk, Horst Puschmann commented that useful subroutines are available for use in home programming projects.

A high point of the program was an informative talk by **Bruce Foxman**, Brandeis U, about software that he has written over a half-century, including a recently written program for determining twin obliquity. The talk was dedicated to Howard Flack, and touched on a number of programs that Bruce has written. Full information can be found at Bruce's web site, ***http://people.brandeis.edu/~foxman1/***.

The near-capacity audience in Celestin A hall engaged the speakers in lively discussion. Sponsored by the Small Molecule SIG and organized by Victor Young and Larry Falvello, this session provided a good survey of the diversity of form and function that can be found in home-built software. The great success of this half-day session suggests that ACA should consider similar themed sessions in years to come.

Larry Falvello
Victor Young

2.2.3: General Interest I

L-R: John Rose, Carla Slebodnick, Igor Nederlof, Bi-Cheng Wang, Oleg Borbulevych, Madushani Dharmarwardana, Gerald Audette, Gloria Borgstahl, Bill Duax, Andrey Kovalevsky. Photo by Vicky Doan-Nguyen.

This session focused on topics of broader interest to the macromolecular crystallography community, including historical overviews, recent scientific results, and new or improved software and instrumental techniques. The session started with **John Rose**, U Georgia, presenting a historical overview of the first structure solved by ISIR methods. **Bill Duax**, Hauptman-Woodward Medical Research Institute, followed with a thorough analysis of the importance of glycine conservation toward conservation of structure in different families of ribosomal proteins.

Bi-Cheng Wang, U Georgia, gave an overview of a pilot program at the SER-CAT facility involving collecting complete datasets on a metalloprotein crystal at multiple wavelengths across the metal's absorption edge, giving simultaneous crystallographic and spectroscopic data.

Igor Nederlof, Amsterdam Scientific Instruments B.V., The Netherlands, outlined possibilities, limitations, and recent advances in solving protein structures on nanocrystals using electron crystallography. **Gerald Audette**, York U, Toronto, Canada, presented recent progress toward determining the structure of TraF, a component protein of the *Escherichia coli* F-plasmid type IV secretion system. **Gloria Borgstahl,** U Nebraska Medical Center, provided an introduction to incommensurately modulated protein crystals, superspace groups, and recent software advances toward processing the complex datasets from these systems. **Andrey Kovalevsky**, Oak Ridge National Laboratory, presented the structure of the PLP-dependent enzyme aspartate aminotransferase (AAT) and highlighted the power of neutron crystallography by identifying different protonation states of both the ground and substrate-bound states of the protein. **Eric Zhou**, Formulatrix, outlined advances in macromolecular crystal screening and growth optimization through use of Second Order Nonlinear Imaging of Chiral Crystals (SONICC) to differentiate between chiral protein, RNA, and achiral salts on crystals as small as submicron size. The session concluded with **Oleg Borbulevych**, QuantumBio Inc., explaining the use of the DivCon plugin to complete mixed-QM/MM computation during structure refinement to give lower residual electron densities and better refinement statistics than traditional stereochemical restraints.

Madushani Dharmarwardana
Carla Slebodnick

2.2.4 Integrative Approaches to Structural Biology (NMR, cryo-EM, SAS)

L-R: Michal Hammel, Yuba Bhandari, Gabriel Valez, John Tanner, Sangita Sinha, Greg Hura, Kushol Gupta, Daniel Saltzberg, John Tainer. Photo by Kushol Gupta.

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2.2.4 Integrative Approaches to Structural Biology (NMR, cryo-EM, SAS), ctd.

Cutting-edge insights into structural biology require comprehensive approaches to the determination of structure and dynamics in macromolecular assemblies to elucidate their complex macromolecular structures and function. This session featured a breadth of experience across these areas and highlighted integrative approaches to challenging questions in structural biology, with a focus on small-angle scattering. Small-angle X-ray and neutron scattering (SAXS/SANS) provides information that is highly complementary to other well-established structural approaches including NMR, cryo-EM, and X-ray crystallography.

Invited speaker, **John Tainer**, MD Anderson Cancer Center, U Texas, presented an overview of the state-of-the-art in biological small-angle X-ray scattering (BioSAXS), using ongoing studies of dynamics complexes acting in DNA replication and repair as examples of how SAXS can be applied to distinguish different conformational states, intrinsic flexibility, and as a screen in high-throughput under most solution conditions. Our next invited speaker **Yuba Bhandari**, NIH, presented general methods for high-throughput topological structure determination of RNAs, guided by SAXS-based rigid-body modeling, secondary structure constraints, and additional long-range interaction information. He also demonstrated the applicability and feasibility of the approach to derive low-resolution topological structures of relatively large multi-domain RNAs. **Greg Hura**, Lawrence Berkeley National Laboratory, presented current methods development at the ALS SIBYLS beamline with the focus on describing dynamic solution states of macromolecules using an integrative structural approach combining crystallography and SAXS. **Gabriel Valez**, U Iowa, presented a new crystal structure of the catalytic core domain of human Calpain-5. In comparison to the calcium-bound state observed in the crystal, SAXS and molecular dynamics revealed a highly open conformation of the domain in solution. This in turn provided insight into the molecular mechanisms that regulate this family of proteins and inform the design of specific inhibitors. **Sangita Sinha**, North Dakota State U, presented an integrative approach to the study of structure and function in BECN and ATG/BARKOR, key components of the autophagy nucleation complex. X-ray crystallography, SAXS, isothermal titration calorimetry, and site-directed mutagenesis revealed possible mechanistic differences among the BECN paralogs that enable dynamic exchange between diverse coiled-coil containing partners within the cell. **John Tanner**, U Missouri, demonstrated the integration of SAXS, crystallography, hot-spot mutagenesis, and analytical ultracentrifugation, which provide the tools to understand the role of oligomerization in the function of enzymes of the aldehyde dehydrogenase (ALDH) superfamily. **Kushol Gupta**, U Pennsylvania, presented the crystal structure of allosteric inhibitors of integrase (ALLINI) bound to viral-encoded integrase (IN). The structure reveals for the first time the complete ALLINI-binding interface, comprised of both IN C-terminal and catalytic core domains. Our last invited speaker for the session, **Daniel Saltzberg**, U California San Francisco, presented structural modeling using Integrative Modeling Platform (IMP) with particular focus on development and implementation of structural restraints for hydrogen-deuterium exchange data.

Kushol Gupta
Michal Hammel

2.2.5: Electron Diffraction of Solid-state Materials

This symposium, supported jointly by the Powder Diffraction, Materials, and Neutron Scattering SIGs, was the first in several years dedicated to the use of electron scattering to understand the structure and crystallography of solids with materials science applications. The goal of the symposium was to represent a broad range of topics at the state of the art of electron scattering in both real and reciprocal space applied to problems in nanoscience, spanning timescales from static to ultrafast, and in crystallography from bulk defects in crystalline materials through surfaces and amorphous structures.

To begin the symposium, **Laurence Marks**, Northwestern U, presented an overview of the competing driving forces controlling the surface crystallography in single- and multi-element nanoparticles with ample historical perspective on the use of electron scattering to study nanoparticle surfaces and growth. An important growth area in electron scattering involves the collection of full 2D diffraction patterns from a 2D map of rastered electron probe positions, producing very large 4D or 5D (*in-situ*) datasets ripe for many and varied analyses. **Paul Voyles**, U Wisconsin – Madison, reported on the efforts of his group to determine the differences in local medium-range order in metallic glasses through fluctuation electron microscopy and the effect of slight composition variations on glass-forming ability. The use of scanning diffraction data to recover the full electron phase at atomic resolution through ptychographic methods was presented by **Hao Yang**, Lawrence Berkeley National Laboratory (LBL). These methods were applied by **Roberto dos Reis**, also from LBL, to determine local nanoscale variations in space-group symmetry of beam-sensitive $CsPbBr_3$ and $CsPbCl_3$ halide perovskite materials, revealing the mosaic nature of octahedral disorder. 4D scanning diffraction data was also analyzed by **Yu-Tsun Shao**, U Illinois Urbana-Champaign, to uncover the local symmetry breaking at nanoscale resolution in the vicinity of relaxor ferroelectric domain boundaries $(1-x)Pb(Zn_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$, elucidating the interaction of 1D and 2D topological defects through lattice rotation vortices in these materials. To conclude the symposium, **Jing Tao**, Brookhaven National Laboratory, outlined the challenges and early results using megavolt ultrafast electron diffraction to study metastable charge-density waves in transition-metal dichalcogenide materials.

This year's symposium received positive feedback from the community, and there is momentum to organize a similarly focused symposium at ACA 2018.

Jim Ciston
Olaf Borkiewicz

2.3.1: Evening Session on Diversity and Inclusion

L-R: Krystle McLaughlin, Cheryl Stevens, Bernard Santarsiero, Oluwatoyin Asojo

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

The first talk was by **Bernard Santarsiero**, U Illinois at Chicago (UIC), who described the L@S GANAS program at UIC. Funded by the U.S. Department of Education, the L@S GANAS program aims to improve outcomes for Latino STEM students, including academic performance as well as persistence and graduation rates. L@S GANAS targets Latinos and low-income undergraduate students, and aims to support the whole student through strong ties to their heritage. For this holistic support approach, the program places students in a structured, intensive, and intrusive environment, including a special fall-term course to improve their academic and professional skills, while providing an emphasis on creating supportive diverse networks to improve students' sense of belonging and develop "social capital." Participants also receive active and collaborative learning opportunities to improve their success in gateway courses. Additionally, significant financial support is provided to students in the program in the form of research fellowships, to sustain interest and to assist with "unmet needs." Often these "unmet needs" can derail students, and addressing them can improve outcomes. Santarsiero also described another project that involved community members and the underrepresented STEM students, bringing them together to promote citizen-science. The UIC administration has given its full support to the program, and this emerged throughout the rest of the session as a common theme: To tackle diversity and inclusion issues, you need "buy-in" from your administration!

The next talk by **Oluwatoyin Asojo**, addressed some strategies to do this, and how to communicate the significance of diversity and inclusion issues. She noted that one of the main questions you may get when trying to start any discourse on diversity and inclusion or any programs targeting underrepresented scientists is, "Why do we need to do this?" Asojo provided several resources, including published papers to help answer this question.

https://www.scientificamerican.com/article/how-diversity-makes-us-smarter/

https://psmag.com/news/here-are-four-myths-about-diversity-in-science

Lu Hong and Scott E. Page, *Groups of diverse problem solvers can outperform groups of high-ability problem solvers, Proc. Natl. Acad. Sci. U. S. A.* **2004**, *101(46)*, 16385–16389 ***http://www.pnas.org/content/101/46/16385.full***

Hannah A. Valantine and Francis S. Collins, *National Institutes of Health addresses the science of diversity*, *Proc. Natl. Acad. Sci. U. S. A.* **2015**, *112(40)*, 12240–12242 ***http://www.pnas.org/cgi/doi/10.1073/pnas.1515612112***

Asojo discussed methods used since 2001 to engage high-school and undergraduate students in crystallographic research in her laboratory and identified successes and failures involved in the process of fully integrating these pre-baccalaureate students in crystallography research. The need for "buy-in" from the host-institutions, strategies for recruiting and retaining students, and major barriers to operating these summer research programs were also discussed. Additionally, Asojo identified potential funding sources such as NSF, NIH, ACS, and foundation grants.

In the third talk of the session, *Diversity and inclusion – steady progress by degrees*, **Cheryl Stevens**, Western Kentucky U (WKU), shared her experience addressing the issue of diversity in the faculty through her position as the Dean of the Ogden College of Science and Engineering at WKU. Stevens described the strategy she took, adapted from Wittenberg-Cox, *How Women Mean Business* (2010): (1) Take a look at where we are, and be aware of the problems; (2) Collect data to actually prove there is a problem, and (3) Develop a plan to address the problem. Addressing the problem, for example, might include strategies to address campus attitudes, processes/procedures, financial challenges, and culture. When Stevens arrived in 2012 at WKU from Xavier University, an HBCU in New Orleans, she was surprised at the low diversity in her environment. For example, out of 90 tenured Associate Professors in her college, there were only 14 women and few people of color overall. First, Ogden College defined overall goals that included diversity and inclusion. These became a core value for the college, providing the necessary institutional "buy-in." Some strategies they undertook to address the problems were refining the search committee process for new faculty hires, recruiting underrepresented faculty candidates at conferences, and creating a college level Task Force on Diversity. They also introduced strategies for increasing faculty retention, including a welcome reception for new faculty and spouses, meetings 2-3 times during the academic year, faculty mentors, research mentoring for setting up labs and proposal writing, a luncheon for international female junior faculty, and the initiation of a Women in Science and Engineering group. Together, these strategies have enabled a positive increase in diversity and inclusion for faculty in the Ogden College at WKU. With the implementation, the aim is to focus on sustainability, making sure there is long-term success, to keep making positive progress. Hiring diverse faculty, said Stevens, is the short-term goal, but culture change and longevity is the long-term objective.

Krystle McLaughlin
Oluwatoyin Asojo

3.1.1: Materials for a Sustainable Future

L-R: Sofia Antal, Kamila Wianderek, Ryan Hadt, Andrea Bruck, Alfred French, Vicky Doan-Ngyen, Cheng Wang, Craig Bridges

The **Materials for a Sustainable Future** session focused on innovative characterization techniques and materials development for energy production and storage. Research areas covered included scattering studies done on materials for energy-related technologies such as batteries, solar conversion, hydrogen storage, and carbon capture. **Cheng Wang**, Advanced Light Source, opened the session with a presentation of resonant soft X-ray scattering (RSoXS) as an important complementary tool for studying polymeric and biological materials. **Sofia Antal**, New Mexico Highlands U, reported on investigating crystalline products of CO_2 capture by carboxyamines. **Ryan Hadt**, Argonne National Laboratory, pivoted the topic to energy conversion by cobalt and nickel oxygen-evolving catalysts and their role in O–O bond formation for oxygen evolution reaction. **Craig Bridges**, Oak Ridge National Laboratory, discussed computational design and development of ion-conducting oxides for solid oxide fuel cells. **Albert French**, U. S. Department of Agriculture, continued the discussion of sustainability with the topic of crystallography and computed charge density of aged cellulose chromaphores. The session's final speaker, **Andrea Bruck**, Stony Brook U, received the **Margaret C. Etter Student Lecturer Award** from the Materials SIG. Andrea presented on the roles of composite electrode constituents in the electrochemistry of $Li/Ag_2VO_2PO_4$ batteries.

Vicky Doan-Nguyen

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

This session considered innovative ways to obtain crystallographic data using standard methods and tools. A wide range of non-standard protocols was discussed, tackling topics from K-edge mass absorption coefficients to centering samples. **Michael Ruf**, Bruker AXS, described enhancements in hardware and software to increase the completeness in high-pressure experiments using multiple samples in a Diamond Anvil Cell. **Arturas Vailionis**, Stanford U, discussed grazing incidence diffraction using a single-crystal diffractometer with a kappa goniometer. **Randy Alkire**, Argonne National Laboratory, described a method developed for determining the near K-edge mass absorption coefficients for Ni, which shows good agreement at the 1% error level. **Martin Adam**, Bruker AXS, focused on optimizing sample centering through automation, while **Milan Gembicky**, U California San Diego, demonstrated ingenuity by customizing a multi-purpose diffractometer to analyze biological calcification. Finally, **Cary Bauer**, Bruker AXS, demonstrated how powder diffraction could be investigated with a single-crystal diffractometer.

Tiffany Kinnibrugh

Session 3.2.2: Complementary Methods

L-R: Craig Bridges, Avni Bhatt, Haydyn Mertens, Leiah Carey, Leighton Coates. Photo by ACA Meeting student volunteer.

This session focused on the need to combine multiple advanced analytical methods to properly understand complex materials and phenomena. The initial concept was found to be relevant for both the biological and materials tracks of the ACA meeting, and thus it was constructed as an interdisciplinary session. The session therefore attracted wide-ranging talks, from proteins to inorganic materials. The session was well attended, with good discussions following each talk, and the mix of subject matter was useful in promoting the sharing of ideas across different fields. The opening talk of the session was given by **Edward Snell**, U at Buffalo

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and Hauptman-Woodward Medical Research Institute, in which he showed that a combination of particle induced X-ray emission (PIXE) and comprehensive analysis of crystallization screening outcome can identify erroneous metals that would otherwise compromise the study of metalloprotein structure. The second talk by **Haydyn Mertens**, European Molecular Biology Laboratory, Germany, focused on membrane proteins and discussed the wide range of methods used to uncover structural information in these complex systems, with a particular focus on the complementarity of SAXS and SANS. Next, **Leighton Coates**, Spallation Neutron Source (SNS), Oak Ridge National Laboratory, discussed the current state of neutron protein crystallography at SNS, with the application to structure-derived information on enzyme mechanisms, and how neutrons can be used with X-ray scattering to determine both heavy atom and light atom positions.

After the break, **Luke Daemen**, also of SNS, discussed how neutron vibrational spectroscopy could be used to derive structural information that can be combined with diffraction studies, and the advantages of the high intensity of the VISION beamline in performing studies of small samples or weak scatterers that were not previously possible. **Leiah Carey**, North Carolina State U, then discussed the first neutron diffraction structure of a multifunctional heme protein, in particular the heme reactive center of the enzyme dehaloperoxidase (DHP) from the marine worm *Amphitrite ornata*; this structural information is combined with spectroscopic analysis of substrate binding to better understand the differing functionalities that exist on the heme active site. Finally, the Etter award-winning talk of **Daniel Olds**, SNS, was presented by **Matt Tucker**. This talk ended the session on a high note by showing how new analysis of data collected with total scattering and pair-distribution function (PDF) methods at time-of-flight neutron sources can improve the quality of fit, and allow detailed study of atomic order that is complementary to traditional wide-angle scattering (Rietveld) methods. The session benefited greatly by receiving sponsorship from Douglas Instruments and Art Robbins Instruments.

Craig Bridges
Avni Bhatt

3.2.3: Crystal Structure and Property Prediction

This session, very kindly sponsored by Boehringer-Ingelheim, showcased some of the challenges in the prediction of crystal structures and their properties as well as the interpretation of this structural information.

Our session opened with an entertaining and thought-provoking presentation from **Joel Bernstein**, Ben-Gurion U of the Negev, Israel, on the relationship between chemistry, fuzzy logic and patent law (the true sport of kings!). Chemists, particularly academic ones, often think in terms of exact answers or observations – discussing rules and scientific laws. In practice, a lot of the structural chemistry questions that come up in patent litigation, such as that around pharmaceutical solid form patents, is concerned with the exceptions to these rules or grey areas where interpretation is required. Joel took us through some intriguing examples of real patent litigation cases where "fuzzy logic" came into play to tackle these grey areas (see also: *Israel Journal of Chemistry*, **2017**, *57*, 124-136).

Angeles Pulido, U Southampton, UK, next introduced us to the design of porous organic molecular crystals using Crystal Structure Prediction (CSP) techniques. Awkwardly shaped molecules that form strongly-directional intermolecular interactions can potentially be arranged into unusually stable porous frameworks. The use of CSP along with energy-structure-function maps provided guidance as to which molecules can actually form these surprisingly stable honeycomb-like frameworks (see also: *Nature*, **2017**, *543*, 657-664).

Juan Manuel German Acacio, National Autonomous U of Mexico, then shared with us some recent results illustrating the inclusion of unexpected guests in a series of Pd-complex crystal structures.

The second half of the session started with **Joost van den Ende**, Hoffman-La Roche, who spoke about energy barriers and mechanisms in solid-state transitions. Joost presented several interesting cases of polymorphic transitions, such as DL-norleucine and fatty acids in chocolate. He also discussed the role of predictions, based on various theoretical and semi-empirical tools, to explain and rationalize mechanisms of solid-solid phase transitions (see also: *CrystEngComm*, **2016**, *18*, 4420-4430).

Victoria Soghomonian, Virginia Tech, presented an interesting topic of structural aspects of electrical conductivity as a function of pressure. Victoria discussed a family of mixed vanadium gallium hexafluorides, which undergo a monoclinic to cubic phase transition upon heating or under high pressure. She presented a very interesting case relating structural chemistry with electrochemistry in the context of a highly important research of energy storage.

Our final speaker of the day, **Madushani Dharmawardana**, U Texas at Dallas, was awarded the Industrial SIG **Etter Student Lecturer Award** for her talk on a thermo-mechanical responsive crystalline organic semiconductor. Madushani discussed polymorphic transitions in the context of thermal expansion and thermochromism. She presented several studies of naphthalene diimides and other compounds that exhibit a color change during polymorphic transition, gave structural reasons for color change with temperature, and discussed cases of unusual thermal expansion.

Peter Wood
Mariusz Krawiec

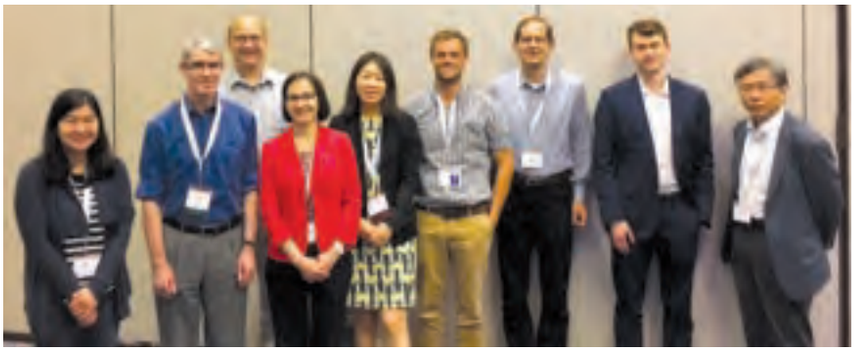
Neela and Hemant Yennawar. Photo by Richard Bromund.

3.2.4: Hot Structures

The **Hot Structures** Session was co-chaired by Elizabeth Goldsmith, U Texas Southwestern Medical Center, and Sangita Sinha, North Dakota State U. Several speakers presented breakthrough research. **Nicholas Noinaj**, Purdue U, presented data on how bacteria load proteins into their outer membranes. **Kerry Goodman**, Columbia U, presented new data on how cadherins mediate neuronal self-vs.-nonself-discrimination. **Diana Tomchick**, U Texas Southwestern Medical Center, presented the structure of the long-sought multi-domain vesicle fusion protein MUNC13. **John Tainer**, U Texas MD Anderson Cancer Center, spoke about higher-order oligomerization of AIF, and how AIF sites of allostery link to the NADH-binding site. Talks on enzymology and drug discovery were presented by **Andrzej Joachimiak**, U Chicago, and **Margarita Tararina**, Boston U, while session co-chair **Elizabeth Goldsmith** described conformational regulation in WNK protein kinases by environmental factors. All-in-all, brain-food for a structural biologist!

Elizabeth Goldsmith
Sangita Sinha

3.2.5: Crystal Growth



L-R: Miki Senda, Kenneth Harris, Tom Friedlander, Magdalena Owczarek, Yi-Yeoun Kim, Benjamin Palmer, Travis Gallagher, Daniel Wrapp, Rui Tamura

The session on **Crystal Growth**, organized by Kenneth Harris, Cardiff U, UK, covered a range of different aspects of crystallization sciences, including fundamental understanding of crystallization processes in both biological systems (e.g., biomineralization) and laboratory contexts, and developments in experimental techniques for the preparation of high-quality crystals.

Benjamin Palmer, Weizmann Institute of Science, Israel, opened the session with a beautifully illustrated lecture on biologically controlled crystal growth, focusing on the image-forming mirror in the eye of the scallop. He demonstrated that each eye of the *Pecten* scallop contains a concave mirror to focus light onto a retina, operating on principles similar to a reflecting telescope. The hierarchical organization of the multi-layered mirror is exquisitely controlled for image formation, both with regard to the structure of the component guanine crystals at the nanoscale and the complex morphology of the crystals at the millimeter level. Amazingly, each layer of the mirror is formed from a tiling of regular square guanine crystals. The ability of the scallop to form almost perfectly square crystals for a monoclinic crystal structure is believed to be achieved by controlling crystal twinning and by carrying out crystallization inside a confined environment.

Yi-Yeoun Kim, U Leeds, UK, then gave a very enthusiastic presentation of her research to develop bio-inspired strategies aimed at incorporating organic components within crystals of calcite (calcium carbonate). The strategy recognizes that the nano-composite structure of biominerals derives from an intimate association of organic molecules with a mineral host. She demonstrated that the strategy has been applied successfully to prepare single crystals of calcite as a host mineral, precipitated in the presence of a wide range of guest species, encompassing commercial latex particles, organic/inorganic nanoparticles functionalized with block copolymers, and small molecules such as amino acids. Using several experimental techniques for rigorous characterization of the composite systems, she revealed insights into the mechanism of occlusion within the host crystals, and the relationships between macroscopic physical properties and the microscopic structure of the composite materials.

Over several years, **Rui Tamura**, Kyoto U, Japan, has pioneered a strategy – named "*preferential enrichment*" – for spontaneous enantiomeric resolution, which relies on two processes: (i) a solvent-assisted polymorphic transition, and (ii) subsequent selective dissolution of the excess of one enantiomer from the transformed disordered crystals into the mother liquor. Rui's lecture described the latest developments in this fascinating process, including *in-situ* XRD and microscopic observations of the polymorphic transition, as well as kinetic and thermodynamic studies to understand the chiral symmetry breaking. His research has applied the preferential enrichment concept to a range of co-crystal systems, including those containing chiral drugs.

Magdalena Owczarek, Northwestern U, gave a very enthusiastic presentation of some remarkable recent results on crystals formed from derivatives of imidazole (containing at least one halogen substituent), selected on the expectation that they may exhibit desirable properties such as ferroelectric or piezoelectric behavior. Magdalena discovered that several materials in this class have a strong propensity to form curved crystals, and demonstrated through rigorous experimental studies that halogen bonding may play a key role in the tendency for the crystals to exhibit curved morphologies. Furthermore, by extending this idea, she has shown that co-crystallization of different haloimidazoles gives rise to flexible crystals, many of which do indeed exhibit ferroelectric and piezoelectric properties.

The remaining talks in the session covered different aspects of protein crystallization. **Miki Senda**, Photon Factory, Japan, focused on improving the reproducibility of producing high-quality crystals for protein crystallography. She

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demonstrated that carrying out crystallization under anaerobic conditions in carefully designed apparatus could have significant advantages, including the reproducible formation of crystals of larger size and higher quality than under aerobic conditions. Next, recognizing that vapor diffusion is the most commonly used method for protein crystal growth, **Tom Friedlander**, Formulatrix, described systematic studies of the effects of humidity on the rate of drop evaporation, demonstrating that precise humidity control is a significant advantage in ensuring reproducibility of protein crystallization processes. On a related theme, **Daniel Wrapp**, Dartmouth College, described an automated strategy for iterative optimization of protein crystallization screens. His method takes the results from an initial set of crystallization trials, and then iteratively adjusts the conditions (e.g., precipitant concentrations) to be used in the next crystallization trials. Repetition of this iterative optimization process was shown to lead to a substantial increase in the probability of achieving successful crystallization of a protein from a limited set of reagents. Finally, **Travis Gallagher**, NIST, concluded the session by describing a model for the crystallization of proteins based on concepts of helical pseudosymmetry.

Kenneth Harris

Session 3.3.1: How Do I Get My Data? (Beamlines and Their Capabilities)

L-R: Sanjit Ghose, Tiffany Kinnibrugh, Allen Orville, Marian Szebenyi, Christian Feiler (at rear), Randall Winans, Ashfia Huq. Not shown: Christine Beavers. Photo courtesy of Ashfia Huq.

Facilities that host synchrotrons, neutron sources and free-electron lasers are extremely useful resources for the crystallography community. This evening session hosted several speakers from various facilities to provide information about proposal process, access mode and also beamline description that enables a wide range of materials research from macromolecular crystallography to materials diffraction and studying large-scale structures using small-angle scattering.

First speaker of the session **Marian Szebenyi** from MacChess, Cornell High Energy Synchrotron Source (CHESS), described the NIH-funded resource that provides support for structural biologists collecting data at CHESS, one of the five high-energy synchrotron sources in the United States. State-of-the-art support is provided for macromolecular crystallography (MX) and BioSAXS. The next speaker **Randall Winans** is a Senior Scientist and the leader of the Chemical and Materials Science Group in the X-ray Science Division of the Advanced Photon Source (APS) at Argonne National Laboratory. He is responsible for the beamlines in Sector 12 and the USAXS beamline at 9-ID. Recently, Winans was interim head of the Structural Sciences group, Sector 11 and 17-BM. He went over a wealth of information regarding APS. **Christine Beavers** covered the resources available at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory, followed by **Christian Feiler** who described three MX beamlines at the electron storage ring BESSY II operated by Helmholtz-Zentrum Berlin (HZB), Germany. **Allen Orville**, the Principal Scientist of the UK XFEL Hub, described the mode of operation for larger collaborations mode at the free-electron laser facilities. The last two speakers **Sanjit Ghose** and **Ashfia Huq** gave brief descriptions of beamlines available for crystallography and small-angle scattering at NSLS II, the new synchrotron source located at Brookhaven National Laboratory, and the two neutron facilities Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) located at Oak Ridge National Laboratory. More detailed information from all these facilities can be downloaded from the ACA New Orleans program website: ***http://www.amercrystalassn.org/documents/2017%20Meeting/HowToGetMyData.pdf***

The session organizers are thankful to CHESS and ORNL for providing funding to serve snacks at this evening session.

Ashfia Huq
Tiffany Kinnibrugh

3.3.2: Would You Publish This?

This ever-popular session was held for the 7th year (originally held in 2009) and was generously supported by Crystallographic Resources, Inc. The session began with **Victor Young**, U Minnesota, presenting compounds that undergo temperature-dependent phase transitions between 'better' and 'poorer' quality structures. Discussion centered on the trade-off between the commitment of time and resources to obtain the structures of both phases vs. the value to the crystallographic community in reporting both phases. **Laura McCormick**, U St Andrews, UK and Advanced Light Source, presented a conundrum where attempts to hone in on reaction scale-up conditions produced five different phases! All but one of the phases were structurally characterized. The 5th phase gives clean diffraction, but a poor structure model. To what extent should the 5th phase be reported, if at all? **Carl Schwalbe**, Aston U, UK, provided examples relating to publication practices. Carl discussed eliminating weak high-angle data to improve statistics. Although truncating data might be interpreted as 'trying to satisfy ones vanity' by improving data and refinement statistics, there can also be real consequence, for example fewer flags in *CheckCIF* or meeting the R-factor < 0.05 filter to achieve more hits in *CSD Conquest*. **Danielle Gray**, U Illinois Urbana-Champaign, presented a trend in her lab of obtaining quick datasets as part of the screening process. The datasets provide enough information to identify the substance and refine isotropically – i.e., enough to satisfy the scientist. The

3.3.2: Would You Publish This?, ctd.

L-R: Laura McCormick, Carl Schwalbe, Christine Beavers, Carla Slebodnick, Danielle Gray, Victor Young. Photo courtesy of Victor Young.

ramifications of this new trend are both local (e.g., lab not bringing in data collection fees) and broader (structures never being published). **Carla Slebodnick**, Virginia Tech, presented a system with space group ambiguity between *I*4/*m* and *I*-4. *I*4/*m* introduces disorder into a significant portion of the molecule, but no disorder is present when refining in the lower symmetry space group, *I*-4. Unfortunately, in *I*-4, the remainder of the molecule is related by mirror symmetry and strong correlation between atoms required heavy restraints to stabilize the refinement. Opinions differ on best choice of space group. The session concluded with **Christine Beavers**, Advanced Light Source and U California, Santa Cruz, presenting the 'low resolution' structure of a single-molecule magnet. The structure model allows identification of the geometry at the Ni_{18} core of the molecule, but not the coordinated ligands. When publishing such structures, what compromises are acceptable?

Carla Slebodnick
Danielle Gray

4.1.1: Etter Symposium for Young Scientists

L-R: back row – Nico Giordano, Justin Kurian, Matthew McLeod, Avni Bhatt, Zhelong Xiang; front row – Roberto dos Reis, Kyle Stiers, Stanislav Stoyko, Anastasiya Vinokur, Daniel Mast, Thomas Bohl, Margarita Tararina. Photo courtesy of Roberto dos Reis.

This half-day session, following the **Margaret C. Etter Early Career Award** presentation, brought together young scientists to present their works for a broad audience at ACA. The session provided a platform of discussion for graduate, postdoctoral fellow, and early career scientists who want to pursue their careers as part of the crystallographic community. The session featured ten exceptional speakers covering a range of subjects from X-Ray crystallography to cryo-electron microscopy (cryo-EM), exhibiting the diversity of the crystallographic sciences. The session started with work presented by **Zhelong Jiang**, U Illinois Urbana-Champaign, on the application of *in-situ* X-ray diffraction to analyze the progress of reactions leading to the formation of inorganic crystal Fe_2SiS_4, followed by **Anastasiya Vinokur**, U Wisconsin – Madison, who presented a combination of X-ray

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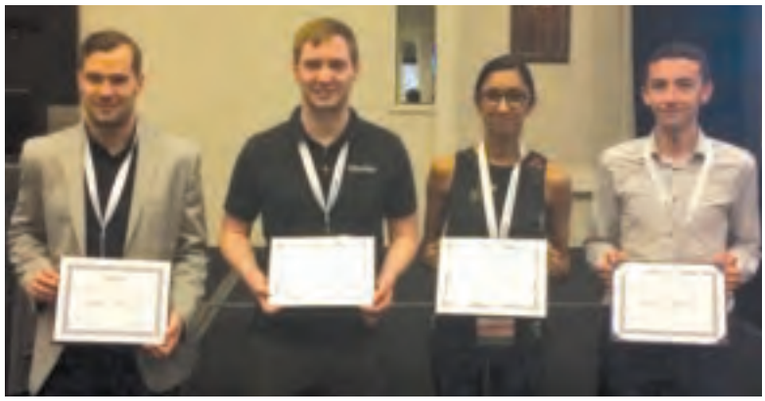
diffraction, NMR, and mass spectrometry data to elucidate molecular structure of natural products extracted from *Millettia versicolor*. An excellent example of combining both theory and experimental methods was given by **Daniel Mast**, U Nevada Las Vegas, who was able to model the negative thermal bond expansion in Tc_2O_7 using variable temperature single-crystal diffraction and Langevin molecular dynamics. Cryo-EM was a highlighted topic at this years' ACA meeting and was represented in the Etter Symposium by exceptional talks from **Justin Kurian** and **Avni Bhatt**, both of U Florida.

In this symposium, ACA has honored students with awards for their outstanding work. The awards were sponsored by the ACA SIGs: Biological SIG award to



2017 Etter Student Lecturer Award Winners honored at this session, L-R: Matthew McLeod, Kyle Stiers, Avni Bhatt, Nico Giordano. For the complete list of 2017 Etter Award winners, turn to p. 44. Photo courtesy of Roberto dos Reis.

Avni Bhatt for her abstract entitled *Crystallographic insight into enhanced catalytic activity of carbonic anhydrase II using "activating" ligands*; Service Crystallography SIG award to **Nico Giordano**, U Edinburgh, UK, for *A pressure induced phase transition of 4-iodobenzonitrile*; Young Scientist SIG award to **Kyle Stiers**, U Missouri, for *Personalized biophysics of human PGM1 deficiency*; and Canadian Division award to **Matthew McLeod**, U Waterloo, Canada, for *Anion inhibition of PEPCK manifested as substrate inhibition; Using crystallographic methods to determine thermodynamic data*.

The YSIG is pleased to have opened this excellent opportunity for young scientists and looks forward to next year's meeting.

Roberto Dos Reis
Margarita Tararina

4.1.3: Conformational Dynamics of Ligand Binding

Session 4.1.3 was organized by Michael James, U Alberta, Canada, and Barry Finzel, U Minnesota, to provide a forum for discussion of the effects of conformational change induced by ligand binding by proteins. Speakers included **Gyanendra Kumar,** St Jude Research Hospital, **Denis Kudlinski**, DKFZ, Heidelberg, Germany, and **Suzanne Mays**, Emory U. **Henry Tang**'s (Lawrence Berkeley National Laboratory) studies with phosphoenolpyruvate kinase combining single-crystal work and HT-SAXS provided a nice example of how point mutations can influence protein dynamics and ligand selectivity. **Michael James** presented a comprehensive summary of published work that enabled the precise quantification of the entropic penalty paid in binding a peptide inhibitor of penicillopepsin with rotational degrees of freedom. Conformational restriction of each rotamer accounts for 0.9 Kcal/mol of binding affinity. **Emil Pai**, U Toronto, Canada, presented some fascinating observations made regarding the conformational dynamics of fluoroacetate dehydrogenase. These confirm the existence of a dynamic cooperativity between subunits of the homodimer that seems to allow the entropic cost of ligand binding in one subunit to be distributed and offset by increasing the conformational dynamics of the other subunit. It will be interesting to see if this turns out to be a more generalizable feature exploited by many homodimeric enzymes.

Barry Finzel

4.1.4: In situ and Operando Measurements

This half-day session covered cutting-edge applications of *in situ* and operando techniques in the areas of chemistry, material sciences and solid-state physics. A total of eight speakers presented their research. **John Parise** from Stony Brook U and Brookhaven National Laboratory led with the opening talk, on combining *in situ* diffraction-DSC experiments with theoretical predictions and data mining to guide the search or synthesis of metal-organic frameworks (MOFs) promising for gas sorption and separation usage. **Tao Sun**, Argonne National Laboratory, introduced the audience to the ultrafast diffraction and imaging applications on his beamline, which pushed the temporal resolution to the microsecond range and opened a door to study very fast transformation processes. Following Tao, **Amy Marschilok**, Stony Brook U, talked about mesoscale to nanoscale investigations of battery materials using both energy and angle dispersive XRD. Amy examined how silver formed and localized in the vanadium phosphate framework upon fast or slow charge and discharge cycles, and the impact on battery capacity and lifetime.

After the coffee break, **Anna Plonka** from Yeshiva U presented her study of Zr-based MOFs for filtrating and degrading simulants of nerve-agent materials. Anna used multiple *in situ* methods including XRD, XAFS and infrared spectroscopy to probe the capturing and degradation of the simulants within the MOFs. The next three talks were about *in situ* synthesis, but with different scattering techniques and for different types of materials. **Michael Campos**, Columbia U, used both small-angle and wide-angle X-ray scattering to understand the nucleation and growth of colloidal quantum dots in the PbS and PbSe systems. Michael's talk was particularly well received by the audience, with four questions about the experimental details and alternative oxide precursors for the synthesis. **Ashfia Huq**, Oak Ridge National Laboratory, talked about her study on solid-state synthesis of lanthanum molybdenum oxide with neutron diffraction, which yielded crucial information on the intermediate phases

and formation temperatures that could only be obtained with the *in situ* measurements. Following Ashfia, **Chunhua Hu** from New York U showed his research on determining the crystal structure of a glycine polymorph that might exist on extraterrestrial bodies. Chunhua applied a flash-cooling method with *in situ* synchrotron XRD to obtain the powder profile of the target phase that led to the structure. **Scott McCormack** from U Illinois Urbana-Champaign gave the final talk of the session, on negative thermal expansion materials. Scott illustrated an *in situ* diffraction setup with a quadrupole lamp that could supply heat to 2000 °C, which he used to study hafnium titanium oxide. He analyzed the evolution of the sample's zero thermal expansion directions with 3D plot and pole figures.

Wenqian Xu
Sanjit Ghose

Session 4.1.5: Enabling New Science with Light Sources and Hybrid Methods

L-R: Alke Meents, Jeney Wierman, Alexey Rozov, Lois Pollack, Seth Cory, Chelsy Chesterman, Armin Wagner, Steve Meisburger

At this year's annual meeting, **Session 4.1.5** was made possible by generous support from Dectris, Xenocs/SAXSLAB, ACA, MiTeGen, and Rigaku. The session was organized by Nozomi Ando and Armin Wagner, and chaired by Armin and Steve Meisburger. Talks ranged over topics from enzyme structure to novel X-ray methods. Highlights included **Lois Pollack**, Cornell U, who spoke about the use of time-resolved SAXS to study nucleosomes. **Seth Cory**, Texas A&M U, winner of the Light Source SIG's **Etter Student Lecturer Award**, gave an excellent talk on the structure of the human cysteine desulferase complex. Two talks addressed aspects of the emerging field of serial protein microcrystallography at synchrotrons. **Jeney Wierman**, Cornell U, a veteran speaker at the ACA, reported on latest results from CHESS using monochromatic X-rays, while **Alke Meents**, DESY, Germany, spoke about recent low-background pink beam experiments at BioCARS.

Armin Wagner
Nozomi Ando Steve Meisburger

4.2.1: Communicating Science to the Public

As Ambassadors for Crystallography we must convey the utility and excitement of our scientific advances to friends, family, funding agencies, legislators, and the general public. This session, organized by Katrina Forest, U Wisconsin – Madison, and Jim Fettinger, U California Davis, and sponsored by the ACA Communications Committee and the Young Scientist SIG, provided enabling advice for connecting with the public audience. The broad appeal of the topic was evident from the 76-attendee crowd.

The session opened with the introduction of **James O'Brien**, Missouri State U, the 2017 winner of ACA's **Wood Science Writing Award**. O'Brien was gearing up for his speech at the Tuesday evening banquet and was not a scheduled speaker for our session, but came as a guest. Moreover, in a last-minute surprise gesture, he provided a copy of his hot-off-the-presses book, *The Scientific Sherlock Holmes*, officially released in paperback on June 1st. This treasure may have been one reason 59 intrepid souls remained spellbound until the session close, when prizewinner Randy Alkire was drawn. O'Brien had explained to the organizers that his winding path to book authorship was not necessarily one that would be easy to follow. He was asked to speak at an ACS symposium on chemistry and science fiction, which led to writing a book chapter, which was nicely contemporaneous with the "flap" about Sherlock as the eponymous BBC series took off, which lead a publisher to invite him to write *The Scientific Sherlock Holmes*. The lesson was to be ready to take advantage when opportunity presents itself.

Coming off a very busy week as co-organizer of the EM **Transactions Symposium**, **Stephen Burley**, RCSB Protein Data Bank, Rutgers U, *Demonstrating the value of 3D macromolecular structures*, described the history of the PDB, the pioneering organization for open-access science. Beginning with seven structures in 1971, the PDB has over 130,000 structures today and grows a little over 10% a year. With 1.5 million hits per day, PDB public access serves as validation, as consumers can readily see the quality of the product. From blind methods development challenges at the cutting edge of research, to outreach and education such as David Goodsell's wildly popular PDB-101 series, the PDB has become essential to biomedical research and education. Major pharmaceutical companies use the PDB databases for structure-based drug design, with a sterling example being the treatment of leukemia, with such drugs as Gleevec (2001), Sprycel (2006), and Tasigna (2007) playing a role in the doubling of patient survival rates since their discoveries. The annual cost of maintaining the PDB is $6.9 million, mere pennies per download, as the institution approaches its 10-year funding renewal in 2018.

Brian McMahon, IUCr, Chester, UK, *Showing that crystallography matters*, described numerous public resources created by the IUCr Outreach group to, "increase public awareness, inspire young people and promote the universality of science" for the occasion of the

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International Year of Crystallography in 2014. A moving video "Welcome to the World of Crystallography" (***http://www.iycr2014.org/about/video***) was spearheaded by Juan Manual Garcia-Ruiz; remarkably the YouTube version has now been subtitled into 29 languages! A short film starring young Johanna as she learns about discoveries in crystallography (***https://www.youtube.com/watch?v=AlBPajICFIU***) is promoting crystallography to children. The IUCr makes available shareable PDF posters, organizes photo competitions, and manages worldwide outreach such as crystal growth contests. An interactive time line in which one can map one's own events onto crystallographic landmarks (***http://www.iycr2014.org/timeline***) provides a personal link to crystallographic milestones. Recognizable and breathtaking stamp collections from nations worldwide broadcast the beauty of crystals and crystallography.

Beamline scientist, ACA member, author of the banquet review in the Fall 2016 *Reflexions*, and major proponent of social media **Christine Beavers**, Advanced Light Source and U California Santa Cruz, gave a juicy, engaging talk, *Using social media for #SciComm: An interactive tutorial*, in which she encouraged members of the ACA to take full advantage of social media and provided a real-time lesson for audience members to become Twitter users. As Beavers advised, think of these as 140 character microblogs and boil down the essence of your message. Take advantage of searchable hashtag links (like #ACANOLA). Remember that Tweets are dynamic messages and that the time and even time zone you are in when tweeting will impact your readership. Case in point, there were multiple tweets within our session including this one from Camelia Stan, "Learning about Twitter by listening to @XtalGrrl talk about Twitter at #ACANOLA is a bit meta." Was it coincidence that there were 41 new @ACAXtal followers in May and 49 in June compared to 8.5 per month the previous 6 months?

Diane Dickie, Brandeis U and Sandia National Laboratory, *From magic show to crime scene analysis – getting kids interested in science with hands-on investigations*, described her 12 year-long and still-going-strong project at Sandia designed as a collaborative (not competitive) "CSI Dognapping" case to engage children from Title I schools to experience the thrill of laboratory science. As described in a recent *Chemical & Engineering News* article, this program recognizes that "we decide early what we do not want to be when we grow up." Dickie and her colleagues, knowing that kids choose to pursue what they know, show them science is a real future career option so that they may keep it in mind. Knowing just how to engage kids of this age, the scientists bring the children into a "surprise" case involving broken equipment, a missing dog, ID cards so they feel a sense of belonging, and a good dose of yuck factor along with serious experimental analysis of clues and statistical significance. The team has collected data to demonstrate the impact of their program; the children's knowledge increases and is retained at least 2-3 months later when the post-test is repeated.

As the recipient of an ACA Outreach Grant (did you know about these – apply!), **Katharine Page**, Oak Ridge National Laboratory (ORNL), *Uniqueness and you: How the disorder of atomic structure enables your world*, set out to sell Materials Science to the public. Wanting to avoid old and outdated memes, she focused on three components: Inspiration Through Observation, Hands on Structure Activity, and a Web-Based Simulator to help young students engage in materials science. Kids don't get bored building models! As **Thomas Proffen**, also of ORNL, shared with the audience, tool building for kids can turn into tool building for research. Symmetry and structure are fascinating to children, and the ORNL project has now grown into a traveling science fair with six installations. Check for yourself at ***www.myatomicstructureworld.org*** and ***www.orcsgirls.org***.

Representing the AIP, science journalist **Catherine Meyers** of *Inside Science*, *Talking science with journalists*, provided imminently usable advice for communicating with the public by working with science journalists. In a Pew Research Center survey of Americans in 2015, 59% declared themselves very interested in science, which is a heartening figure until you learn that only 2% of all stories in the paper are science-related. Meyers relayed that writing science is hard for journalists due to the real culture clash between them and scientists. So, as a scientist how can you help these fantastic professionals convey your message? According to Meyers, consider the true essence of your story; what you did and why it matters. Be ready to discuss these points with a journalist in every-day language using creative analogies and metaphors; try your talking points out on a neighbor. Another strong recommendation is to get to know the public information officer at your institution, and go to her or him right away when you know an article will be published, as the clock is ticking. Apropos an earlier talk, Meyers confirmed, journalists do follow Twitter, so tweet. And, show your human side. If the public likes scientists, they will like science.

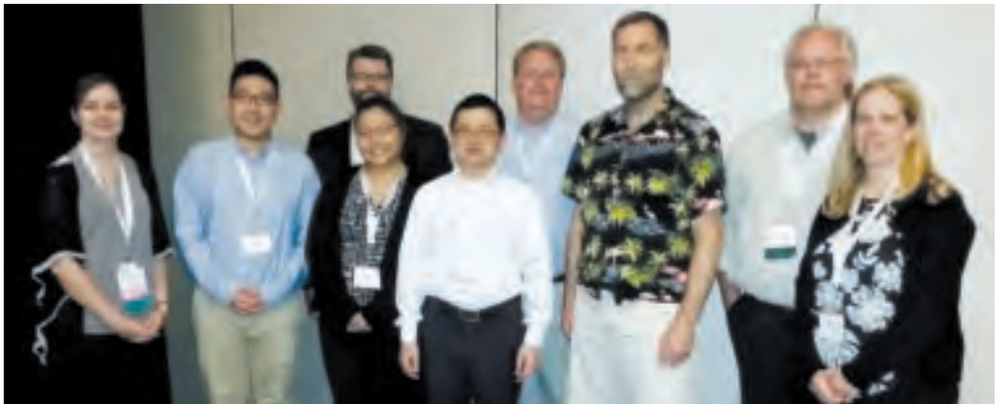
See you at #ACA_TO in 2017!

Katrina Forest
Jim Fettinger

2017 Margaret C. Etter Student Lecturer Awards

Biomac	**Avni Bhatt, U Florida**	**Powder Diffraction**	**Ying Zhang, Brigham Young U**
Canadian	**Matt McLeod, U Waterloo**	**Small Angle Scattering**	**Eric Manley, Northwestern U**
Industrial	**Madushani Dharmarwardana, U Texas**	**Small Molecule**	**Korey Carter, GWU**
Light Sources	**Seth Corey, Texas A&M U**	**Service Crystallography**	**Nico Giordano, U Edinburgh**
Materials Science	**Andrea Bruck, Stony Brook U**	**Young Scientist**	**Kyle Stiers, U Missouri**
Neutron Scattering	**Daniel Olds, ORNL**		

4.2.2: General Interest



L-R: Anastasiya Vinokur, Lawrence Wong, Eric Reinheimer (at rear), Suyin Grass Wang, Shiao-Liang Zheng, Jefffrey Lovelace (at rear), David Schuller, Allen Oliver (at rear), Jennifer Aitken. Absent: Dubravka Jung. Photo by Mark Mashuta.

Despite being one of the final sessions of the ACA conference, the second **General Interest** symposium opened with some 30 audience members in attendance. The session commenced with **Dubravka Jung**, Dectris, who presented advances in the EIGER detector over previous versions of hybrid detectors. **Shao-Liang Zheng**, Harvard U, presented the first of several educational talks, detailing his experiences in developing a course that involves a research visit by undergraduate and graduate students to the Advanced Photon Source. This course is well received by the students and underpins three key philosophies: to encourage and educate students; to incorporate crystallography into chemistry courses; and to develop undergraduate involvement in the science of crystallography. **Jeffrey Lovelace**, Eppley Institute, discussed how one can treat a commensurately-modulated structure as a supercell structure and how to interchange between the two. The discussion on modulation was insightful and clearly explained the underlying features of commensurate vs. incommensurate structures. Prior to the coffee break, **Eric Reinheimer**, Rigaku, gave an enthusiastic talk on how to organize a simple, one laboratory-session experiment involving crystal growth, sample selection and data acquisition. Eric's focus was on an undergraduate laboratory session and how to introduce the topic of crystallography to students. The three key ingredients are: an accessible instrument, software and, most critically, crystals. Eric passionately described how to overcome all three challenges.

The second half of the session was led off by **Lawrence Wong**, Hong Kong U of Science and Technology, who presented his work on using spinols to assist in chiral resolution of a number of new co-crystallant compounds. **Jennifer Aitken**, Duquesne U, followed with a presentation of the emerging classes of lithium chalcogenide materials that her group is synthesizing. These new materials exhibit excellent non-linear optical properties and show promise for their absorption/emission properties. The breadth of resources available at the ChemMatCARS beamline at the APS was detailed by **Suyin Grass Wang**, Argonne National Laboratory. Her talk covered diverse topics such as: extreme conditions (high pressure, extreme cryogenic temperatures), charge density and diffuse diffraction studies, and photocrystallography and time-resolved measurements. In short, the scientists at ChemMatCARS can work with researchers and develop a broad range of crystallographic methodologies to answer the researcher's questions. Rounding out the symposium was **David Schuller**, Cornell U, who discussed the upgrades to the automated mounting hardware at MacCHESS. Upgrades to both the robotic hardware and controlling software have significantly improved automation. The breadth of topics covered in this session demonstrates the scope of the General Interest topics: every field is welcome.

Allen Oliver
Anastasiya Vinokur

4.2.3: Structural Biology of Infectious Diseases

L-R: Erica Ollman Saphire, George Lountos, Oleg Volkov, Christopher Colbert, Marzena Pazgier, Thomas Edwards, Toshiya Senda

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4.2.3: Structural Biology of Infectious Diseases, ctd.

The current status of the contributions of structural biology to the study and development of therapeutic agents against infectious diseases was highlighted at this year's ACA meeting in New Orleans. Erica Ollmann Saphire, Scripps, opened the session with an outstanding talk presenting her lab's ground-breaking work, which required several years of perseverance to solve the crystal structure of the Lassa virus surface glycoprotein bound to a fragment of a neutralizing antibody from a surviving patient. The structure provides the basis for the development of a potential Lassa virus vaccine, for a disease that currently is 50-70% fatal. **Marzena Pazgier**, U Maryland, described crystal structures of a construct of the inner domain of gp120 (HIV-1) complexed with an antibody, and efforts to induce a protective antibody response to HIV-1 with the inner domain of gp120. **Toshiya Senda**, High Energy Accelerator Research Organization, Japan, described the deletion mechanism of SHP2 by CagA from *Helicobacter pylori*, while **Thomas Edwards**, Beryllium Discovery, described the novel crystal structure of acid deoxyribonuclease and insights into its catalytic mechanism. **Oleg Volkov**, UT Southwestern Medical Center, presented crystal structures of *Trypanosoma brucei* S-adenosylmethionine decarboxylase and discussed how allostery activates the enzyme. The mechanism of peptide editing by the TAPBRP/MHC-1 complex, which provides insights into understanding tapasin function, was presented by **Jiansheng Jiang**, NIH. Finally, **Christopher Colbert**, North Dakota State U, presented his laboratory's work on elucidating the structural basis of cell-surface signaling by the sigma-regulator, PupR, in *Pseudomonas putida*. The afternoon's collection of outstanding talks and engaging audience questions demonstrated that structural biology continues to provide major contributions toward our understanding of the molecular basis of infectious diseases and will continue to provide critical information needed for the development of novel therapeutic agents.

George Lountos

4.2.4: Frontiers in SAS

L-R: Youngha Hwang, Soren Skou, Martha Brennich, Thomas Weiss, Timothy Ryan (at rear), Sai Venkatesh Pingali, Volker Urban

This session focused on new developments and latest advances in the experimental protocols and data analysis methods for small-angle scattering. The session was opened by **Martha Brennich**, European Molecular Biology Laboratory, Grenoble Outstation, France, who showed how the idea of online purification of the sample can be carried further from the established size-exclusion chromatography to methods such as ion-exchange and nickel affinity chromatography. She discussed further how, in order for these methods to work, the correct buffer background must be carefully determined before subtraction, and pointed out the advantages and challenges brought about by these new methods. In the following presentation **Volker Urban**, Oak Ridge National Laboratory (ORNL), standing in for Hugh O'Neill, showed how time-resolved neutron scattering helps to elucidate the complex thermochemical processes that take place during pretreatment of biomass. **Youngha Hwang**, Purdue U, presented a numerical analysis on how, e.g., organo-metallic gold clusters attached to icosahedrally-symmetric particles (such as certain viruses) can be used to resolve ambiguities in the radial density function obtained from solution-scattering experiments. Following the coffee break **Soren Skou**, Xenocs, presented the current status of protein solution scattering in a home-lab setting and showed how dedicated instrumentation

combined with a high level of automation facilitates the SAXS data collection and analysis. **Sai Venkatesh Pingali**, ORNL, showed how the increased angular coverage achieved by the recent detector upgrade at the Bio-SANS instrument at HFIR increases the data collection efficiency and enables new scientific capabilities. In the final presentation of the session **Timothy Ryan**, Australian Synchrotron, showed how the use of a novel co-flow sample cell for size-exclusion chromatography coupled solution scattering improved the data quality by eliminating the capillary fouling during the experiment and making it possible to perform the experiment at a higher flux level without significant radiation damage issues on the sample. He further discussed the detail of the flow cell design and its implementation at the SAXS/WAXS beamline at the Australian Synchrotron.

Thomas Weiss

4.2.5: Advances in Structure Solution from Powder Data

This session covered both results and new tools for solving crystal structures using powder diffraction data. **Branton Campbell**, Brigham Young U, gave a brief introduction to group theory and showed how irreducible representations provide the basis for understanding symmetry lowering of a parent space group. Symmetry modes can provide a simplification (smaller number of parameters) of a refinement. In the transformation between the alpha- and beta-$Bi_2Sn_2O_7$ pyrochlore structures, only 13 symmetry modes are important. Characterizing the structures of nanomaterials and systems with significant local distortions requires more information than just the diffraction data, and tools are needed that can accommodate such additional information. **Pavol Juhas**, Brookhaven National Laboratory, described the DiffPy-CMI software toolbox for such complex modeling. Applications of this software included $Au_{144}(p\text{-}SC_6H_4CO_2)_{60}$ metal clusters and CdSe quantum dots. The new hollandite $K_2Sn_3O_7$ was predicted as part of the Materials Project (***materialsproject.org***). **Dan Shoemaker**, U Illinois Urbana-Champaign, described characterization of the structure using both synchrotron and neutron powder data. The neutron data were critical, as the structure falls apart in the 30 keV synchrotron X-ray beam.

Jim Kaduk, North Central College, described the structures of a set of lithium alkali hydrogen citrates, $LiMHC_6H_5O_7$ (M = Li, Na, K, Rb), solved from laboratory X-ray powder data and optimized using DFT techniques. The structures are layered, with metal-oxygen coordination in the center of the layer, and chains of very strong carboxylic acid-carboxylate hydrogen bonds on the surfaces of the layers. **Matt Tucker**, Oak Ridge National Laboratory, showed how the RMCProfile software (*rmcprofile.org*) expands the reverse Monte Carlo (big box) modeling technique to take explicit account of the Bragg intensity from crystalline materials. Matt's example was $SrTiO_3$ at 296 and 5K. He showed how superposition of the RMC results on the average structure gives insight into the local displacements in the structure. **Silvina Pagola**, William & Mary, described the workflow and operation of the new WinPSSP program for applying direct-space methods to crystal structure solution. Her examples included a rigid molecule, a simple co-crystal, and a molecule with a flexible sidechain. The software is freely available at: ***http://users.uoi.gr/nkourkou/winpssp***.

Saul Lapidus
Jim Kaduk

L-R: Benjamin Apker, Garrett Ginell, Krystle McLaughlin. Photo courtesy of Krystle McLaughlin.

Joel Bernstein explaining "fuzzy logic" while addressing the audience in Session 3.2.3. Photo by Peter Müller.

Sue Byram and Ilia Guzei. Photo by Dick Bromund.

Amy Sarjeant presenting the ACA Service Award to retiring ACA RefleXions Co-Editor Tom Koetzle. Photo by Peter Müller.

ACA Summer Course in Chemical Crystallography 2017

ACA Summer Course 2017, L-R: back row – J. Lee, A. Foerster, J. Li, E. Abucayon, M. Imer, B. Bouley, O. Esarte Palomero, G. Díaz de Delgado, R. von Dreele, Y. Liu, J. Kaduk, E. Dolgopolova, A. Peixoto de Abreu Lima, D. Ferreira, C. Lake, M. Crawley, S. Adas, C. Webb, K. Pringouri, J. Sears, S. Antal, H. Munasinghe, E. Eitrheim, D. Gray, K. Storms, N. Henderson, R. Papoular; front row – C. Malliakas, C. Stern, A. Filatov, Y. Kim, M. Ramirez, J. McMahon, E. Reinheimer, A. Sarjeant, A. Oliver, C. Chappell, B. Noll, R. Sommers, C. Powell, V. Sena. Photo by Yuyang Wu.

The University of Notre Dame and Northwestern University have co-hosted the **ACA Summer Course in Chemical Crystallography** since 2012. This year the course was held at Northwestern University from June 25th – July 2nd. Course organizers were: **Charlotte Stern** and **Christos Malliakas** of Northwestern U, **Allen Oliver**, U Notre Dame, and **Amy Sarjeant**, CCDC. For more information, please see the course website: ***http://acasummercourse.net***.

This was the second year we opted to run the course in 7 days instead of 10, which we discovered helps with scheduling. It still remains an intense course with lectures starting at 8:30 am and finishing at 8:30 pm, when everyone is ready for a dinner in town with their new friends. The mornings were devoted to lectures on theory while the afternoons were filled with workshops on the interpretation of the *International Tables*, Symmetry and Space Group analysis, and practical work on sample preparation for both single-crystal and powder-diffraction experiments. Later in the week this practical work included hands-on use of software with students' own data that either they brought with them, or that were collected on Northwestern's single-crystal and powder instruments or on the demo powder units that were on loan for the course. We have noticed that students now have more basic knowledge than in the past, so we divided attendees into groups depending on their ability. We have also incorporated some challenging sample and structural problems that crystallographers might encounter, so that when the students see them in the future they might know where to go or whom to ask for assistance.

Together, students and instructors collected 18 successful single-crystal data sets and a number of powder diffractograms as well. As in past years, we encouraged publication of these data with a request that an acknowledgment to the ACA summer course be included.

This year we had 26 attendees from across the globe, including Canada, South Korea, Uruguay, Venezuela, and the U. S., from academia and industry. Many of the same faculty have continued to be involved, which makes the course run smoothly. We had 18 faculty experts in the field of either or both single-crystal and powder diffraction. This is a wonderful ratio that promotes individual, one-on-one interaction. This has already proven to promote networking among all that are involved.

Overall the course is very well received by both students and instructors. Some remarks given in this year's survey at the end of the course were:

"This community of faculty has been overwhelmingly hospitable. Thank you for taking the time to share your love for crystallography. It's encouraging and inspiring!"

"Is there an ACA summer course part II? After a year of intense practice, I'd love to come back for additional training!"

"The course was an incredible experience that I will carry with me for the rest of my life. Course material and instructors were phenomenal. I'm very thankful for this opportunity."

"This course was a great help in first steps in crystallography. The great team of faculties makes this a great experience."

"The faculty were absolutely amazing and the perfect choices for presenting such difficult materials in such a condensed period of time."

We would like to thank the following vendors and associations for their kind and generous support of the course: The American Crystallographic Association, The U. S. National Committee for Crystallography, Bruker AXS, Cambridge Crystallographic Data Centre, Pittsburgh Diffraction Society, The International Centre for Diffraction Data, MiTeGen, STOE, Olex2, Rigaku Americas, and Dectris. We would especially like to thank all of the Faculty for their time and dedication to the course.

Charlotte Stern

Remembering Philip Coppens

Philip Coppens, SUNY Distinguished Professor Emeritus and Distinguished Research Professor of Chemistry at the University at Buffalo-SUNY, passed away on June 21, 2017, at the age of 86. Chair of Chemistry at UB David Watson said, "Philip was a giant in his field and pioneered the technique of time-resolved X-ray crystallography … He was renowned for promoting the discipline, organizing international meetings and mentoring younger colleagues in his field." A memoir written by Philip can be found in the History Portal of the ACA (***http://www.amercrystalassn.org/h_coppens_memoir***). What follows are the remembrances of several of our crystallographic community who knew him well.

Jane Griffin

I was an older graduate student in the Chemistry Department of SUNY at Buffalo in 1968 when Philip Coppens came to give a seminar for an open position in the Department. It was on his X-N work on triazine. It was exciting to see experimentally produced electron-density maps that showed bonding and lone-pair density. Philip was hired, and I took his first course in X-Ray Crystallography in 1968.

How many professors would take a mother of four young children as their first graduate student? Philip brought the world to Buffalo. He never went to a meeting that he did not return with a new collaborator, post doc, or graduate student. In my time in the lab my mentors included Finn Larsen from Aarhus University; Pierre Becker from France; Dan Jones, South Carolinian fresh out of Lipscomb's lab at Harvard; Niels Hansen, Aarhus; and Bob Blessing from University of Pittsburgh and Lund University in Sweden. Life was never dull in Philip's lab. He was a wonderful teacher, well prepared, clearly explaining the mathematics involved in every aspect of crystallography. He was an expert at using time as efficiently as possible. Every morning he walked into the lab to ask, "How's it going?", and you better be prepared to answer. When you made a presentation in his group meetings, his first question was always, "So what is your major conclusion?" What had you learned?

Philip in his office at UB. Photo by Nancy J. Parisi.

Philip never rested on his previous accomplishments; he was always looking for what new scientific question could be solved by an advance in crystallographic technology. Although recently retired and relocated to be near his sons and grandchildren, he had returned to Buffalo to work on a joint paper when he died.

Finn Krebs Larsen

I came across Philip's seminal *Science* paper entitled *Comparative X-ray and neutron diffraction study of bonding effects in s-triazine* (*Science, vol. 158 (Dec. 22, 1967), 1577-1579)* during studies for my degree in X-ray and neutron diffraction. Subsequently I very much wanted to learn more about what could be achieved by X-N studies. I got in touch with Philip and persuaded him to take me on. I arrived in Buffalo in late 1969 with my wife and small daughter and became one of Philip's first post docs after he moved from Brookhaven National Laboratory to his new chair at SUNY at Buffalo.

It was a tumultuous time there, with student demonstrations against the war in Vietnam and with groups of police patrolling campus; very exciting and a little scary for a small family from peaceful Denmark. Philip and Marguerite were extremely helpful in getting us started. Philip helped us buy a car and Marguerite drove us around town until we found an apartment.

My main project was to help develop low-temperature X-ray equipment and also to go on measuring trips to Brookhaven National Laboratory. Our collaboration continued after I, in 1971, returned to a position in the Department of Chemistry at Aarhus University, Denmark, and it endured right up to my retirement. The most important way I kept close collaborations with Philip was by stationing some of the best of my Ph.D. students in Buffalo for extended stays as part of their education. Some remarkable works and noteworthy theses resulted from these contacts with Philip. It should be mentioned that Niels K. Hansen (sadly, now deceased), during such a stay, tested aspherical atom refinements of small molecules and developed, with Philip, the MOLLY program, which later was extended to the most successful program system XD2006.

Very early on Philip realized the great potential of synchrotron radiation for crystallography. He involved himself deeply by raising funds and building a beamline at the National Synchrotron Light Source at Brookhaven and later at the Advanced Photon Source in Chicago. The very intense synchrotron X-radiation beam with variable wavelength and low-temperature capability opened new and exciting crystallographic research and made the use of such beamlines an irresistible goal for many, including myself. Fortunately it was possible even for an outsider from Denmark to be allocated beam time through application and according to scientific merit. We from the Department of Chemistry, Aarhus University have continued to benefit to this very day.

There is another extremely important side to Philip's impressive achievements that I will laud and praise, namely his never failing willingness to help educate students. Many Nordic students have benefitted greatly from this. The governments of the Nordic countries – Denmark, Sweden, Norway, Finland and Iceland – give substantial sums of money to finance Ph.D. courses, summer schools in advanced subjects. About 10 Ph.D. students

from each of these countries get all expenses paid for taking weeklong courses. I have for many years arranged such Nordic Research Training Courses, every three to four years since 1988. The subject is: *The application of X-ray synchrotron radiation in chemistry, physics and biology*. Lecturers are well-renowned scientists from the Nordic countries, but also some top experts from other parts of the world. Philip was extremely kind and came to lecture whenever I asked. He was a most popular lecturer at every single one of the courses. I want to mention that he did not – like some busy lecturers unfortunately do – just turn up to deliver the lecture and then leave immediately afterwards. In fact, every time Philip spent several days with the students and they appreciated it.

Philip has had a deep impact on my entire professional life – indeed, my life in total. My life would have been completely different had I not seen Philip's *Science* paper on the X-N study of *s*-triazine. This was a defining moment for which I am, Philip, eternally grateful.

Pierre Becker

When doing my Ph.D., I was stymied by the abstract nature of wave-functions until I saw the *Science* paper by Philip Coppens that showed the bonding density observed through X-ray scattering in *s*-triazine: so, the square of a wave-function was a reality! That's why I got in contact with Philip. In 1972-1973 I joined him in Buffalo for six months and brought my family. He immediately exposed me to the reality of scattering experiments: absorption, thermal effects, extinction, the difference between X and N atomic data, optimization of signal/noise ratio. He had me work with his young collaborators (including Bob Blessing and Jane Griffin). We had a weekly meeting where everyone shared his or her work with the whole group. This was when Philip started time-resolved research, since every 15 minutes he came to ask about our progress!

I was always impressed by Philip's chemical intuition. We solved several interesting problems. What a joy to obtain (in cooperation with Fred Ross) the experimental electron density of tetracyanoethylene showing single, double, and triple bonds and lone pairs: this gave sense to LCAO approaches in quantum chemistry.

Such a fantastic time, where we also discovered the strong human qualities of Philip and his wife Marguerite (in particular at the occurrence of two dramatic family events in France).

It was a great pleasure to continue working with Philip and his international collaborators. This strengthened my scientific life immensely. During my whole career, I kept in mind fantastic lessons from Philip: when working with other people find complementary skills and give priority to strengthening their talent, put their name first on publications, and see that they are invited to international lectures. Another valuable point: when publishing a rather theoretical model – which is often complex to read – provide a simple strategy to apply your model. This was the case with our work on extinction. Philip was a man who made his work open to the whole community. He never said or wrote, "I did," but always put emphasis on his co-workers.

And how was he able, starting in 1997, to develop a new field of time-resolved crystallography? He attracted so many young, talented scientists and structured a revolutionary time-dependent crystallography, which let us go from pictures towards molecular movies.

Philip's retirement symposium, organized by Jason Benedict last October, was an unforgettable event where we all felt as if we were members of a family!

Philip Coppens was a fantastic man and scientist. Sadly, he has left us, but his spirit is present in our lives. I personally cannot give a course or work with a scientist without having him present in me. And all my family loved him, Marguerite and their sons.

James Phillips

My professional association with Philip Coppens began when my phone rang in my office at the EMBL Outstation in Hamburg. A woman's voice announced, "United States calling," and Philip came on the line. He offered me a job to coordinate the building of a beam line for SUNY at NSLS (the old one). I had applied for the job, as advertised in the ACA newsletter, but a direct offer amazed me. I asked for an interview and to see NSLS. To say it succinctly, as I found out Philip often did, I went to New York and soon accepted the job. I did have to tell Sir John Kendrew that I was no longer working for him!

Thus began an eight-year period of working closely with Philip Coppens. Many people remember his scientific achievements, but I also saw him as a wise administrator. As part of the SUNY beam line management team, and eventually as its leader, he helped steer the project through the difficult priority decisions necessary for the construction of a facility that would serve the diverse experiments needed for five SUNY campuses. In short, he had my back. I found that he drove me hard but drove himself harder.

Philip's original scientific concept for his synchrotron radiation work was to expand the charge-density field, perhaps with anomalous dispersion techniques. Soon, though, he had the idea of time-resolved crystallography. An NSLS bending magnet line proved inadequate so his vision came to fruition with his work at APS. This illustrates Philip's determination to see his visions through. It also shows his ability to innovate the instrumentation necessary for time-resolved work.

When I moved to industry I saw Philip in a new light, as a customer. Siemens/Bruker salesmen will tell you how tough a bargainer he was. However, he did let us use the SUNY facilities to test some variations on phosphors used in the detectors of the time. Again, he showed wisdom. He knew what improvements in instrumentation would benefit all.

It is said that we all stand on the shoulders of giants. Though Philip is gone, crystallographers of the future will be standing on his shoulders.

Jason Benedict

I joined Philip's research group as a post doc in 2008. In a word, his style as a research supervisor was "demanding." It was not uncommon for Philip to request that you present at

group meeting – with only a few hours' advance notice. The first time this happens, which is often shortly after joining Philip's group, the experience is rather jarring. Only when it's over and you debrief with other group members do the intensity and high expectations of being a Coppens group member become apparent. When I had the opportunity to organize a symposium at the 2011 ACA Annual Meeting, I had the chance to meet Coppens' group members who pre-dated me by decades, all of whom assured me that this older Philip was now a real softy – I had it easy!

While I was fortunate enough to forge countless scientific memories with Philip and crew in his lab at the University at Buffalo and at the APS (he was an active member of the Scientific Advisory Committee of the ChemMatCARS beamline), some of my fondest experiences occurred outside of science, for instance, swimming get-togethers in the Coppens' pool at their Amherst home. Marguerite would prepare an amazing fruit salad and make sure we all departed with a bounty of chives, an herb that overtook much of the free space in their back yard. Many reading this will also recall the group hikes in the serene wilderness just outside of the city.

Much is omitted when my memories of Philip are distilled into a couple of short paragraphs, but the following is absolutely certain: Philip was a great friend and mentor and will be missed dearly.

Connie Rajnak

My first memory of Philip was way back when I was a novice crystallographer and my boss, Dave Duchamp, drove me to hear him speak. Philip's talk was something to do with monopoles, and he made them sound so easy to understand that I imagined I did in fact understand. From then on I admired Philip from afar until I started going to ACA meetings, and, subsequently, IUCr meetings. In 1978 Philip was President of the ACA and from 1993 to 1996 he was President of the IUCr.

We somehow became friends and when I eventually married Stan, in 2007, we put Philip and Marguerite on our Christmas letter list. Marguerite decided Stan must be British or at least have spent a long time in the UK (not true). They wrote, *"Your poem reminded us of the many limericks we heard and read and we enjoyed it equally (no Schadenfreude)."* After another Christmas letter (2011) describing our travels in South Africa they wrote, *"We were in Kruger Park and the Cape Province about 10 years ago, but did not see a quarter of what you people managed to see and photograph. What beautiful pictures. We will follow your trail next time we may get to South Africa!"*

I sent Philip congratulatory notes when he was awarded the Gregori Aminoff Prize in 1996, the Ewald Prize of the IUCr in 2005, and the Kołos Medal in 2013, which he always politely acknowledged. But what I admired most about Philip was that in his talks he always, always showed photos of the people in his lab, and gave them the credit he claimed they deserved.

When I co-edited *ACA RefleXions*, Philip was a frequent contributor so we corresponded often. In 2009 Philip provided a *RefleXions* cover based on his Plenary Lecture at the Toronto ACA meeting on *New developments in X-ray photocrystallography*. Dick van der Helm's obituary appeared in the Fall 2010 issue and Philip helped with that – they were both Dutch and neither of them ever lost the Dutch accent. After the Boston ACA meeting in 2012, I requested and promptly received an image from Philip to include in the *Transactions* report. In the Fall 2013 issue his article *Workshop on dynamic structural photocrystallography in chemistry* appeared.

I was profoundly saddened to hear of Philip's (much too early) death.

Bob Blessing

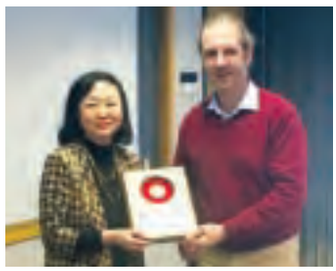
A signal characteristic of Philip Coppens' research career was his uncanny ability to quickly see through to the central questions in a new, emerging field of research on chemical structure and energetics. As a result of an insightful focus or refocus of the work in Philip's laboratory, the lab was consistently an innovative leader at the frontier of new research areas.

Philip's lab at the University at Buffalo (UB) and at his synchrotron beamline stations at Brookhaven and Argonne were for fifty-some years strong attractors for a steady succession of international students, fellows, collaborators, and colleagues. Many in that group became and remain good friends and continuing research collaborators and colleagues. Philip was our nexus for the growth of worldwide friendships and cooperation in ongoing research. Happily, it was the good fortune for many of us to be able to assemble in Buffalo in October 2016 to salute Philip on the occasion of his UB retirement at the fest-symposium organized by Jason Benedict.

Editor's Note: *This remembrance was assembled by Kay Onan.*

News & Awards

ICDD Announces New Distinguished Fellow



Winnie Wong-Ng receiving her Distinguished Fellow Award from ICDD Board of Directors Chairman Matteo Leoni

In March, 2017, the Board of Directors of the International Centre for Diffraction Data (ICDD) awarded **Winnie Wong-Ng**, Research Chemist at the National Institute of Standards and Technology (NIST), the ICDD's **Distinguished Fellow Award**. This award is given to a member, currently recognized as an ICDD Fellow, who has given long and meritorious service to the ICDD. Besides serving the ICDD, Winnie has given sustained and meritorious service to the ACA as indicated by her being named an ACA Fellow in 2014.

"Visionary" Speaker

Majed Chergui, Professor of Chemistry and Physics at the Ecole Polytechnique Fédérale de Lausanne, Switzerland, ACA member and founding Editor-in-Chief of the ACA's flagship journal *Structural Dynamics*, was invited to be one of the visionary speakers at the 2017 Frontiers in Optics + Laser Science conference. Majed was chosen to discuss the future of innovation

Majed Chergui

and to provide insight into cutting-edge advances in optics and photonics. He is most noted for his contribution to the development of new ultrafast spectroscopic techniques with which he addresses fundamental questions in, for instance, the photophysics of transition-metal complexes and the charge-carrier dynamics in semiconductors.

ACA Member Receives ASBMB Award

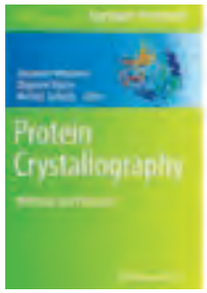
Leemor Joshua-Tor

Leemor Joshua-Tor, Professor and Howard Hughes Medical Institute Investigator at Cold Spring Harbor Laboratory, has won the 2018 **Mildred Cohn Award in Biological Chemistry** from the American Society for Biochemistry and Molecular Biology (ASBMB). The Cohn Award was established to honor the pioneering scientific accomplishments and the spirit of the late Professor Cohn, who was the first female president of the ASBMB. The award recognizes and honors scientists who have made substantial advances in understanding biological chemistry using innovative physical approaches.

Joshua-Tor's lab studies the molecular basis of nucleic acid regulatory processes using the tools of structural biology, biochemistry and biophysics. They study proteins and protein complexes associated with these processes to elucidate how they work. The use of X-ray crystallography, electron microscopy, and other structural techniques enables them to obtain the three-dimensional structures of these molecular machines. Biochemistry, biophysics and molecular biology allow them to study properties that can be correlated to their function and biology.

Kay Onan

Book Reviews



Protein Crystallography: Methods and Protocols: Alexander Wlodawer, Zbigniew Dauter and Mariusz Jaskólski, Eds., Springer Science+Business Media, New York, 2017, 672 pp., ISBN-13: 978-1-4939-6998-2

This book is a compilation of 27 reviews by 50 contributors on current methods in protein crystallography. Each contributor is recognized as a leader in their area of specialization, adding gravitas to each review.

The book starts with a chapter (1) on expression and purification, followed by a chapter (2) on traditional crystallization. The micrographs in this chapter of growth steps are beautiful and instructive. Three more chapters (3-5) cover state-of-the-art processes in crystallizing problem proteins. Another chapter (6) on finding crystals for the diffraction experiment illustrates the problems of selecting an object from the background when there is little contrast.

Once crystals are grown, the next step is data collection. The ensuing five chapters (7-11) cover conventional data collection, microbeam data collection, serial synchrotron data collection and time-resolved data collection. Chapter 12 covers structure determination with X-ray free-electron laser data while Chapter 13 reviews the problems of data processing from XFELs.

Chapters 14-19 cover experimental solutions to phasing with derivatization, anomalous diffraction and long-wavelength data collection, and computational methods via Patterson and direct methods and molecular replacement. Chapter 20 covers the issues of radiation damage and even loops back to experimental phasing using radiation damage.

With an initial model, the book flows through five chapters (21-25) on modeling, refinement and validation before closing with two chapters (26 and 27) on databases in crystallography.

What is missing from this tome are reviews on cryo-techniques and conventional data processing. Nevertheless, I believe this modern volume will replace the venerable Volumes 276 and 277 of *Methods in Enzymology* on many shelves.

Back in January the *1A* podcast did a special on dystopian novels because of the surge in sales of books in that genre since November 2016. *1984* was at the top of the list, but because I've read it once a decade since high school I didn't reread it this year. I picked up two of the novels on the list, *It Can't Happen Here* and *A Handmaid's Tale*, and also found a Great Course titled *Great Utopian and Dystopian Works of Literature*.

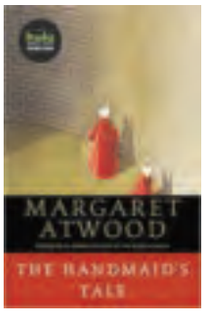
Great Utopian and Dystopian Works of Literature: Pamela Bedore, Ph.D., The Great Courses, Chantilly, VA, 2017

Pamela Bedore is an English professor at the University of Connecticut. She is the recipient of an Excellence in Teaching Award, and when you listen to the course you will understand why. I wish my English teachers in college had been as animated as she is. The course begins with an analysis of Thomas More's *Utopia*. The next few lectures cover the classics by Voltaire, Swift, Hawthorne, Alcott, Butler and Bellamy. For me, things began to get interesting with the analysis of H.G. Welles' *The Time Machine*. Here is where I realized one being's utopia is another's dystopia, a fact Bedore points out in a later lecture. The mid-20th century classics are included for analysis: Huxley's *Brave New World*, Orwell's *1984*, one of my favorites, Dick's *Minority Report*, and Burgess' *A Clockwork Orange*. Here Bedore begins

the analysis of movie versions of the studied novels. More recent classics are also studied: Atwood's *A Handmaid's Tale*, Collins' *The Hunger Games* trilogy and McCarthy's *The Road*. I found this a fascinating and rewarding series of lectures and highly recommend it as a diversion from current events.

It Can't Happen Here: Sinclair Lewis, Signet Classics, New York, 1935-2014, 416 pp., ISBN: 978-0451465641

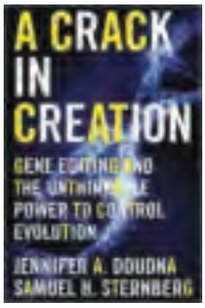
The novel is set in the 1930s and is based on the premise that Franklin Delano Roosevelt loses the 1936 election to a fictional character, Buzz Windrip, modeled on Huey Long (who was assassinated just before the election). Dystopia arises from Windrip's destruction of American democracy and imposition of totalitarian rule through a paramilitary force created from unemployed workers. The hero is Doremus Jessup, a journalist, who fights Windrip throughput the novel. I don't want to spoil the ending, but I really enjoyed the book.



A Handmaid's Tale: Margaret Atwood, Houghton Mifflin Harcourt, New York, 1986, 320 pp., ISBN: 978-0385490818

The novel is a first-person narrative provided by the protagonist, a woman renamed Offred, who has been forced to become a handmaid (surrogate for infertile wives) in an America that has become a theocracy called Gilead based on the Old Testament. Since women have been relegated to subservient tasks throughout society, one wonders how Offred manages to write the account. You will find out in the last chapter; to provide any more information will spoil the ending. Hulu has produced a miniseries based on the novel, which has received a lot of positive press, at least in the periodicals I read; however, I always recommend reading the book before seeing any screen adaptations.

Joseph Ferrara



A Crack in Creation: Gene Editing and the Unthinkable Power to Control Evolution: Jennifer Doudna and Samuel H. Sternberg, Houghton Mifflin Harcourt, New York, 2017, 282 pp., ISBN-13: 978-0544716940

CRISPR is one of the hottest buzzwords in the biotech world right now. The ability to edit genes directly in living things – plants, animals, and even maybe one day soon humans – is here. And Jennifer Doudna is one of CRISPR's foremost pioneers. In her lab at Berkeley, she helped start the CRISPR revolution. Sternberg is one of her fellow researchers, and their book (according to the jacket cover, a favorite of *Star Wars'* creator George Lucas) reads a bit like "CRISPR for Dummies" – but in the best way possible.

Doudna and Sternberg break down CRISPR – which stands for Clustered Regularly Interspaced Short Palindromic Repeats – into plain, simple English. Even someone without a strong science background could probably understand the basic principle behind CRISPR. It allows scientists to edit DNA – remove bad genes or add good genes. It can help us make cows more muscular so that more meat comes from each animal, or make plants less susceptible to fungal outbreaks.

But the most interesting part of Doudna and Sternberg's book wasn't the specifics of CRISPR and how it works. It was the dissection of the ethical and moral implications of direct germline editing. They detail the obvious possible pitfalls of the process – like eugenics – and even detail a Chinese experiment where attempts were made to edit the germline in embryos – an experiment that failed.

CRISPR represents a tremendous breakthrough – but the most important lesson in the book isn't about what it can do, it is about what we choose to do with it.

Jeanette Ferrara

Editor's Note: *Joe Ferrara has pointed out to us that the reviews of The Glass Universe and Shoot Like a Girl in our summer issue were actually authored by Jeanette, rather than by Joe himself as we erroneously indicated in the by-line. Our apologies to Jeanette!*

10 Reasons Why ACA Partners with the American Institute of Physics (AIP)

In the early 1930s amid the Great Depression, five scientific societies banded together to amplify efforts at a time when resources were scarce and to leverage economies of scale for scholarly publishing. The societies served a diversity of communities – physics, optics, acoustics and rheology. They settled on the name American Institute of Physics, as Physics was widely understood as the foundational science from which all other physical sciences emerge. Over the years, AIP has grown its services for its Member Societies, and for the greater good. The ACA became a member in 1966, and several others joined in the ensuing years. AIP now has 10 Member Societies with a collective 120,000 members.

Membership in AIP allows the ACA to extend our influence beyond our membership, to connect with the broader physical sciences community, to support programs that raise the profile of the physical sciences to policy makers and the public, and to

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strengthen our voice and capacity to address mutual concerns.

Below are a few ways in which ACA benefits from belonging to AIP:

1. To be a part of a bigger physical sciences community

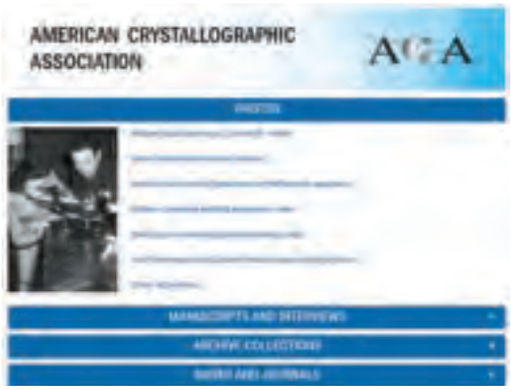
We share a common mission with AIP and their Member Societies to inspire and improve human lives through the knowledge of the physical sciences and their applications to human welfare. Through leadership meetings and committees, we routinely exchange information and expertise on areas of common interest. Thus, we are better equipped to serve our own communities and to partner as needs and opportunities arise.

2. To keep current about other areas of research

Physics Today keeps all 120K Member Society members informed about technological advances and ground-breaking research across the physical sciences, including crystallography. See the July 2017 editorial, *Electron cryomicroscopy comes of age* (***http://dx.doi.org/10.1063/1.882609***). ACA members receive *Physics Today*, AIP's flagship magazine, in print or electronic format each month, at no extra charge.

3. To preserve our history and make it available to thousands of researchers

The Niels Bohr Library & Archives is the collecting repository of AIP and its Member Societies with over 30 collections connected to ACA. To learn more about the treasures the Library holds for ACA, see AIP's archives portal online (***http://history.aip.org/society-portals/aca/aca.html***). See the article on page 5 for news on the ACA History Project.



4. To promote increased diversity and inclusion in the physical sciences

The ACA serves on the AIP Liaison Committee for Underrepresented Minorities (LCURM), which fosters collaboration to increase these groups' representation in the physical sciences. This year, LCURM helped to launch a national task force to increase the number of bachelor's degrees in physics and astronomy among African Americans.

AIP's Statistical Research Center also produces data-driven reports on the representation of women and minority populations in the physical sciences, and is conducting a membership survey for the ACA in the fall.

5. To engage in public policy

AIP offers the ACA an opportunity to advance science policy campaigns, increasing visibility and representation through Executive Branch and Congressional visits, to sign on to statements for endorsement, and to enhance other policy efforts. Only Member Society members may apply for AIP science policy fellowships offered each year. ACA members, Caitlin Murphy, Christopher Cahill and Matthew McGrath are a few of the most recent beneficiaries of this program (***https://www.aip.org/policy/fellowships/overview***).

6. To educate the public and raise awareness

As a Member Society, ACA supports programs that promote the physical sciences, inform the public, and illustrate how scientific advancements influence our way of life. *Inside Science* (***www.insidescience.org/***) brings science news into mainstream media. AIP has also promoted compelling research presented at ACA meetings, writing press releases and pitching them to the media. *FYI science policy news* (***www.aip.org/fyi***) helps researchers, policy makers, and the public keep current on policy and funding developments in Washington, DC that affect the physical sciences.

7. To attain funding for innovative, collaborative projects

This year, AIP launched a new program to encourage partnerships with its Member Societies. Next year, the *Venture Partnership Program* (***www.aip.org/aip/member-benefits/venture-partnership-fund***) will increase the total award amount to ~$250K for strategy- and growth-driven innovation. Submissions for this program were due this year on September 25.

8. To extend our ability to reach students

The Society of Physics Students' (SPS) (***www.spsnational.org***) joint membership program introduced 200 undergraduate physics majors to ACA in 2016. The year of free membership gives the ACA the opportunity to engage these prospective crystallographers and attract new members among the best and brightest. SPS works with the ACA's Young Scientists Interest Group to hold student-focused sessions and awards at ACA meetings.

9. To bring in exhibit revenue

AIP Publishing manages the ACA's meeting exhibits. This not only yields ~$60K in revenue, it also enables the ACA to focus on meeting content.

10. To leverage publishing expertise

AIP Publishing worked closely with the ACA to launch our flagship journal – *Structural Dynamics* – in January 2014. In just a few years, the journal has reached an impact factor 2.968 putting it well within the top third of highest ranking scholarly journals. We are optimistic about its future development. See pp. 7-9 for an update on *Structural Dynamics* (***http://aca.scitation.org/journal/sdy***).

Amy Sarjeant
2017 ACA President

Spotlight on Stamps

A Special Kind of CAT

Daniel Rabinovich

Computer-assisted tomography (CAT) is a medical diagnostic technique in which X-ray scans taken from multiple angles are used to generate cross-sectional images of the bones and a variety of soft tissues inside the body, including the brain, heart, lungs, and the gastrointestinal tract, which cannot be visualized with conventional X-ray techniques.

The original ideas behind computed tomography were conceived in 1967 by Godfrey Hounsfield (1919-2004), a British engineer at Electric and Musical Industries (EMI), where he had also worked on research projects ranging from guided weapon systems and radar to the UK's first all-transistor computer, the EMIDEC 1100. Hounsfield, an expert on pattern recognition problems, designed and built several prototypes of head scanners during the next four years and, on October 1, 1971, CT scanning was introduced into medical practice when the first image of a patient with a potential brain tumor was obtained at Atkinson Morley Hospital in London. Remarkably, Hounsfield was not aware at the time that South African physicist Allan Cormack (1924-1998) had devised a mathematical method in the late 1950s and early 1960s for measuring different tissue densities within the body and, in fact, had predicted that such calculations could be used to create X-ray images of cross-sections or "slices" of organs like the brain.

Hounsfield and Cormack shared the 1979 Nobel Prize in Physiology or Medicine "for the development of computer-assisted tomography," the same year that H.C. Brown and G. Wittig were recognized with the Chemistry Prize and Mother Teresa was honored with the one for Peace. Interestingly, Hounsfield and Cormack not only worked independently from one another to bring about CAT, but also had never met in person until they attended the Nobel presentation ceremony in Stockholm in December of that year. During his Nobel Banquet speech, Cormack also stressed the irony of the award since neither he nor Hounsfield were physicians, and proclaimed that Alfred Nobel himself would have been pleased that an electrical engineer and a physicist had contributed in their own way to the advancement of medicine.

Although CAT gets some serious competition these days from Magnetic Resonance Imaging (MRI) in medical diagnostics, it has a number of noteworthy applications in other fields, including precision metrology, reverse engineering, failure analysis, airport security, and art conservation.

Daniel Rabinovich

Puzzle Corner

For this issue, we have a word-search puzzle by **Guest Puzzler Joe Ferrara**, a new **Crystal Connections** and solution to the previous one, mention of those who provided solutions to previous puzzles, the solution to the baseball-themed **DISORDERED** puzzle, and a few comments about it.

You'll find Joe's word-search puzzle right here in the adjoining column. It contains names of Nobel laureates associated with crystallography. There are 51. How many can you find?

Turn the page for the new **Crystal Connections** and the solutions to previous puzzles.

Turn to p. 56

Crystal Connections #12

What do the answers to these clues have in common?

1) Deck _____: for transmitting natural light below deck in sailing ships

2) Full-page illustration; scute

3) "Well I headed for Las Vegas, Only made it out to _____"

4) Highest symmetry hexahedron

5) _____ of the Moon, Teotihuacan

6) A one-person hot air balloon; type of rail car

7) The Doric temple at Segesta is thought to have never been completed, since these are not fluted

8) _____ Runner: 1982 movie based on *Do Androids Dream of Electric Sheep?*

9) The _____: *Prelude and Fugue in E Minor*, J.S. Bach; a golf club

10) A 3-ball in the Manhattan L_1 Metric, taxicab geometry

Solution to Crystal Connections #11 - Names of diffractometers

1) Banjo player or gleaner – Picker (FACS-1)

2) Polar rhombohedral space group lacking glides – R3 (Nicolet, then Siemens)

3) To abstain from food; very sensitive film – Fast (Nonius)

4) Second most common Sohncke space group – $P2_1$ (Syntex)

5) Acronym for engineering software, followed by space group number for 4) - CAD4 (Enraf-Nonius)

6) Smart Museum of Art, at the University of Chicago - (Bruker)

7) Major source of elements heavier than oxygen – SuperNova (Rigaku/Oxford)

8) Lies on the ecliptic. *Castor*, *Pollux* and *Alhena* are its brightest – Gemini (Oxford)

9) The Italian *tarantella* dance is thought to have origins in the bite of this animal – Spider (Rigaku R-axis)

Marian Szebenyi, Cornell U, submitted the correct solution for Crystal Connections #11.

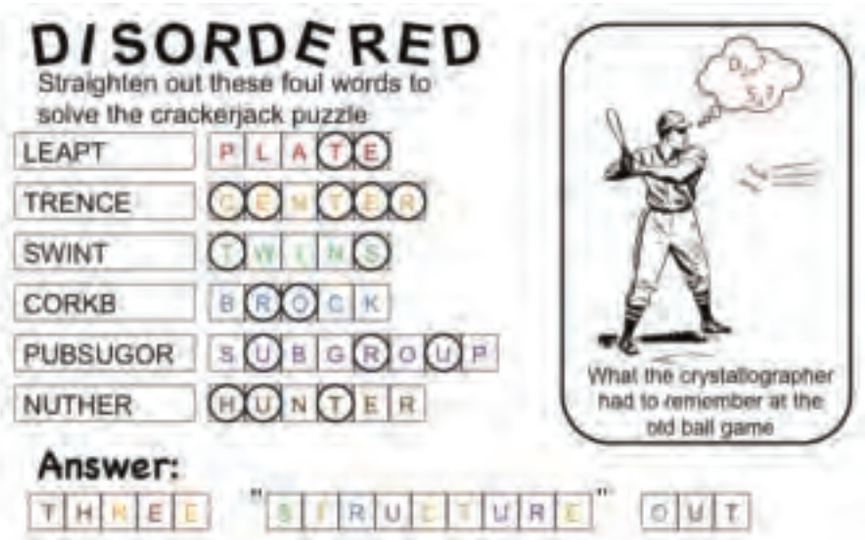
Tim Royappa, U West Florida, provided the solution to the baseball **DISORDERED** puzzle, shown at left below.

Notes on the answers: **PLATE** is a bad habit or home base; **CENTER** is a field or a symmetry element; **TWINS** are a Minnesota baseball team or a crystallographic nuisance; Lou **BROCK** and Jim (Catfish) **HUNTER** are baseball Hall-of-Famers, Carol Brock, Allen Hunter and Bill Hunter are not; point group S_4 is a **SUBGROUP** of D_{2d}. Concerning the latter, a favorite point symmetry question for students is to assign the point group of a tennis ball or *baseball*, including the seams, and the accepted answer is D_{2d}. However, note that the stitching makes the seams of a baseball *directional*, as seen at right below, viewed down the direction of one of the potential dihedral twofolds.

The directionality destroys not only these twofolds, but also the vertical mirrors, and only the S_4 remains, as is being contemplated by the batter.

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

Frank Fronczek
ffroncz@lsu.edu



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ACA TORONTO

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Travel Grant Application Deadline: March 31, 2018
Abstract Deadline: March 31, 2018
Early Registration Deadline: May 31, 2018
Hotel Reservation Deadline: June 18, 2018

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

Program Chair - Gerald Audette
audette@yorku.ca

Program Chair - Tiffany Kinnibrugh
kinnibrught@gmail.com

Posters Chair - Louise Dawe
ldawe@wlu.ca

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

OPENING SESSION KEYNOTE SPEAKER

John Polanyi - 1986 Nobel Laureate in Chemistry

WORKSHOPS

Cryo-EM – A Guide to High-Resolution Structure Determination
Molecular Art and Animation in 3D
X-Ray Crystallography: Structure Preparation, Electron Density and Solvent Analysis
Applications of Small Angle Scattering to Structural Biology: An Introduction
Rietveld Refinement and pdf Analyses of in situ X-ray Scattering Data within GSAS-II

EDUCATIONAL SESSIONS & YSIG EVENTS

3-Minute Thesis Session
YSIG Orientation and Networking Mixer
Career Development Session
Engaging Undergraduates with Crystallographic Research
Diversity & Inclusivity Session

ACA AWARDS

Buerger Award honoring Frank Hawthorne
Warren Award honoring Simon Billinge
Margaret C. Etter Early Career Award honoring Jason McLellan

SESSIONS

Transactions Symposium – Shining a Light on Structure-Based Drug Design
Structural Dynamics – in Honor of Philip Coppens
Special Sessions in Honor of Dick Marsh
Crystallography on the International Space Station
Advances in Biological Cryo Electron Microscopy
Structural Biology of Pathogens
NMR Crystallography
Neutron and X-ray Scattering of Correlated and Quantum Materials
Dynamic Crystals as Molecular Materials
Mineralogical Crystallography

Transactions Symposium – Shining a Light on Structure-Based Drug Design

Organizers: **Stephen Soisson** (Merck; *stephen_soisson@merck.com*) and **Vincent Stoll** (AbbVie, *Vincent.Stoll@abbvie.com*)

Meeting participants working in the area of protein crystallography, cryo-electron microscopy, and with an interest in drug discovery will have an opportunity to learn from experts how cutting-edge technologies are being applied to next-generation drug discovery. Unique facets of industrial structural biology will be highlighted in the course of discussing small-molecule hit-finding efforts, such as fragment-based drug discovery, and the integration of structural and computational approaches to facilitate structure-based drug design. The role of structural information in "new" modality discovery such as vaccines, biologics and peptides will also be discussed. Unique opportunities to increase the breadth and scope of structural impact in drug discovery will be presented in context of new methods to access traditionally challenging targets such as ion channels and GPCRs, and how next generation synchrotrons, XFELs, and serial data collection techniques could play key roles in the future.

General Meeting Information

As the 2018 ACA Meeting is taking place outside of the United States, advanced planning by US and foreign travelers is critical. Thorough research should be completed on the documentation needed to access Canada and what is needed to return to your country of origin.

The following links may be helpful:

US Department of State: US Passports & International Travel (https://travel.state.gov/content/passports/en/country/canada.html)

US Customs & Border Protection: Travel to Canada & Mexico (https://www.cbp.gov/travel/us-citizens/canada-mexico-travel)

Government of Canada: Traveling to Canada (https://travel.gc.ca/returning/travelling-to-canada)

Government of Canada: Visa Information (http://www.cic.gc.ca/english/visit/apply-who.asp)

Canadian Tourism Commission (http://caen-keepexploring.canada.travel/)

To request a letter of participation from ACA contact the Meeting Registrar at ***aca@hwi.buffalo.edu.***

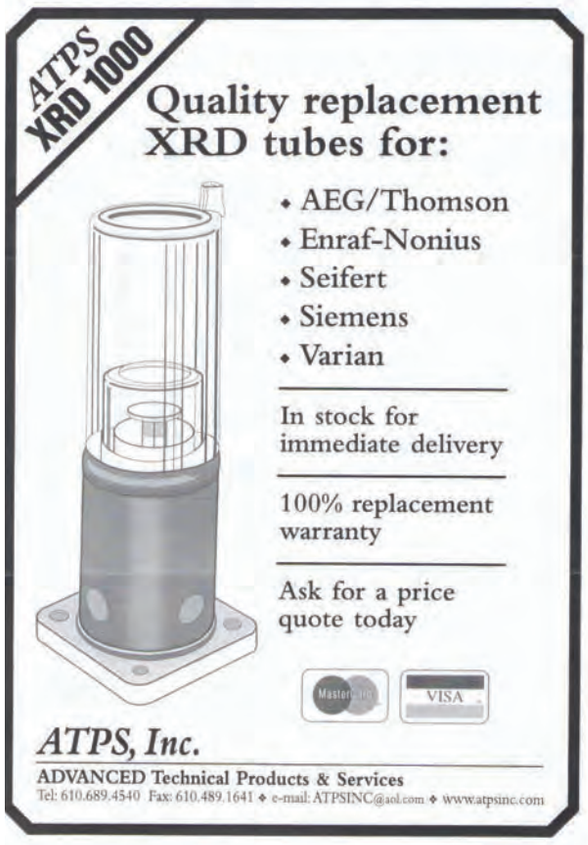
Staying Green: All attendees will receive a hardcopy of the ***Program Book***, but the full set of abstracts will only be available online. We are not planning to have a meeting bag, so if you would like one you should remember to bring your favorite from an earlier meeting.

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

Room rates, in Canadian dollars, are $199 CAN for one or two people, per night and plus taxes. A special rate of $169 CAN has been negotiated **for students and post docs only**. Room sharing can make these rates even more reasonable – use the e-mail ***Room Sharing*** feature under accommodations on the meeting web site at ***http://www.amercrystalassn.org/2018-accommodations***.

Financial Support: Travel support will be available for young scientists. Applications for travel support should be made by March 31, 2018. For additional information see ***http://www.amercrystalassn.org/2018-young-scientists***.

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



FEBRUARY 2018

13-15 **5th BioXFEL International Conference**. New Orleans, LA
https://bioxfel.org/events/details/1155

17-21 **Biophysical Society. 62nd Annual Meeting**. San Francisco, CA
https://www.biophysics.org/2018meeting

MARCH 2018

1-14 **Cryoelectron Microscopy**. Cold Spring Harbor, NY
https://meetings.cshl.edu

APRIL 2018

2-6 **MRS Spring Meeting & Exhibit**. Phoenix, AZ
http://www.mrs.org/fall2018

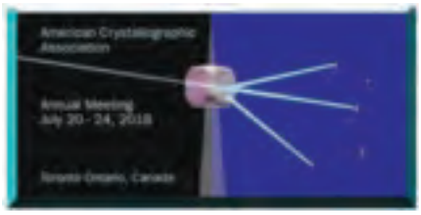
10-13 **BCA Spring Meeting**. University of Warwick, UK
http://ww.bcaspringmeetings.org.uk

22-27 **RapiData 2018**. Menlo Park, CA
http://smb.slac.stanford.edu/rapidata/rapidata-2018

JUNE 2018

1-10 **51st Erice Course: Electron Crystallography** &
52nd Erice Course: Quantum Crystallography. Erice, Italy
http://crystalerice.org

JULY 2018



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

24-28 **ACNS-2018**. College Park, MD
https://www.mrs.org/acns-2018

AUGUST 2018

19-24 **XXVII International Materials Research Congress**. Cancun, Mexico
http://www.mrs.org/imrc-2018

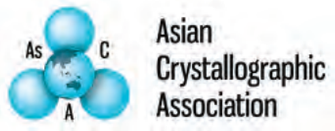
22-27 **31st European Crystallographic Meeting**. Oviedo, Spain
http://ecm31.ecanews.org

OCTOBER 2018

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

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

DECEMBER 2018



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

JULY 2019

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

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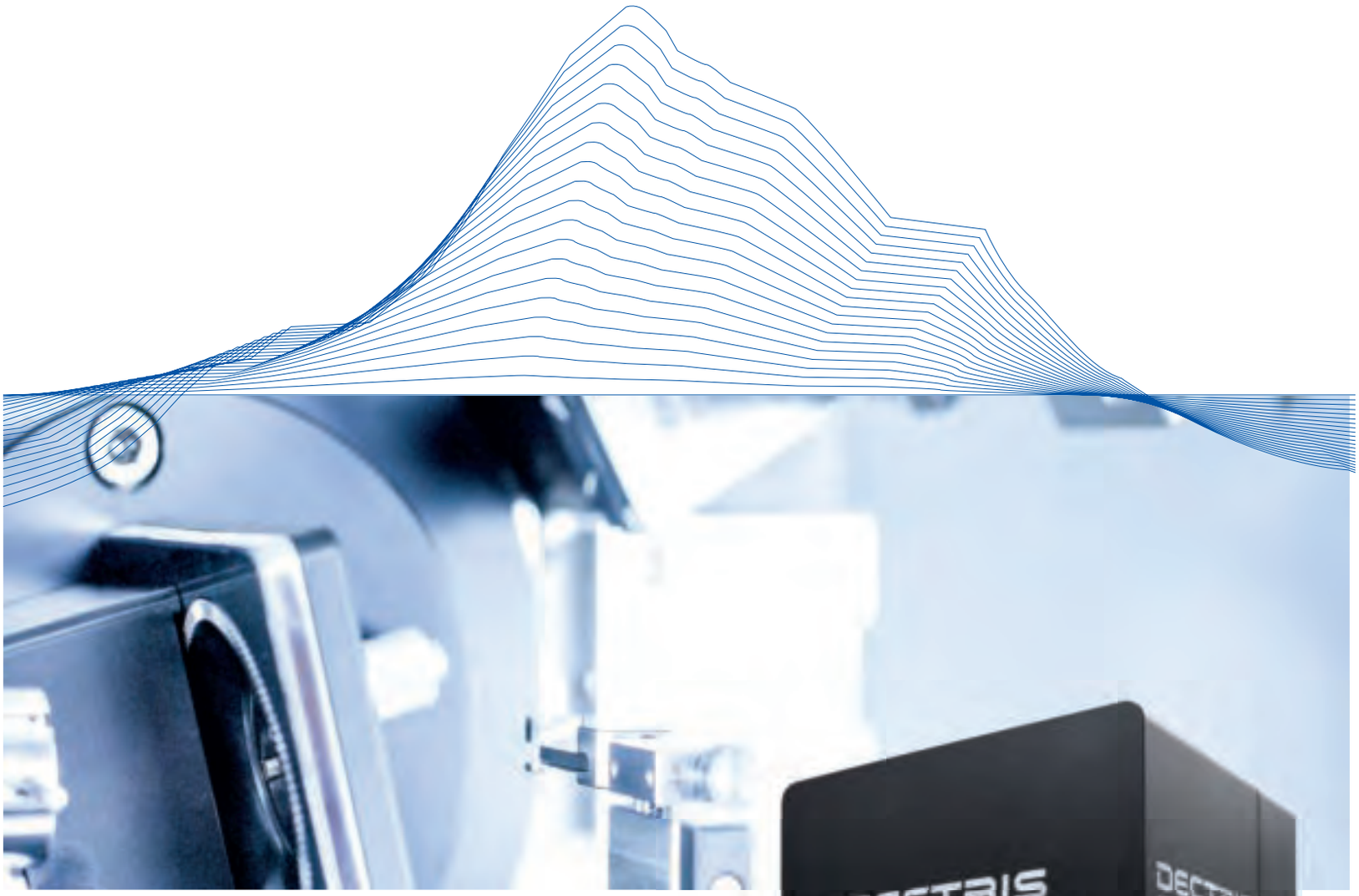

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ACA President

Sir James Fraser Stoddart
Special Opening Plenary Lecturer in New Orleans

What's on the Cover. The image is from Zbigniew Dauter, who received the 2017 Patterson Award at the ACA Annual Meeting in New Orleans. See p. 10.

Contributions to ***ACA RefleXions*** may be sent to either of the *Editors*:

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Thomas F. Koetzle ..... tkoetzle@aol.com

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

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President's Column

Amy Sarjeant

Dear Colleagues,

With our annual meeting long past, I'm sure many of us have been able to exhale a little and enjoy a lazy day or two of summer. I've always liked the peaceful time on campus in the summer: more parking, shorter lines for coffee, and the quiet industry of students focused on research. But, like most of you, my life is never peaceful for long. Soon after New Orleans, I headed off adventuring in the realm of structural chemistry.

Shortly after returning from the ACA meeting, I was off again to the **Midwest Organic Solid State Chemistry Symposium**, or MOSSCS for short, at Kansas State University. This informal, student-focused meeting has its roots at the University of Illinois, starting out there in 1988 as a retirement celebration for David Curtin. At this year's Symposium I thoroughly enjoyed the presentations of the students, who were passionate about their research. The informal atmosphere led to a lot of great discussions, both scientific and not, among all the attendees. I came away truly inspired by the science, and pleased to note that many of the organizers and attendees – both past and present – are active members of the ACA community.

After a few days at home to re-pack my bags, I headed out again, this time to the **ACA Summer Course in Chemical Crystallography,** held at Northwestern University. It was a delight to be back on campus and to see how the X-ray Crystallography facility has changed in the two years since my departure. But of course the real pleasure was in helping the class of 26 attendees who came for an intense week of chemical crystallography. I'm eternally grateful to my co-organizers Allen Oliver, Charlotte Stern and Christos Malliakas for keeping the show on the road, to all the instructors who volunteer their time and expertise to make this such an informative and rewarding experience for the students, and to all our sponsors whose donations keep the course running. We send around a survey to the participants every year, and it's a joy to read the comments that come back. Especially ones like this, "The course was an incredible experience that I will carry with me for the rest of my life. Course material and instructors were phenomenal. I'm very thankful for this opportunity." However, the best part of the summer school comes years afterwards when I see alumni presenting their work at ACA meetings.

After the ACA Summer Course, I've had about a month off from traveling leading up to the **IUCr Congress** in Hyderabad, India. As of this writing (mid-August) the IUCr has yet to happen, but the enthusiasm for crystallography is clearly building in advance of this much-anticipated event. I hope I will be seeing many of you there!

But enough about me. What about you? What do crystallographers and structural scientists get up to in the summer? Folks at the APS have been busy hosting a symposium on drug discovery in recognition of 25 years of pharmaceutical research at the synchrotron, as well as the **CCP4 Workshop** and the **National School on Neutron and X-ray Scattering**. I know several of my colleagues hightailed it up to Canada to attend the 100th meeting of the **Canadian Society for Chemistry** (CSC) just after our annual meeting. Jim Britten ran his **Chemical Crystallography Workshop** and Louise Dawe hosted the **4th Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec** (CEMWOQ-4, for short) in the lead-up to the CSC meeting. Once again, two long-standing ACA members spreading the word about crystallography to the broader community of structural scientists!

In addition to spreading the word of crystallography like a scientific Johnny Appleseed, members of Council are still hard at work on the business of ACA. We met briefly in Buffalo over the summer to work through several issues we're facing with our transition. We're pleased to say that both our CFO and CEO, Rao and Bill, will be staying on board for the next few years. We've been investigating website and membership database options. Thanks to all the donations to the website fund, we should be able to see some real improvements on our site. We continue to work with AIP to make sure we get the most out of our relationship with them (see the article beginning on p. 53 for more details).

I hope your summer has been relaxing and productive and that you are ready to tackle the newest challenges of structural science this Fall.

Amy Sarjeant

RefleXions from Canada

Tomislav Friščić

As I write this, we have just returned from the **24th Congress & General Assembly of the IUCr** that took place August 21-28 in Hyderabad, India. It has been a busy and event-packed meeting for everyone, and the Canadian delegates have been no exception. Two Canadians were keynote speakers at the meeting: **David Bryce**, U Ottawa, one of the pioneers of the emergent area of NMR Crystallography, a topic that he addressed in his lecture *Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables*; and **Farideh Jalilehvand**, U Calgary, who is an expert in speciation of sulfur and metal species in biologically-relevant environments, a topic that she presented in her lecture *X-ray absorption spectroscopy and chemical speciation: from archaeology to biology*. At the IUCr Congress, Farideh also co-chaired a workshop dedicated to **X-Ray Absorption Spectroscopy for the Crystallographer**.

It therefore appears particularly suitable to highlight these eminent speakers in this, and in coming editions of ***RefleXions from Canada***. Here I start with David Bryce, currently Full Professor and University Research Chair in Nuclear Magnetic Resonance at the University of Ottawa, and the Chair of the Department of Chemistry and Biomolecular Sciences. He earned his B. Sc. (Hons) in Chemistry in 1998 from Queen's University (Kingston, Ontario), followed by a Ph.D. in 2002 from Dalhousie University, where he worked with Rod Wasylishen. Following postdoctoral work with Ad Bax at the Laboratory of Chemical Physics at NIH, David took up a faculty position in his home

Fig. 1: (left) David Bryce and Yijue Xu discuss the results of some mechanochemical milling experiments; (right) L-R: Cesar Leroy, Patrick Szell, and David Bryce get ready for some NMR crystallography.

city of Ottawa in 2005. His current research interests include solid-state NMR spectroscopy of low-frequency quadrupolar nuclei, NMR studies of materials, NMR crystallography, halogen bonding, mechanochemistry, and quantum chemical interpretation of NMR interaction tensors. His group (Fig. 1, above) has authored NMR software products downloaded >500 times in 25 countries.

The Bryce group are pioneers and promoters of NMR Crystallography, an emergent field that employs NMR spectroscopy data to refine or solve crystal structures. While this hot area of research has strongly focused on the interpretation of ^{1}H chemical shifts, the Bryce group have provided novel contributions and advances by recognizing that the majority of the elements in materials are quadrupolar, and that special experimental and analytical methods are required to use their NMR spectra to their full potential. The group's initial proof-of-principle work focused on simple systems, wherein unambiguous results were achievable (*Phys. Chem. Chem. Phys.* **2009**, *11*, 7120-7122). They followed on by developing a more sophisticated experimental and computational protocol in which structural models of solids can be refined jointly against experimental quadrupolar couplings and a DFT-optimized energy term – as described in examples of their work in *J. Phys. Chem. C* **2012**, *116*, 19472-19482, and *CrystEngComm* **2013**, *15*, 8727-8738. There is particular interest in the use of this methodology for understanding and characterization of pharmaceutical materials, such as polymorphs, and solvates, and this has also been addressed in the group's publications, including *J. Pharm. Sci.* **2012**, *101*, 2930-2940 and *Can. J. Chem.* **2014**, *92*, 9-15. Beyond NMR crystallography, the Bryce group have been active in a wide range of topics, notably for making major, internationally-noticed contributions in utilizing NMR spectroscopy for understanding supramolecular chemistry in the solid state, particularly for studying the behavior of halogen bonds – an area in which they have provided a series of articles describing pioneering studies of the halogen bond with multinuclear solid-state NMR spectroscopy. Historically, NMR spectroscopy of solids has played a key role in the understanding of *hydrogen* bonding, and the Bryce group are now making in-roads in its use in the hot area of *halogen* bonding. In that context, they have reported the first measurement of spin-spin (J) coupling within a halogen bond, and have established a novel reporter on the strength and geometry of these bonds – you can check these out in their paper: *CrystEngComm* **2014**, *16*, 7285-7297. In *J. Am. Chem. Soc.* **2014**, *136*, 6929-6942 they reported how NMR is characteristic of halogen bonds in solids, and utilized DFT approaches to interpret spectroscopic data, revealing a unified NMR description of halogen bonds and hydrogen bonds. These pioneering early steps towards NMR understanding of halogen bonding have led David to join the IUPAC commission on *Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements*.

Besides David and Farideh, there have been a number of Canadian contributions at the IUCr congress in Hyderabad. Louise Dawe tells me that there have been a total of two Keynote Lectures, nine Conference Lectures and twelve Poster Presentations. On top of all these, Canadian contributors have co-chaired four Microsymposia: **Patrick Mercier**, National Research Council Canada, co-chaired the microsymposium **Minerals/gems in Industrial Applications**; **Natalie Strynadka**, U British Columbia, co-chaired the microsymposium **Mechanisms of Bacterial Resistance**; **Louise Dawe**, Wilfrid Laurier U, co-chaired the microsymposium **New Approaches in Crystallographic Teaching**; and **Hanna Dabkowska**, McMaster U, co-chaired the microsymposium on **Crystallography for Space Sciences**.

A list of all these contributions can be found (with cool pictures!) in the carefully assembled and maintained Twitter stream of the Canadian National Committee for Crystallography (CNCC), with the Twitter handle:**@CNC_Crystals**.

For me it was a particular pleasure to contribute a little bit towards the functioning of the IUCr, as a member of the Canadian

Turn to p. 4

Delegation (Figs. 2a,b, below), chaired by Louise Dawe, and including also Pawel Grochulski, Canadian Light Source, and Patrick Mercier. For us it was especially delightful to see Hanna Dabkowska elected (Fig. 2c, below) as the Vice-President of the IUCr – Congratulations Hanna!

Fig. 2 - Canadian Delegates at the 24th IUCr Congress: (a) L-R: Pawel Grochulski, Louise Dawe, Tomislav Friščić, McGill U; (b) L-R: Pawel, Louise, and Patrick Mercier; (c) Hanna Dabkowska (right) moments after being elected IUCr Vice-President.

The representatives of the CNCC also had the opportunity to meet all Canadian contributors to the IUCr Congress during a casual get together at the local Le Cafe. The get together gave us all a fantastic opportunity to meet and chat over a cup of coffee, and to acknowledge the student recipients of the Larry Calvert Travel Awards administered by the CNCC: **Naheda Sahtout** and **Thirumalai Ulaganathan**, U Saskatchewan, and **Jenna Skieneh**, Western U (Fig. 3, below).

Fig. 3: (left) Canadian participants of the 24th IUCr Congress having a good time over a coffee at Le Cafe; (right) Chair of the Canadian Delegation Louise Dawe congratulating the Larry Calvert Travel Award winner Jenna Skieneh.

Again, if you wish to know more about our Canadian National Committee for Crystallography and its activities, a lot of information can be found on the exciting and frequently updated webpage that has been put up and is constantly improved by Louise Dawe: ***http://xtallography.ca/***.

Fig. 4. Logo of the upcoming 2018 Annual ACA Meeting in Toronto from: http://www.amercrystalassn.org/2018-meeting-homepage.

I would like to conclude this brief update from Canadian crystallographers by alerting you to the coming 2018 ACA Annual Meeting (Fig. 4, left) that will be taking place in Toronto, Ontario – with Gerald Audette and Tiffany Kinnibrugh as Program Chairs, as well as Louise Dawe and David Rose as Poster Chairs. For more information, see pp. 58-59.

Hopefully you will all be able to join us in Toronto in July 2018!

So much for now – as always, if you would like me to address or highlight any special topics or events, or if there are activities that I have missed covering, or if you simply want to share stories of Canadian crystallographers, please share them with me by e-mail (***tomislav.friscic@mcgill.ca***), and I will do my best to include them in a forthcoming column.

Best regards from increasingly cold Montreal in October!

Tomislav Friščić

From the Editor's Desk

This issue features reports from the ACA's Annual Meeting in New Orleans. Connie Rajnak has put together the cover and ***What's on the Cover*** (see p. 10) featuring our 2017 Patterson Award winner, Zbigniew Dauter.

Our coverage of the Annual Meeting depends upon the efforts of many people. These include the session organizers and poster prize judges, who have drafted reports. We owe a special thanks to our *ACA RefleXions* Photographer Peter Müller and to Richard Bromund for their fabulous photos, along with our student volunteers responsible for the session group photos coordinated by Vicky Doan-Nguyen, Chelsy Chesterman and Anastasiya Vinokur with assistance from Kristina Vitale.

Our gold open-access journal, *Structural Dynamics*, published jointly by ACA with AIP Publishing, continues to grow and thrive. Majed Chergui, our *Structural Dynamics* Editor-in-Chief, was pleased to have the opportunity to meet many of you in New Orleans.

For additional information on *Structural Dynamics*, see pp. 7-9. ACA members can take advantage of a special discounted rate when publishing their work in our journal!

In this, my final ***From the Editor's Desk***, I want to say how much I've enjoyed serving as your Co-Editor these past four years. We are indeed fortunate that Ed Stevens will be taking over my Co-Editor duties beginning with our Spring 2018 issue. Welcome aboard, Ed! In closing, I would like to thank everyone, including Marcia Colquhoun and the team in Buffalo, and especially my Co-Editor Judy Flippen-Anderson, for all of their invaluable help!

Tom Koetzle

ACA History Project News

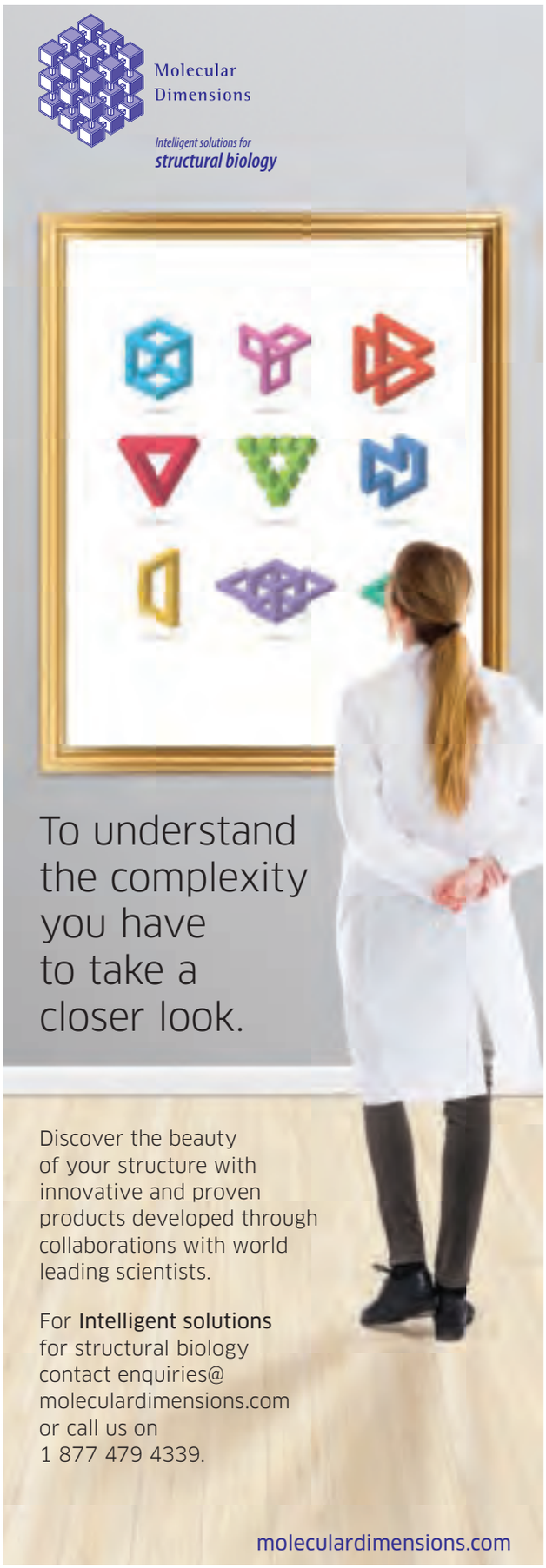
As of August 25, the ACA History webpages have had **207,447** unique visitors in 2017! The average visitor came to the site 1.5 times, and while they were at the site they viewed 2.4 different pages. Clearly, the public is interested in the history of 20th century crystallography as told through memoirs and biographies, ACA award lecture videos, and articles describing the significance of structural science.

In keeping with our aim to encourage more interest in ACA History pages, Webmaster Vanessa Reitz has revamped the ACA History Home page with an appealing, graphic interface. We'd like to hear your reactions to the new design: ***http://www.amercrystalassn.org/history_home***.

Winnie Wong-Ng's full-length Living History autobiography is now online. It describes Winnie's odyssey from China and Hong Kong to the U.S. and Canada, then finally to the National Institute of Standards and Technology (NIST), where the broad scope of her research illustrates the wide variety of questions that can be answered by X-ray diffraction.

Also online now is the video of Elspeth Garman's Fankuchen Award lecture, in which she gives some humorous anecdotes from her "Travels in Protein Crystallography" as well as how she determined the radiation dose maximum for protein crystals. See Elspeth's page for links to her other videos, "From chocolate to drug discovery – what crystallography has done for the world" and "Crystallography one century AD (After Dorothy)."

Virginia Pett
pett@wooster.edu



Net RefleXions

Anastasiya Vinokur

I don't know about you, dear reader, but in the opinion of this young crystallographer, the 2017 ACA meeting in New Orleans was a real blast. It especially was a treat to attend so many sessions that addressed one of the central questions for crystallography (and science in general): that is, how to effectively communicate our work. As reaching the public with good, sound science and engaging a new generation of researchers becomes even more of a hot topic, from a sampling of multiple talks from this meeting on online resources to enhance laboratory modules, effective tweeting, and the values of online tutorials, it is very clear that the web plays an integral role in our pursuits of outreach.

But although there has been a lot of discussion with regard to the content of our websites and tutorials, there was one dimension of web design that we did not address in New Orleans. An all-important aspect of user experience: accessibility. Most of us most likely have never considered how our color choices or font sizes might affect a user with color blindness (which affects 8% of men and 0.6% of women, according to *Wikipedia*) or how a hearing-impaired member of the public can engage with our crystal growing videos. These are the questions that, as responsible web designers, whether amateur or professional, we should ask ourselves so that our websites are not only aesthetically pleasing but also functional.

For example, to reach users with a wider range of seeing abilities, we can insure that our contrast between font and background is at least 7 to 1 and use additional cues besides colors to communicate information such as links for further content. Leaving breadcrumbs (showing the user their progress through the website) could help mentally-challenged site visitors more effectively navigate through our tutorials, and including transcripts of the spoken portions of our videos or providing closed captioning will enhance our reach to users with auditory disabilities.

It may seem like a lot to consider, but luckily there are many resources from tutorials to blog posts to shorthand lists that are available to help improve accessibility of online content. A great starting point on your quest for greater accessibility is the website for Web Accessibility Initiative (***https://www.w3.org/WAI/intro/accessibility.php***), which provides not only solid advice on web design but also includes user experiences that help drive the point about how vital seemingly small design decisions are in narrowing or expanding our web traffic.

Armed with this knowledge, I wish you all the best of luck as you put together new amazing web content. Sadly, this will be my last installment of ***Net Reflexions***. I hope you have enjoyed the column as much as I enjoyed writing it for you, dear reader. It has been a real honor.

Anastasiya Vinokur

Zbigniew Dauter, Senior Investigator at the Macromolecular Crystallography Laboratory and Head of the Synchrotron Radiation Research Section at the National Cancer Institute, received the **2017 Patterson Award** and presented his lecture: *The Patterson Award for a lucky crystallographer* at the annual meeting of the ACA in New Orleans.

The cover image depicts the crystal structure of a fungal CAP protein[1], solved in the laboratory of Oluwatoyin Asojo (Baylor College of Medicine) with the use of selenourea, the novel anomalously scattering reagent introduced by Zhipu Luo, a member of the Dauter lab (see below). In this structure, seven protein molecules pack according to an unusual non-crystallographic 7_5 screw axis.

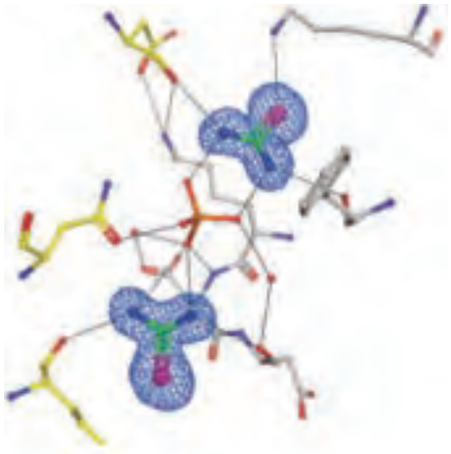
Dauter's research group (a part of the Macromolecular Crystallography Laboratory of NCI) is located at the synchrotron site of Argonne National Laboratory and specializes in biostructural research based on the unique properties of synchrotron radiation. Its high intensity makes it possible to record very high resolution diffraction data, and its wavelength tunability allows recording anomalous diffraction signals of various scatterers used for phasing novel crystal structures of macromolecules. The previously established "quick cryo-soaking of halides" approach[2] has been responsible for a number of crystal structures not amenable for other types of derivatization.

Recently, Zhipu Luo, a member of the lab, introduced a new practical and effective reagent, selenourea[3], which can be soaked for a short time into native crystals of proteins or nucleic acids, providing a significant anomalous signal of selenium atoms. The chemical properties of selenourea molecules differ from other derivatization reagents, as selenoureas can serve both as donors and acceptors of hydrogen bonds formed with polar groups of macromolecules. Selenourea is an effective and easy to use reagent with a potential to gain popularity in the crystallographic practice.

[1] Baroni, RM, Luo, Z, et al., Asojo, OA (2017). Crystal structure of MpPR-1i, a CAP protein from *Moniliophtora perniciosa*, the fungus that causes Witches' Broom Disease in Cacao. *Sci. Rep.*, in press.

[2] Dauter, Z, Dauter, M, Rajashankar, KR (2000). Novel approach to phasing proteins: derivatization by short cryo-soaking with halides. *Acta Cryst.* **D56**, 232-237.

[3] Luo, Z (2016). Selenourea: a convenient phasing vehicle for macromolecular X-ray crystal structures. *Sci. Rep.* **6**, 37123.



At right: The anomalous difference peaks (red), and

at left: The 2Fo-Fc map (blue) of selenourea molecules bound at the surface of a protein.

Contributors to this Issue

Milinda Abeykoon, Alberto Albinati, Oluwatoyin Asojo, Gerald Audette, Christine Beavers, Pierre Becker, Jason Benedict, Herbert Bernstein, Avni Bhatt, Simon Billinge, Bob Blessing, Olaf Borkiewicz, Craig Bridges, Richard Bromund, Stephen Burley, Korey Carter, Jim Ciston, Zbigniew Dauter, Madushani Dharmarwardana, Vicky Doan Ngyen, Martin Donakowski, Roberto dos Reis, Larry Falvello, Jeanette Ferrara, Joseph Ferrara, Jim Fettinger, Barry Finzel, Katrina Forest, Paul Forster, Ben Frandsen, Tomislav Friščić, Frank Fronczek, Allyson Fry-Petit, Sanjit Ghose, Elizabeth Goldsmith, Danielle Gray, Kushol Gupta, Michal Hammel, Kenneth Harris, John Helliwell, Ashfia Huq, Mariusz Jaskólski, Jim Kaduk, Tiffany Kinnibrugh, Mariusz Krawiec, Saul Lapidus, Finn Krebs Larsen, Bernhard Lechtenberg, George Lountos, Krystle McLaughlin, Wladek Minor, Peter Müller, Allen Oliver, Kay Onan, Kate Page, Virginia Pett, James Phillips, Rachel Powers, Przemyslaw Porebski, Daniel Rabinovich, Connie Rajnak, Aaron Robart, Michael Rossmann, Amy Sarjeant, Nicholas Sauter, Carl Schwalbe, Sangita Sinha, Carla Slebodnik, Charlotte Stern, Marian Szebenyi, Joe Tanski, Margarita Tararina, Anastasiya Vinokur, Thomas Weiss, Armin Wagner, Carrie Wilmot, Peter Wood, Wenqian Xu, Victor Young

Pauling Poster Prizes

The Pauling Poster Prize was established by the ACA and is supported by member contributions to honor Linus Pauling, a pioneer in American structural research and a very supportive member of ACA for many years. At each annual meeting up to seven of the best trainee (*postdoctoral*, *graduate* or *undergraduate*) poster presentations receive Pauling awards. Some of the awards consist of a certificate, a $250 prize, and a copy of a Linus Pauling book. Up to three **ACA Pauling Poster Prizes** honor Linus Pauling's contributions to science and U.S. crystallography; the **Herman R. Branson Pauling Poster Prize** recognizes the contributions of Herman Russell Branson, one of the first African American physicists to make crystallography the focus of his research. The **Muttaiya Sundaralingam Pauling Poster Prize** recognizes the ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids done by Muttaiya Sundaralingam and his colleagues. The **Louis Delbaere Pauling Poster Prize** in honor of Louis Delbaere, former Canadian President of the ACA, and sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, is given to the highest ranked *graduate* or *undergraduate* poster from a Canadian laboratory. Finally, the **IUCr Pauling Poster Prize** is sponsored by the International Union of Crystallography and is given to a *graduate* or *undergraduate* poster selected by the committee. The winner of the IUCr Pauling Prize receives complimentary online access to all IUCr journals for one year or a complimentary volume of *International Tables* or other IUCr publication, a copy of *The Little Dictionary of Crystallographic Terms* and an IUCr-2017 polo shirt.

In New Orleans, eligible posters and presenters were evaluated for the Pauling Prize by a panel of 14 judges. Trainees were judged both on the work presented on their posters and on their general knowledge of the subject and crystallography. All posters and presenters were found to be of very high quality, which made the task of determining the best posters very difficult. Following are the winners of the 2017 Pauling Poster Prize, as well as one honorable mention. Photos are shown of winners who were able to attend the conference banquet and accept their awards in person. The majority of the awardees are also shown with their prize-winning posters.

The committee to review posters for the Louis Delbaere Pauling Poster Prize, consisting of Mariusz Jaskólski and Lisa Keefe, reluctantly concluded that there were not enough eligible contenders for a serious competition, and that no presentation qualified for the distinction. The 2017 Delbaere Prize was not awarded.

New Orleans Posters Chair Bruce Noll announcing the Poster Prize presentations at the Awards Banquet

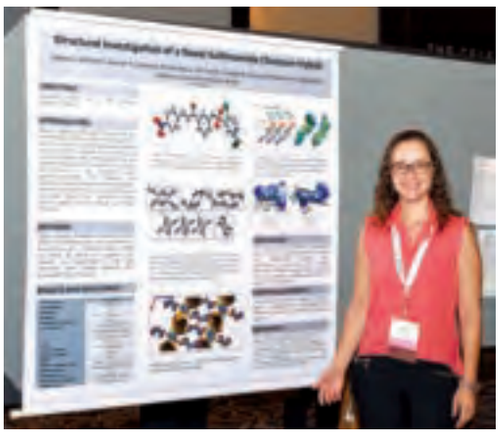
The ACA Pauling Poster Prizes (*presented by Gerald Audette*)

Brinda Selvaraj, Oak Ridge National Laboratory, poster **11-Su**: *Investigation of the Bacteriochlorin rings and its environment in Fenna-Matthews-Olsen antenna complex revealed by neutron and ultra-high resolution X-ray crystallography*.

Brinda Selvaraj, at left, with Gerald Audette

Lidiane Michelini, Universidade Federal de Goiás, Brazil, poster **17-Su**: *Structural investigation of a novel sulfonamide chalcone hybrid*.

L-R: Amy Sarjeant, Lidiane Michelini, Gerald Audette



Lidiane Michelini with her prize-winning poster

Herman R. Branson Pauling Poster Prize (*presented by Allyson Fry-Petit*)

The Branson Pauling Poster Prize was given to **Fiyinfoluwa Adesioye** of the Centre for Microbial Ecology and Genomics in the Genomics Research Institute at U Pretoria, RSA. Her poster **131-Su** was titled, *The crystal structure of a novel Carbohydrate Esterase 7 family esterase from a hot desert metagenome*. The presentation highlighted Fiyin's important work on solving the structure of a novel CE7 acetyl xylan esterase, NaM1. In addition to the structure solution her work encompassed the encoding of

Turn to p. 12

the esterase, chemical synthesis of the gene, cloning, expression, purification, crystallization, and thermal analysis. This research provides an interesting piece in the puzzle of understanding substrate specificities and thermolability in deacetylases.

Fiyinfoluwa Adesioye, at left, accepting the 2017 Herman R. Branson Pauling Poster Prize, presented by Allyson Fry-Petit

Fiyinfoluwa Adesioye with her prize-winning poster

Honorable Mention – **Kartik Manne**, U Alabama at Birmingham, poster **5-Su**: *Structural biology of proteins responsible for biofilm regulation and dispersion*.

L-R: Kartik Manne, Amy Sarjeant, Allyson Fry-Petit

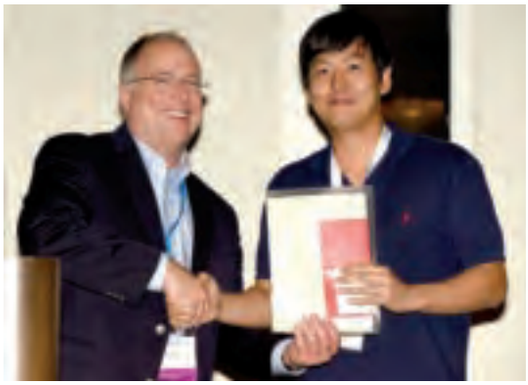
Muttaiya Sundaralingam Pauling Poster Prize (*presented by Christopher Colbert*)

Ashley Campbell, U Missouri, poster **29-Su**: *Trapping conformational states of the SidA ornithine hydroxylase in crystallo*.

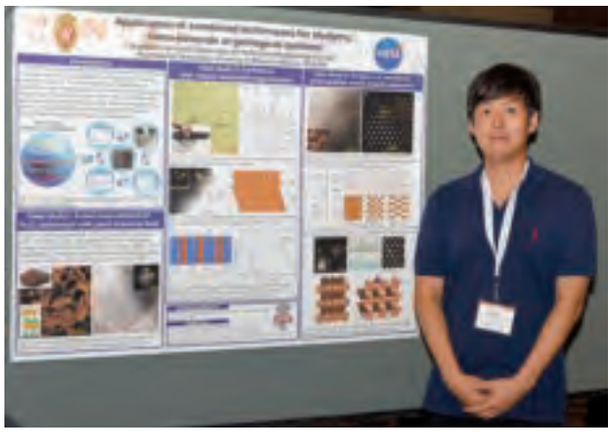
Ashley Campbell, at right, with Christopher Colbert

IUCr Pauling Poster Prize (*presented by Bruce Noll for Frank Fronczek*)

Seungyeol Lee, U Wisconsin – Madison, poster **23-Su**: *Application of combined techniques for studying nano-minerals in geological systems*.



Seungyeol Lee, at right, with Bruce Noll



Seungyeol Lee with his prize-winning poster

Gerald Audette

Structural Dynamics Poster Prize

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

The winner of the Structural Dynamics Poster Prize at ACA 2017 was **Nicholas Keul** from Athens, Georgia for his poster **40-Sa**: *The role of intrinsic disorder in human uridine diphosphate glucose dehydrogenase*.

Nicholas Keul, at right, with John Helliwell

Nicholas Keul with his prize-winning poster

Nicholas is in the fourth year of his graduate program of research at U Georgia. Building on open and closed form crystal structure knowledge of the enzyme he combined mutagenesis and biophysical characterization methods to show that a disordered functionally important tail of the polypeptide acted as what he vividly called a "Brownian motion antenna."

The various candidate posters were of a very high quality. The Editor-in-Chief of *Structural Dynamics* Majed Chergui was very impressed by these and by the winning poster especially.

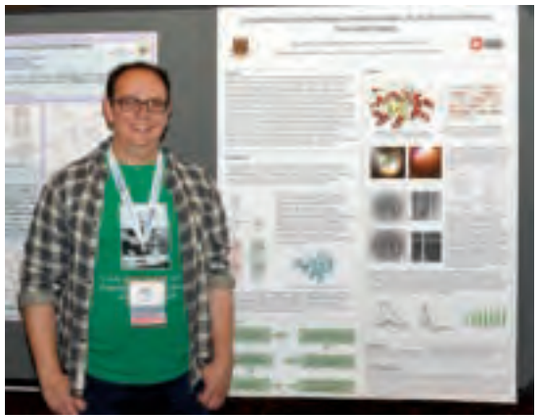
John Helliwell

RCSB Protein Data Bank Poster Prize

The **RCSB (Research Collaboratory for Structural Bioinformatics) Protein Data Bank Poster Prize** recognizes a student, *graduate* or *undergraduate*, poster presentation involving macromolecular crystallography. The award consists of two educational books, and the winner is acknowledged in the RCSB web site and newsletter. This year there were six entrants to be judged by a committee consisting of Marian Szebenyi, Jan Abendroth, and Greg Hura.

The winner was **Miguel Torres** (with co-authors Mehran Dastmalchi, Peter Facchini, and Kenneth Ng), a graduate student at U. Calgary, Canada, for his poster **110-Su**, *Crystallization and preliminary structural studies of an aldo-keto reductase from opium poppy*. Miguel clearly has a talent for making good posters, as he won the same award at the Denver meeting (the judges had no idea!).

Miguel Torres, at right, with Marian Szebenyi



Miguel Torres with his prize-winning poster

The judges also recognized **Makayla Anderson** (and co-authors David Roberts and Jacqueline Roberts), of DePauw U, with an Honorable Mention for their poster **113-Su**, *Unique crystal structures of an SmtB/ArsR transcriptional factor from Methanosarcina acetivorans*. The project described in the poster represents dedicated work by a succession of undergraduate students, of whom Makayla is the latest.

Marian Szebenyi

L-R: Marian Szebenyi, Makayla Anderson, Bruce Noll (at rear)

CrystEngComm Poster Prize

CrystEngComm, published by the Royal Society of Chemistry, is aimed at the materials, chemistry, crystallographic, and crystal engineering communities and is committed to, "covering all aspects of crystal engineering – the design, including synthesis of crystals and crystal growth, synthesis and evaluation of solid-state materials with desired properties." The RSC sponsors the **CrystEngComm Prize** for, "the best student, graduate or undergraduate, poster presentation in the area of crystal engineering/supramolecular chemistry." This year's judging committee for the *CrystEngComm* Poster Prize was Christine Beavers and Tony Hu.

The 2017 winner of the CrystEngComm Prize is **Raúl Castañeda**, New Mexico Highlands U. Raúl's poster **13-Sa**: *Co-crystals of dithieno[3,2-a:2',3'-c]phenazine derivatives and trimeric perfluoro-ortho-phenylene mercury* described his work with a series of co-crystals. His goal was to determine the structural ramifications of functionalizing one component

Raúl Castañeda, at right, with Christine Beavers

Raúl Castañeda with his prize-winning poster

with various halogens or substituting a pyridyl ring in place of a phenyl. Starting with dithienophenazine (DTPhz) and trimeric perfluoro-ortho-phenylene mercury (TPPM), he did not observe any co-crystallization. He was able to observe two distinct 1:1 co-crystal structure types, once the DTPhz was functionalized with halogens, and intriguingly, a non-centrosymmetric structure resulted when the halogen was fluorine. The pyridyl substituted DTPhz did co-crystallize with TPPM, but this structure also incorporated a water molecule. As Raúl stated in his abstract, the focus of this study was to understand how, "small changes in substituents [can] give a variety of packing motifs and interactions." The judging committee for the poster prize felt that Raúl's poster was well presented and fit nicely within the scope of *CrystEngComm*. We congratulate Raúl for his achievement!

Christine Beavers

Taylor & Francis Biomolecular Crystallography Poster Prize

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

The 2017 prize was awarded to **Sharrol Bachas** from Adrian Ferré-D'Amaré's lab at National Heart, Lung, and Blood Institute, NIH, Bethesda for his poster **112-Sa**: *Induced fit in the specific recognition of transition metal ions by a gene-regulatory RNA*. Sharrol presented a crystallographic analysis of alternative metal ion recognition by yybP-ykoY riboswitches. Proper data collection strategy, and challenging and rigorous structure determination

Sharrol Bachas, at right, with Przemyslaw Porebski

Sharrol Bachas with his prize-winning poster

and refinement allowed him to observe a flexible binding site that adopts variable coordination schemes with different metal ions. Sharrol demonstrated that the analogous mechanism is employed by gene-regulatory proteins functioning in the same pathway as the yybP-ykoY riboswitches.

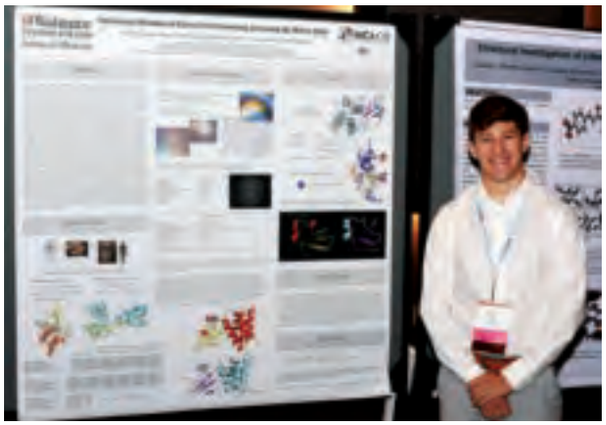
Przemyslaw Porebski

MiTeGen - Society of Physics Students Undergraduate Poster Prize

The **Undergraduate Poster Prize**, co-sponsored by the AIP Society of Physics Students (SPS) and MiTeGen, was established in 2014 to recognize the best undergraduate poster presentation at ACA. The recipient of this award receives a $250 cash prize, generously donated by MiTeGen and SPS, along with a gift card for crystallographic supplies though MiTeGen.

This year's winner was **Garrett Ginell** from Cornell College for the excellent presentation of his research on poster **129-Su**: *Structural studies of Ebola viral homolog encoded by Microbats*.

Garrett Ginell, at left, with Krystle McLaughlin



Garrett Ginell with his prize-winning poster

Structural Dynamics Editor-in-Chief Majed Chergui, at left, with George Phillips at the Structural Dynamics booth.

Editor's note: Photos in the **Poster Prizes in New Orleans** section are by Peter Müller.

The judges also would like to give honorable mention to another presenter, **Makayla Anderson**, DePauw U, for poster **113-Su**: *Unique crystal structures of an SmtB/ArsR transcriptional factor from Methanosarcina acetivorans*. Makayla also received honorable mention in the **RCSB Protein Data Bank Poster Prize** competition, see p. 13. The judges for the 2017 Undergraduate Poster Prize were Krystle McLaughlin and SPS Director Brad Conrad.

We hope that this prize continues to inspire and encourage young undergraduate researchers in the field of crystallography.

Krystle McLaughlin

Oxford Cryosystems Low Temperature Poster Prize

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

This year's winner of the Oxford Prize was **Carlos Pinheiro**, Universidade Federal de Minas Gerais, Brazil, for his poster **19-Sa**: *Hard X-ray-induced valence tautomeric interconversion in cobalt-o-dioxolene complexes*.

Carlos Pinheiro, at left, with Bruce Noll

2017 Poster Prize Winners, L-R: back row – Sharroll Bachas, Miguel Torres, Posters Chair Bruce Noll, Raúl Castañeda; front row – Garrett Ginell, Fiyinfoluwa Adesioye, Lidiane Michelini, Seungyeol Lee. Not shown – Ashley Campbell, Nicholas Keul, Carlos Pinheiro, Brinda Selvaraj.

The ACA's **67th Annual Meeting** kicked off in New Orleans on Friday, May 26, 2017 with four full-day workshops: a **CSD Workshop – Communication and Innovation**, along with workshops on **CrysAlisPro and Olex2: From Raw Data to Publication**, **Introduction to PHENIX for Beginning and Advanced Crystallographers**, and **Research Data Management**. The latter workshop continued into early evening with a technical sub-session on high-performance computing and networking issues. A **First Time Attendee and Student Meeting Orientation** was held Friday evening. This was followed by a **Special Plenary Lecture** by **Sir James Fraser Stoddart**, 2016 Nobel Laureate in Chemistry. The **Opening Reception Exhibit Show**, generously hosted by the exhibitors, capped off the evening. Reports from the **Workshops** and from this year's **Travel Award Winners** will be featured in our winter issue of *ACA RefleXions*. Watch also for upcoming coverage of Fraser Stoddart's lecture, including Tomislav Friščić's interview with Sir Fraser.

The **Patterson Award** for 2017 was presented to **Zbigniew Dauter**. **Helen Berman** received the **David Rognlie Award**, **Christine Dunham** received the **Margaret C. Etter Early Career Award**, and **James O'Brien** was honored with ACA's **Elizabeth Wood Science Writing Award**. Dauter's Patterson award-winning work is featured on our cover (see also ***What's on the Cover*** on p. 10). The **ACA Transactions Symposium**, *Going beyond PX with cryo electron microscopy, tomography, and diffraction*, was chaired by **Stephen Burley** and **Michael Rossmann**.

The meeting wrapped up Tuesday evening with ACA's annual **Awards Banquet**. The evening's program chaired by ACA President, **Amy Sarjeant**, included the presentation of the **ACA Fellows – Class of 2017**: **Marilyn Olmstead** and **Brian Toby**. The ACA honored this year's 11 **Poster Award Winners** along with two students selected to receive honorable mention from among the exceptional array of posters presented at the meeting (see pp. 11-15 for news on the ***Poster Prizes in New Orleans***). This year's awards banquet program featured a fascinating talk by our Wood award-winner James O'Brien, who regaled us with his *Tales of famous mad hatters* spanning five centuries. To cap off the evening, we were treated to entertainment by New Orleans band, Dr. Jazz.

Yulia Sevryugina and **Ilia Guzei** were **Program Chairs** for the meeting; **Bruce Noll** was **Posters Chair**; **Chelsy Chesterman**, **Vicky Doan-Ngyen** and **Anastasiya Vinokur** coordinated the **Session Photos** with assistance from ACA's **Kristina Vitale**; and **Richard Bromund** and **Virginia Pett**, ACA's **Videography Team**, recorded the award lectures and the Stoddart interview. AIP Publishing's **Robert Finnegan** did his usual great job with the **Exhibit Show**.

Bill Duax, at left, and Tom Terwilliger at the opening reception exhibit show Friday evening

L-R: Wesley Vaz, Lidiane Michelini, and Carlos Pinheiro discussing a point during the Monday evening poster session

James O'Brien, a/k/a The Mad Hatter, delivering his talk at the awards banquet

Sir Fraser Stoddart delivering his opening plenary lecture

Brian McMahon and Virginia Pett

Anthony Solis and Jessica Hoy of AIP Publishing

Photos by Richard Bromund or Peter Müller. New Orleans meeting logo design: Kandis Elliot

Wood Award Winner James O'Brien Entertains New Orleans ACA Awards Banquet Crowd with Tales of Famous Mad Hatters

ACA President Amy Sarjeant presenting James O'Brien with the 2017 Elizabeth Wood Science Writing Award. Photo by Peter Müller.

Attendees of the 2017 ACA **Awards Banquet** in New Orleans got a real treat. Forgoing a more general talk about ways to present science in an accessible manner, this year's **Wood Award** recipient, **James O'Brien**, Missouri State U, gave a stellar example of such an effort when he gave a talk on the fascinating, colorful history of the "Famous Mad Hatters."

O'Brien has been part of the Missouri State Chemistry faculty for 35 years. He has won multiple awards for his teaching and research and was named Distinguished Professor in 2002. Beyond the academic arena, O'Brien is no stranger in sparking interest in science among non-scientists. He uses his passion for history and literature to reach a wider audience. An avid Sherlockian, in 2013 O'Brien published *The Scientific Sherlock Holmes*, where he explored the chemistry, forensic science, and botany utilized by everyone's favorite detective to solve various crimes.

For the ACA, O'Brien presented his lecture on the historical victims of mercury poisoning. From Thomas P. "Boston" Corbett, who killed John Wilkes Booth, to the first tsaritsa Anastasia Romanovna, to even Sir Isaac Newton, the presented list of victims of mercury poisoning was truly illustrious. O'Brien delivered an engaging account of the various forms of mercury and its early medical uses (mainly to cure syphilis) and industrial purposes (for hat making), as well as the common symptoms of mercury poisoning, all entwined with the personal histories of famous men and women. It was truly an artful blend of history, chemistry and medicine.

From O'Brien's talk, not only did we learn to appreciate the medical advances of the 21st century and workplace safety regulations, but also how our hobbies and passions can make us better ambassadors for science!

Anastasiya Vinokur

Scenes from the Awards Banquet

Christopher Colbert and Erica Saphire. Photo by Richard Bromund.

Krystle McLaughlin. Photo by Peter Müller.

Luo Yoyo, center, dancing with Anna Gardberg, at left, and Sangita Sinha, at right. Photo by Richard Bromund.

L-R: top row – Jeffrey Lovelace; Ed Stevens; Hanna Dabkowska and Marvin Hackert; second row – Irina Kriksunov and Jeney Wierman; Tomislav Friščić; third row – Bill Duax and Sue Byram; James Holton and Ana Gonzalez; bottom row –Stephan Ginell, Garrett Ginell and Lisa Keefe; Carl Schwalbe. Photos by Richard Bromund or Peter Müller.

Their ACA Family Turned Out in Force to Celebrate with Jeanette Krause and Allen Oliver on Sunday Afternoon in Storyville Hall at the Hyatt. The Newlyweds Continued Celebrating throughout the Week.

Photos by Richard Bromund or Peter Müller.

Zbigniew Dauter Receives 2017 ACA Patterson Award

Amy Sarjeant presenting the Patterson Award for 2017 to Zbigniew Dauter. Photo by Peter Müller.

Describing himself in his lecture title as a very lucky crystallographer, **2017 ACA Patterson Award** winner **Zbigniew Dauter**'s immediately humble approach resonated warmly with his highly appreciative audience. Many decades of experience in crystallography formed the time line for his talk and of his incisive contributions to new diffraction methods in crystallography, also then resonating with the Patterson Award descriptor itself. Zbigniew paid tribute to the rigorous science training he had received in Poland where he studied chemistry in the Technical University of Gdansk and received an M.Sc. there in 1971. He undertook a Ph.D. under the supervision of Professor Zofia Kosturkiewicz of the University of Poznan and was awarded his Ph.D. by the Technical University of Gdansk on the crystal structure studies of the antitumor derivatives of acridine.

A chance meeting at an Erice School of Crystallography led to a Post Doc job offer for Zbigniew in 1981 with Michael Woolfson in York University, UK. In 1983 he moved across the campus from Physics to the Chemistry Department to work with Guy and Eleanor Dodson. Overnight use was made of the York computer by Zbigniew and his close colleague Zygmunt Derewenda, also working at York, which they had decided was the most effective for their calculations. This stay in York Chemistry included a memorable meeting with Max Perutz, who described how alligators are able to stay under water for relatively long periods of time, based of course on the 3D structures of hemoglobin. While in York, Zbigniew worked on the cadmium and mercury derivatives of insulin in what he referred to as his favorite space group *R*3.

More luck occurred for Zbigniew with an offer of a job in 1985 at the EMBL Hamburg Outstation where Keith Wilson had recently been appointed Head of Outstation. A key development was the image-plate scanner by Jules Hendrix and Arno Lentfer, also in Hamburg. Zbigniew energetically saw the new opportunities it presented on the beamline for protein crystallography. A stream of new studies at atomic resolution became possible, and new collaborations were joined with George Sheldrick in an exciting phase of Zbigniew's already by now internationally recognized research career.

After nine years and a short period back in York, Alex Wlodawer tempted Zbigniew to the USA to work for the NIH at the NSLS in Brookhaven where he would run X9B. A study provocatively entitled, *Can the anomalous signal of sulfur become a tool for solving protein crystal structures?*, published in *J. Mol. Biol.* (1999) caught the wide interest of the protein crystallography community. Working with his wife Miroslawa their publication on the halide soaking method, either sodium bromide or sodium iodide, published in *Acta Cryst.* (2000), proved to be very effective as a new phasing method, there being several hundred structures in the PDB that have used this method so far alone. The theme of ultra-high resolution, with its important impacts in biological chemistry started in Hamburg, continued with a study of Z-DNA at 0.55 Ângstrom resolution that was published in *Nucleic Acids Res.* in 2011. Other examples described by Zbigniew included a complex case of pseudosymmetry undertaken with Joanna Sliwick and Mariusz Jaskólski and most recently introducing a new phasing compound, seleno urea, in work with Zhipu Luo. In an overview of the sources of satisfaction in his career Zbigniew highlighted the chances there were at synchrotron facilities for him to meet many people.

Zbigniew concluded his talk with a tribute to his wife Miroslawa. There were appreciative tributes from many members of the audience to Zbigniew after his lecture and who also inquired as to his thoughts on several topics. He commented on synchrotron radiation crystallography data collection and processing, remarking that these days it is fast, perhaps only taking minutes, but that people could be less than competent in methods. Zbigniew's sage advice was to take time and not rush. On the excellent training that he had received in Poland he again paid tribute to his Ph.D. supervisor, Professor Zofia Kosturkiewicz, who was also a demanding supervisor. In addition the crystallography schools, such as at Erice, were excellent. There was also a high level of rigorous teaching in the Polish schools in mathematics, physics and chemistry. In a memorable remark for all present Zbigniew affirmed that, "Data collection is a scientific process, not a technicality."

John Helliwell

ACA Honors Helen Berman with Rognlie Award

Helen Berman was the first recipient of the newly established **ACA David Rognlie Award** (see below), recognizing "an exceptional discovery or technical development of particularly high impact in any area of structural science." Indeed, it would be hard to find anybody else who has had higher impact on the structural science of macromolecules than Helen, taking into account her outstanding achievements in the fields of crystallography, nucleic acids, proteins, and their systematics.

Helen was initiated into protein crystallography as a student in the laboratory of Barbara Low, and then graduated from the lab of George Jeffrey in Pittsburgh, working on structures of sugars. There she became, in her own words, "enamored of computing," as applied to various structural problems. After a number of years at the Fox Chase Cancer Center in Philadelphia, Helen moved to Rutgers University as a Professor of Chemistry, where she educated a large number of young structural biologists and recently "actively" retired.

Amy Sarjeant, at left, with Helen Berman holding her Rognlie Award. Photo by Peter Müller.

Helen published several hundred publications on structures of various proteins and nucleic acids, their classification, and biological function. In 1971 she was, together with Walter Hamilton, Tom Koetzle, and a few others, one of the initiators of setting up the Protein Data Bank as a repository for protein structures, at first with only seven atomic models. Eventually, her greatest service to the community was her leadership of the PDB, undoubtedly the most important resource of knowledge in biology, which Helen led through over 15 years, when it grew to contain more than 130,000 entries.

In her award talk, Helen first presented the most important events in the history of the PDB, from its inception, through the formulation of data standards and deposition guidelines for scientific journals, establishment of the wwPDB in three sites (Rutgers, Cambridge, and Osaka), requirement of deposition of experimental data (e.g., structure factors), and provision of a wide variety of practical search and analysis tools for PDB users.

Next, Helen discussed the future challenges that PDB will face in the coming era of integrative biology, where diverse kinds of hybrid information and data from various biostructural techniques, such as crystallography, NMR, electron microscopy, small-angle scattering, or bioinformatics need to be stored and analyzed. Mechanisms for processing and presentation of such integrative entries have to be developed, since these types of hybrid entries are expected to grow in the near future, as very large complexes and molecular machines require application of several methods for comprehensive analysis of their structure and function. Members of the wwPDB and community groups are currently actively discussing the best ways to tackle this and some other problems awaiting the PDB, in order to make sure that it will continue to be the most useful and comprehensive repository for the biomedical community.

In her memoir Helen once said that her dream was, "to understand biology and medicine at the molecular level so that it will be possible to circumvent the errors of our genes." Her achievements, full of "exceptional discovery and technical development," have very substantially advanced the fulfillment of that dream.

Dave Rognlie

The David Rognlie Award is named to honor a much loved longtime member of the American crystallographic community, the founder of Blake Industries that was the sole supplier of Huber equipment in North America; equipment that forms the basis of so many X-ray synchrotron beamlines. Many remember Dave as an ever-present fixture at ACA and other crystallography meetings, charming the visitors to the Blake booth in the exhibition with his warm smile, laughter, and excruciating metal puzzles. Dave grew up in a small northwestern Minnesota village, Climax, pop 250. An outstanding student and athlete, he financed his way through college by working summers as a farm hand and "bussing dishes" along with a four-year scholarship from a regional lumber company, graduating from the University of North Dakota with a degree in electric engineering. Dave cut his teeth with 10 years (to the day) of employment at GE before leaving to found Blake. Why the name Blake Industries? It was the maiden name of the wife of his founding partner, who dropped out before the company got going! Learning business at the knee of his Swedish maternal grandfather, who ran an implement dealership where all transactions were verbal (with phone and electricity rare) along with a handshake, he carried these principles to Blake, where many of us remember Dave personally delivering the equipment and supervising the installation. He continued well beyond retirement age because, he would say, "I just love what I do," meaning coming to meetings and engaging and enabling the enthusiasm and enterprise of scientists old, and especially, young. Dave will be remembered with fondness by all those who knew him. But through the Rognlie Award, he will also be honored so that future generations of crystallographers become acquainted with his name through the title of the award, but more importantly through the citation of the award itself, to the values he believed in and embodied in his life: his generosity of spirit, optimism, selflessness, and unstinting desire to help others to succeed in their endeavors.

Zbigniew Dauter
Simon Billinge

Helen Berman. Photo by Richard Bromund.

Christine Dunham Receives Etter Award

Amy Sarjeant presenting the Etter Award for 2017 to Christine Dunham. Photo by Peter Müller.

The **Etter Early Career Award** for 2017 was presented to **Christine Dunham**, Assistant Professor in the Emory University School of Medicine's Department of Biochemistry. 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.

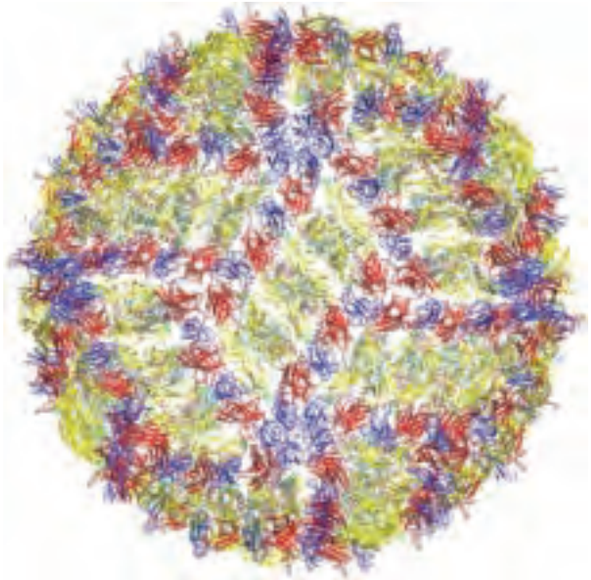
Christine was honored for her impressive work, featured on our spring 2017 cover, which included X-ray crystallography and cryogenic transmission electron microscopy (cryo-EM) to resolve structures of ribosomes and bacterial toxins. In addition to her innovative research, Christine has been dedicated to training and mentoring undergraduate and graduate students to be the next generation of crystallographers. The **Etter Symposium for Young Scientists, Session 4.1.1**, immediately followed Christine's award lecture on Tuesday morning (see p. 41).

Vicky Doan-Nguyen

ACA Transactions Symposium: Going Beyond PX with Cryo Electron Microscopy, Tomography, and Diffraction

This year's **ACA Transaction Symposium** concerned itself with what has become known as the "Resolution Revolution." Structural crystallography of biological substances has been overwhelmed by the growing importance of electron microscopy during the last two or three years. Two factors have contributed to this amazing turn of events. One of these is the sudden development of direct electron counting detectors (DEDs) for use with electron microscopes, and the other is the gradual development of techniques to turn the collection of many thousands of images of a randomly oriented molecule into three-dimensional structure. Each image is a projection of the molecule. Thus if the relative orientation of these images can be determined, then it is not difficult to combine all these images into a three-dimensional structure. However, until recently such structures could not be much better than about 25 Å resolution. Nevertheless that was very useful as most large biological assemblies cannot be crystallized but these "low" resolution electron potential maps could be fitted with the structure of the component molecules determined by X-ray crystallography to give "pseudo atomic resolution" structures of, for instance, viruses and molecular motors that drive bacterial motion. However the advent of the DEDs allowed not only a more accurate response to electrons, but also a very fast read-out that took no more than 1 millisecond – a time shorter than most gravitational or electromagnetic variations. Thus the cryo-EM images could be corrected for motion between successive image records, removing much of the blur that had been typical of most EM observations. As a result in the last two or three years there have been numerous structure determinations, with resolution limits better than 3 Å, of objects whose structure and functional mechanism had heretofore been a mystery.

The meeting opened with **Stephen Burley** (Co-organizer, Rutgers U) giving a short explanation of the events that were changing the biological landscape from the perspective of the RCSB Protein Data Bank. Then **Michael Rossmann** (Co-organizer, Purdue U) followed, describing the structure of Zika virus whose near atomic resolution structure determination



Atomic model of Zika virus. Figure courtesy of Michael Rossmann. Adapted from Sirohi et al., SCIENCE 352: 467 (2016).

had been achieved in about one month. The significance of this structure (see figure above) was not only because Zika virus infections have become a major world health concern, but also because the structure of the homologous structures of other similar flaviviruses (e.g., dengue and West Nile) had been determined previously by a combination of low-resolution electron microscopy and atomic resolution X–ray structures of the component proteins, thus justifying the earlier indirect pseudo atomic methods and demonstrating the far greater speed and simplicity of the new cryo technology.

There followed a variety of examples of the power and versatility of the new cryo-EM technology. **Peijun Zhang**, U Oxford and Diamond Light Source, UK, described the structure of dynamin; **Yuan He**, Northwestern U, and **Seth Darst**, Rockefeller U, showed structures of RNA polymerases; **Hong Zhou**, UCLA, described the structure of a bacteriophage RNA genome; **Shikebi Watanabe**, Johns Hopkins U, showed the structure of neuronal

synapses; and **Wah Chiu**, Baylor College of Medicine, reported on recent high-resolution structure determinations and discussed the importance of validation of both EM image/density map data and structural models derived therefrom.

Most impressive of all for the ACA audience, **Maryam Khoshauer**, MPI, Martinsried, Germany, described a 3.2-Å resolution structure determination of hemoglobin (MW 68KDa). The hemoglobin tetramer is so small that conventional single-particle EM techniques fail to find the orientation of the molecules. However, with the addition of a "phase plate" to increase contrast, this has now been possible. Hemoglobin was one of the first two proteins whose structure had been determined. Thus now there seem to be few limits on where cryo-EM can improve, extend and open new vistas.

In addition there were talks on the new technology. In particular, **Wolfgang Baumeister**, MPI, Martinsried, discussed tomography. Cryo-EM depends on averaging many thousands of presumably identical particles, as is also the case for conventional crystallography. However as biological objects that we wish to study become ever larger, the likelihood of finding a homogenous sample decreases. This is where tomography can take over. Instead of averaging between many randomly oriented particles, in tomography the sample is imaged in a series of known relative orientations. The problem, however, is that the many exposures to electrons will damage the particle. Another consequence of the new EM technology is that many labs are equipping themselves with powerful microscopes. That also makes it possible to use these microscopes for electron diffraction as opposed to imaging. **Tamir Gonen**, HHMI, Janelia Research Campus, gave a talk on how electron diffraction can be used successfully for analyzing very small crystals. Finally, **Elizabeth Villa**, U California San Diego, discussed how specimens can be better prepared for cryo-EM investigations using ion beam milling.

A brief final round-table discussion among the speakers, the leadership of the ACA, and audience members made it clear that structural biology has entered a new era, wherein protein crystallography and nuclear magnetic resonance spectroscopy have found a powerful new partner in cryo-EM.

Symposium speaker registration fees and travel/accommodation expenses were partially reimbursed using contributions from the ACA and four corporate sponsors, including FEI, Jeol USA, Gatan, Inc., and Direct Electron, LLP.

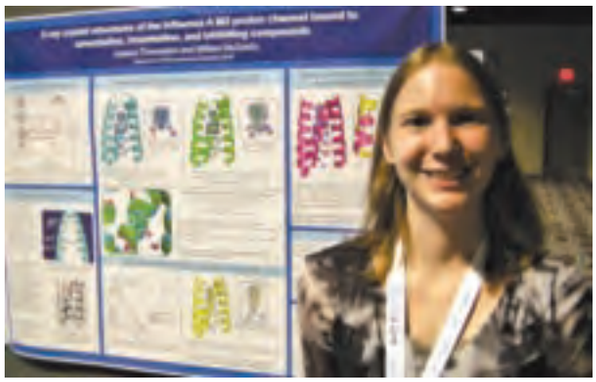
Michael Rossmann
Stephen Burley

Joe Reibenspies, at left, and Richard Staples. Photo by Peter Müller.

General Interest Posters

As usual, I could choose from a wide variety of scientifically stimulating and beautifully presented posters in New Orleans. For this column I have selected four posters that addressed particular interests of mine: drug discovery, drug formulation design, research that extracts the maximum information from crystal structure determinations, and radiation damage. Coming from Hong Kong, Brazil and England as well as the USA, these posters also illustrate the worldwide appeal of this ACA meeting. I had taken notes on a number of additional posters; but in those cases my personal choice was matched by carefully considered evaluation from the poster prize judges, who awarded prizes to these posters. Such posters are included in the section on prize winners, see pp. 11-15.

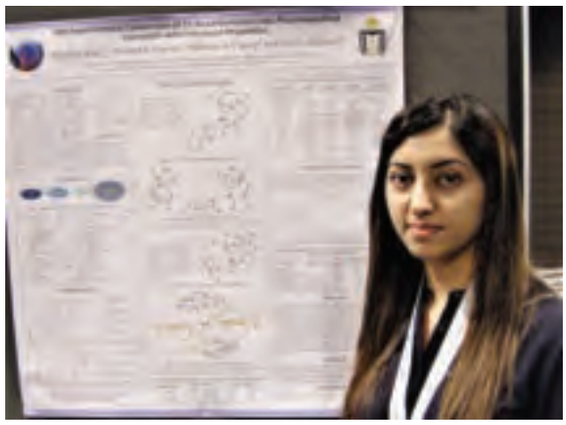
Poster **82-Sa**: *X-ray crystal structures of the influenza A M2 proton channel bound to amantadine, rimantadine, and inhibiting compounds*, presented by **Jessica Thomaston**, U California, San Francisco



The influenza virus continues to be a major cause of illness and a significant cause of death. Once it has obtained access to a host cell by endocytosis, it must unpack its RNA. This process requires an influx of protons via the M2 protein channel. Two drugs from our sparse armamentarium, amantadine and rimantadine, block this channel and abort the infection. Both drugs have an ammonium group attached to an adamantyl cage. Unfortunately, resistance has become widespread in currently circulating viruses. To inform the discovery of new drugs, Jessica has crystallized the protein and determined its structure to much higher resolution than ever before with drugs bound. The extremely difficult task of growing high-quality crystals of this membrane protein was finally accomplished using lipidic cubic phase techniques. Structures of the channel in its $Inward_{closed}$ conformation both with bound rimantadine and with bound amantadine were determined to a resolution of 2.0 Å; the structure of the $Inward_{open}$ channel with bound rimantadine was determined to 2.5 Å. Maps clearly show the orientation of the drugs as well as the positions of ordered water molecules that interact with their ammonium group. Furthermore, the binding mode has been established for a spiroadamantane inhibitor that blocks both the wild-type M2 channel and the heretofore drug-resistant V27A mutant. The binding position of the drug in the wild-type and the V27A channel shifts, but it remains effective. This information helps with the design of drugs to counteract resistance.

Turn to p. 24

Poster **26-Su**: *Mechanochemical conversion of 11-azaartemisinin into pharmaceutical cocrystals with improved solubility*, presented by **Madiha Nisar,** Hong Kong U of Science and Technology (HKUST)

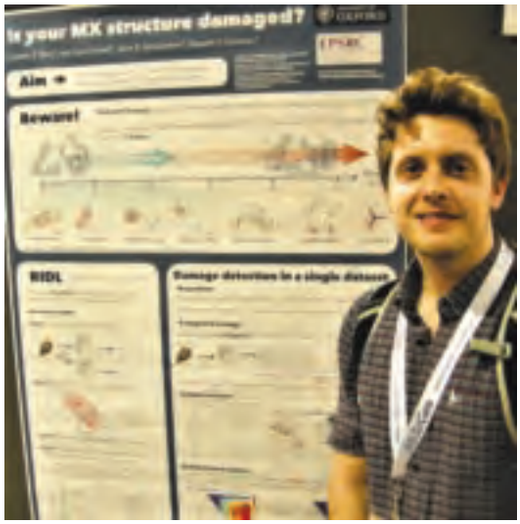


In the ongoing battle against malaria an important advance was the discovery that the natural product artemisinin has antimalarial activity. Subsequently, variants have been synthesized, especially in attempts to improve the bioavailability while retaining or enhancing the activity against *Plasmodium falciparum*, the most dangerous pathogen. While 11-azaartemisinin is effective, it still has poor aqueous solubility. In her poster Madiha reported on cocrystallization experiments by the technique of liquid assisted grinding. Of the 26 coformers tried with 11-azaartemisinin and screened by X-ray powder diffraction, 15 yielded cocrystals, carboxylic acids being particularly effective. The structures of 4 cocrystals subsequently grown from solution were determined, revealing the importance of the introduced nitrogen atom at position 11 in forming a synthon of the type OCNH…OCOH. The cocrystals showed improved solubility and thermal stability. Intriguingly, the cocrystal with another antimalarial drug, mefloquine, gave the highest thermal stability along with much improved solubility.

Poster **38-Su**: *Supramolecular arrangement of two methoxychalcones*, presented by **Hamilton Napolitano**, U Goias, Brazil

Before we discussed his poster, Hamilton and I chatted about his situation in Brazil. His university is located outside of wealthy parts of the country; and therefore his group lacks the resources to produce a blizzard of structure determinations like many groups in the USA or, indeed, Sao Paolo. Instead, this poster, along with two others presented at the ACA meeting by his group members, gave us a helpful lesson in concentrating on a few significant structures and using a variety of techniques to deepen our understanding of them. Chalcone moieties, which are present in many pharmaceutical compounds, have two phenyl rings joined by a prop-2-ene-1-one linker. Two chalcones with constant 4-methoxyphenyl substitution on one phenyl ring but 3,4,5-trimethoxy *versus* 4-ethoxy substitution on the other (MT-TRI *vs*. MT-ETX), were found to differ in degree of planarity and dihedral angles. Intermolecular interactions affecting crystal packing were investigated by Hirshfeld surface analysis, demonstrating the particular importance of C-H…π interactions in MT-ETX. Properties were evaluated by CAM-B3LYP/6-311+G(d) theoretical calculations, which also predicted IR vibrational spectra and enabled the assignment of the normal vibrational modes. Softness and hardness, both obtained from frontier molecular orbitals, showed that MT-TRI is more likely to receive electrons while MT-ETX resists charge transfer.

Poster **125-Su**: *Objective classification of specific radiation damage in macromolecular X-ray crystallography*, presented by **Charles Bury**, U Oxford, UK



Through their publications and by tutoring at crystallography schools Elspeth Garman and her colleagues at Oxford have done much to make us aware of the dangers of radiation damage. Our response to this threat has been rather similar to our response to the threat of burglary: add cryoprotectants and cool to low temperature / install strong doors and windows and keep them locked. Then we settled back and hoped it wouldn't happen to us. However, at 100 K damage can be insidious: specific residues may be widely affected long before diffraction intensities decrease noticeably. Chemical changes include disulfide cleavage, decarboxylation, and methylthiol cleavage. It may become all too easy to misinterpret structure and function around the active site. Charles presented an objective procedure for analysis of a data set to determine whether significant radiation damage has occurred. While $F_{obs}(n) - F_{obs}(1)$ Fourier difference maps based on initial (1) and later (n) data sets have been used in visual searches for signs of damage, interpretation of such noisy maps

can be difficult and may be tainted by preconceived ideas. The RIDL computational method has been developed to quantify specific damage events. Machine-learning algorithms, guided by model protein systems where damage has been well characterized, provide promising ways to identify true damage events. This method can also save beam time: a single dataset is collected, overlapping sub-datasets are defined, and a sliding window can be used to define the boundary between unaffected "early" and damaged "late" data.

Carl Schwalbe

Reception and Symposium for Undergraduate Students

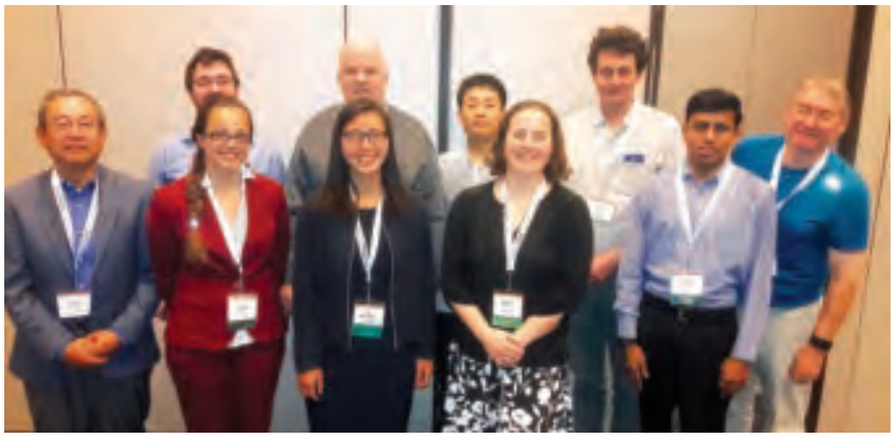
Brad Conrad addressing the group. Dasan Thamattoor is shown seated in the background. Photo by Krystle McLaughlin.

The fourth annual **Undergraduate Student Reception** was held at ACA 2017, in an ongoing collaboration with the Society of Physics Students (SPS), American Institute of Physics. Attendees, mostly undergraduate students, were treated to lunch and then an interactive talk on career pathways and resources for undergraduate students by SPS Director **Brad Conrad**. Brad started off with some interesting employment statistics for students with undergraduate and graduate degrees in the physical sciences, delineating the sectors (i.e., public, private, university, etc.) in which they work. Next he asked the students present to think about where they wanted to be in the next 10 years, and what was their dream job. Students were encouraged to share with their peers, and to also consider the follow-up questions: why and how? What was it about that particular job, at that particular place that made them want it, and how were they going to achieve it? This active examination provided a lot of enthusiastic discussion from the attendees. Resources for undergraduates thinking about different careers were highlighted. Brad also shared a story from his own undergraduate days, which led to the final group activity. One summer, while working as a NIST intern, Brad happened to get into an elevator with Hillary Clinton. Senator Clinton turned to him and said, "So, tell me about what you do here." Brad was caught off guard, and he did not remember saying too much. He told this story as a missed opportunity – if only he'd had an elevator speech prepared! Perhaps it would have led to other opportunities. Attendees were then asked to pair up, create and practice their own elevator speeches – a clear, brief, 30-second summary about research/interests. The reception ended with an open discussion, where many attendees asked questions, as well as gave suggestions for what they would like to see at ACA meetings for students in the future.

Krystle McLaughlin

The audience listening attentively to Brad's talk. Photo by Krystle McLaughlin.

1.1.2: Disorder, Inhomogeniety, and Local Structure in Complex Materials



L-R: Takeshi Egami, Kamila Wiaderek, Martin Donakowski (at rear), Vicky Doan-Nguyen, Thomas Proffen (at rear), Yuanpeng Zhang (at rear), Kate Page, Emil Bozin (at rear), Milinda Abeykoon, Ian Williams (at rear)

Takeshi Egami, Oak Ridge National Laboratory, began the session on **Disorder, Inhomogeneity, and Local Structure in Complex Materials**. He described that in contrast to crystals, many materials – such as glasses, (most) liquids, and many electrochemical materials – exist with their atoms in disordered systems. This can be visualized (see figure below) as ordered, marching soldiers (a 'crystal') versus disordered crowds on the street ('noncrystalline').

Egami introduced PDF, or pair distribution function, to explore disordered systems: PDF examines the entirety of the scattering, not exclusively the Bragg peaks, to produce a histogram of atom-pair distances. He successfully used this methodology to illustrate the structure of the supreme capacitor, disordered hydrous ruthenium oxide ($RuO_2 \cdot xH_2O$). The ruthenia material exists as a nanocomposite of metallic rutile RuO_2 and hydrous water. The water can facilitate proton transfer of the aqueous capacitor while the metallic component is able to facilitate electron transfer.

Vicky Doan-Nguyen, now at The Ohio State U, continued the theme of electrochemical materials with her talk on molybdenum sulfide clusters in a lithium ion battery. With *operando* electrochemical and PDF measurements – coupled with Raman and X-ray photoelectron spectroscopy – she found that the oxidation state of the molybdenum did not change during charge and discharge of the battery. Rather, the sulfide anions of the disordered chalcogenide gel (or 'chalcogel') changed oxidation state and were the redox-active agent in the complex $MoS_{3.4}$ battery electrode.

Emil Bozin, Brookhaven National Laboratory, described how they applied X-ray and neutron PDF techniques to explore dynamic local symmetry breaking in novel materials, emphasizing that this local symmetry breaking is the key for understanding devices from energy conversion to superconductivity. He presented evidence that local, fluctuating broken symmetry states are widespread in functional materials, illustrating this with three examples having implications for photovoltaics, thermoelectrics, and superconductivity.

Kamila Wiaderek, Argonne National Laboratory, presented her work, *Relating ε-$LiVOPO_4$ performance to local environment dynamics and hysteresis*. She used *operando* PDF analysis along with X-ray diffraction to identify potential structural differences between $LiVOPO_4$ synthesized via solid-state and hydrothermal methods, which might affect the diffusion pathways and ultimately limit the cycling efficiency of potential battery applications.

Katharine Page, Oak Ridge National Laboratory, concluded the session by presenting their design for a novel total scattering diffractometer for materials discovery (DISCOVER), proposed for the Spallation Neutron Source (SNS). DISCOVER is expected to be the world's highest resolution dedicated neutron total scattering instrument that will be optimized for studying real materials in their operating environments. Page also explained why the total scattering method holds the key to determine the crystallographic average structure as well as the local structure, often responsible for the physical properties of complex materials.

Milinda Abeykoon
Martin Donakowski

Brandon Mercado, at left, and Mike Takase. Photo by Peter Müller.

Stacey Ortega. Photo by Richard Bromund.

1.1.4: Engaging Undergraduates with Crystallographic Research

This half-day session included an engaging panel of speakers who highlighted the ways in which they are involving undergraduate students in crystallography at their institutions. The talks featured a mixture of topics in both small molecule and protein crystallography. **Tim Royappa**, U West Florida, answered the question of how to teach crystallography without a diffractometer by discussing the incorporation of computational lab modules that use the freely available resources of the Cambridge Structural Database. **Peter Wood**, CCDC, UK, highlighted the benefits of 3D printing to create physical models of molecules for classroom use that are both accurate and inexpensive. **Simon Coles**, U Southampton, UK, discussed ways in which he has embedded real-world aspects in an existing crystallography lab to provide a scaffolded research experience for students. **Rich Matyi**, Florida Polytechnic U, discussed his experience leading a team of undergraduates in the setup and characterization of a new diffractometer system, while **Joe Tanski,** Vassar College, summarized an undergraduate lab module he developed on molecular structure determination, focusing on how students should investigate and describe intermolecular interactions in crystal structures in their reports. **Krystle McLaughlin**, Vassar College, discussed her lab module at Lehigh U that introduces undergraduates to protein crystallography in an effort to excite them about structure. Krystle's series of labs spans crystallization, virtual data collection, model building in Coot, and figure generation with PyMOL. **Bradley Miller**, Bryn Mawr College, wrapped up the session by describing ways in which he incorporates structural biology into the biochemistry classroom, the biochemistry teaching labs and his undergraduate research program.

Joe Tanski
Rachel Powers

1.2.1: Nucleic Acids and Friends

The **Nucleic Acid and Friends** session focused on structures of RNA, DNA, and protein nucleic acid complexes that perform essential tasks in biology. **Hong Li**, Florida State U, presented a tour de force story on how essential snoRNP complexes are formed using a balanced mix of structural and biochemical methods. **Rui Zhao**, U Colorado, Denver, presented her group's exciting new work on a high-resolution cryo-EM structure of the *S. cerevisiae* U1 snRNP spliceosome complex. Alternative splicing allows one gene to code for many proteins, and Rui's talk offered interesting insights into splicing initiation and the choice of performing alternative splicing. **Hideki Aihara**, U Minnesota, presented his group's past and recent work unravelling the complexity and diversity of intrasomes. Hideki highlighted how different viruses use unique combinations of integrases to encase DNA targets. Before the coffee break, **Xinhua Ji**, NIH, took us on his group's decade-long journey examining RNase III enzymes, and how they measure and cut RNA targets using a unique "double ruler" mechanism. **Blaine Mooers**, U Oklahoma, who was in the air flying to the meeting when the session started, heroically arrived just in time to present how local RNA structures and sequence context regulate the fascinating world of RNA editing. Next, the session switched gears to DNA modification and repair. **Alex Drohat**, U Maryland, presented an examination of how epigenetic DNA marks are recognized, decoded, and finally removed. Alex's talk set up **Martin Horvath**, U Utah, who presented a revised mechanism for MutY DNA repair activity. **Fukang Wang**, Zhen lab, Georgia State U, closed the session with a fascinating talk on Se modification of DNA and RNA nucleotides to create a phasing toolbox. Fukang's talk created a lively discussion regarding the versatility of Se-labeled nucleotides and their adaptability to aid the research of the nucleic acids structural biology community.

Aaron Robart

Session 1.2.2: Diffuse Scattering in Complex Oxides

L-R: back row – Daniel Phelan, Richard Welberry, Emil Bozin, Ben Frandsen; front row – Kate Page, Yan Wu, Tedi-Marie Usher, Ying Zhang, Allyson Fry-Petit. Photo by Pavol Juhas.

The session on **Diffuse Scattering in Complex Oxides** featured four invited and four contributed presentations covering a wide range of research utilizing diffuse scattering. The talks highlighted the diversity of experimental techniques related to diffuse scattering as well as the plethora of material systems that can benefit from this type of analysis. On the experimental side, we enjoyed presentations about measuring and modeling single-crystal, three-dimensional diffuse scattering patterns in reciprocal space; real-space based atomic and magnetic pair distribution function (PDF) analysis of powder diffraction data; dynamical pair distribution function (dyPDF) methods using inelastic neutron scattering; and advancements in PDF modeling methods, such as improvements in incorporating particle shape and size into calculated PDFs. The materials investigated included strongly correlated electron systems, relaxor ferroelectrics, magnetoelectrics, magnetic semiconductors, and high-efficiency catalysts. Out of this variety of research emerged a strong common theme: diffuse scattering is rich in information about the local structure of complex materials, which often has direct bearing on their properties and functions. Many thanks to the speakers for their excellent work and engaging presentations!

Ben Frandsen
Kate Page

1.2.4: Important Science from Small Molecules

The **Important Science from Small Molecules** session continued its biennial tradition of bringing together speakers involved in many aspects of chemistry and physics to give presentations involving both theory and experimentation. Speakers came from all levels of academia ranging from second-year graduate students, to post docs, to established professors.

The session began with **Nikolay Gerasimchuk**, Missouri State U, introducing us to recent work from his group on the rich, diverse chemistry of Ag(I) and Tl(I) cyanoximates. Silver cyanoximates were found to display anti-microbial properties while also demonstrating initial promise as battery-less sensors for the detection of UV light. Thallium cyanoximates were shown to form light-insensitive compounds, and demonstrated particularly interesting structural chemistry.

Michael Hall, Texas A&M U, our next speaker, introduced us to the fascinating realm of non-innocent ligands, which were shown to be a particularly intriguing topic for electronic-structure calculations. A range of recently characterized ruthenium and rhenium complexes with non-innocent ligands were described, with selected complexes displaying potential to facilitate the water oxidation of methanol.

Raúl Castañeda, U Ottawa, Canada, followed with an update on his ongoing graduate work focused on using Fe(II) tetrachlorides with pyridinium cations as starting materials for the coordination of imidoyl amines.

Alice Brink, U Free State, Bloemfontein, RSA, wrapped up the first half of the session by providing an excellent overview of the use of rhenium in drug development. Utilizing a new class of ligands, Alice had characterized new Re drug candidates and compared these new compounds to metastable technetium analogues.

The second half of the session started with **Robin Macaluso**, U Texas at Arlington, discussing two Er-Pt-Ga intermetallic compounds that had recently been synthesized by her group via flux synthesis. The two phases were a known modulated structure along with a second new phase, the latter of which was of particular note as magnetic measurements on this new compound displayed geometrical frustration.

Carlos Murillo, Texas A&M U, followed with a presentation focusing on transition-metal complex metal-metal interaction distances, an often-overlooked means of non-covalent assembly, and then detailed the many manifestations of these interactions on structures and properties.

Paul Forster, U Nevada Las Vegas, next introduced us to the mystery that is technetium red, a Tc oxide whose formal oxidation state has remained a bit of a scientific conundrum. Proceeding via a combination of simulation and experimentation, Paul eloquently described the anticipated coordination environment of this unusual phase and finished his talk by highlighting initial experimental results from his group that confirmed theoretical findings.

Gertruida Venter, U Free State, Bloemfontein, RSA, followed with an update on her ongoing work developing new hydroxypyridine-N-oxide (HPNO) ligands and complexation efforts with these ligands and rhodium(I).

Our last speaker of the day was **Jim Donahue**, Tulane U, who reminded us all of the importance of paying attention to the details in crystallography, as he presented two cases of metal-ion misidentification in transition-metal diazadiene chloride complexes. As our previous speakers had detailed the ample ways in which small-molecule structures can provide valuable insights across many disciplines, Jim's talk emphasized the importance of accuracy in small-molecule crystal structures, an important takeaway for all session attendees.

Korey Carter
Alberto Albinati

Training Sessions 2.1.1: Learn Macromolecular Crystallography; Best Practices with Diffraction Images from Known X-ray Structure; and 3.1.4: Apply Macromolecular Crystallography Best Practices to Your Challenging Diffraction Data

***Session 3.1.4** – L-R: Ivan Shabalin, Zbigniew Dauter (at rear), Wladek Minor, Dominika Borek (at rear), Jasmine Young, Maksymilian Chruszcz (at rear), Przemyslaw Porebski, Stephen Burley, Zbyszek Otwinowski (at rear), Paul Emsley. Photo courtesy of Wlakek Minor.*

Both training sessions turned out to be among the most popular and successful sessions of the 2017 meeting. Attendance at both sessions was excellent. The participants could download the content of a bootable USB drive with state-of-the-art software for use during the session. A limited number of USB drives were also distributed during the session 3.1.4. X-ray diffraction data for the session were available from ***http://www.proteindiffraction.org***.

During **Session 2.1.1** five speakers presented different aspects of structure determination and validation. **Janet Smith**, U Michigan, made an introductory presentation. She showed the difficulties related to space-group determination and possible complications that may arise from multi-crystal experiments. **Zbigniew Dauter**, NIH, Chicago, discussed the scientific issues that are behind data collection. **Tom Terwilliger**, Los Alamos National Laboratory, discussed SAD phasing for both easy and challenging cases. **Paul Adams**, Lawrence Berkeley Laboratory, discussed various phasing strategies that should be considered when molecular replacement is used to obtain phases. Finally, **Paul Emsley**, MRC, Cambridge, UK, presented the pitfalls of model building and structure refinement and had a live demonstration of the newest COOT capabilities for building N-linked glycans. Session chairs provided introductions and case studies.

Session 3.1.4 concentrated on a practical approach to structure determination. **Dominika Borek**, UT Southwestern Medical Center, discussed the best practices for data reduction. **Zbyszek Otwinowski**, also of UT Southwestern, presented several difficult cases of space-group determination and methods for troubleshooting such problems. **Maksymilian Chruszcz**, U South Carolina, showed the difficulties of phasing when the data were not collected optimally and demonstrated several cases of crystallization artifacts. **Ivan Shabalin**, U Virginia, showed the complicated cases of refining the structural models, including metal ions, with special focus on refinement and analysis of ADPs. **Przemyslaw Porebski**, also of U Virginia, presented issues related to structure refinement and model building for several difficult cases and applications that simplify model building. Finally **Jasmine Young**, RCSB Protein Data Bank, described the wwPDB OneDep Validation procedure during deposition of macromolecular structures. During the session break Ivan Shabalin carried out live demonstration of structure determination from indexing diffraction images to model refinement.

Stephen Burley
Wladek Minor

2.1.2: Joint Methods for High Rate Data Processing: XFEL and Synchrotron

L-R: Ralf Flaig, Danny Axford, Artem Lyubimov, Aaron Brewster, Nicholas Sauter, James Holton, Herbert Bernstein

Session 2.1.2 on **Joint Methods for High Rate Data Processing: XFEL and Synchrotron** was held the morning of Sunday, May 28. Advances in light sources, detectors, beamline design, sample preparation and crystal delivery enable the generation of diffraction data at unprecedented speeds, with the newest pixel array detectors collecting hundreds of frames per second, and giving terabyte data sets. At the same time, the techniques of serial crystallography, popularized by the femtosecond X-ray pulses found at free-electron lasers, are now being transferred to conventional synchrotron beamlines with notable success, greatly increasing the range of samples available for study. Much of the work reported focused on the data-processing challenges arising from serial crystallography. How will high-rate data be acquired, moved, and stored, and what data analysis pipelines will be needed in order to provide timely scientific feedback to the beamline user? Furthermore, what special treatment is required to merge diffraction data from ensembles of crystals, considering specific problems such as non-isomorphism and the issue of still-shot versus rotation data collection?

The speakers responded to this charge with reports of rapid progress in building the hardware and software infrastructure to collect and process data at very high rates from large numbers of crystals, both at XFELs and at synchrotrons. **Ralf Flaig**, Diamond Light Source, UK, spoke about beamline I04 at Diamond, a fully automated, multiwavelength endstation with multiaxis goniometry, including present efforts to produce a real-time data analysis pipeline. Diamond's **Danny Axford** described their beamline I24, along with the silicon-chip array approach to collecting fixed-target serial crystallography data, both at synchrotrons and XFELs. **Herbert Bernstein**, RIT, spoke on *Synchrotron serial crystallography with multi-stage merging of 1000's of images*, combining a sensitive and accurate cell-based clustering with a reflection-based clustering modified to work with low-completeness datasets. **Artem Lyubimov**, Stanford U, gave details of IOTA, his program to optimize the computational merging of data from large serial crystallography data sets. **Aaron Brewster**, Lawrence Berkeley National Laboratory (LBL), reflected on the integration step itself for still shots, and the importance of devising models that are detailed enough to describe the degrees of freedom in the experiment, and accurate enough to be reproducible. **James Holton**, LBL, examined the question of resolution limit, asking where to cut the data in multi-crystal merging, what limits to use for crystallographic refinement, and controversially, what limits to claim in a publication. **Andreas Foerster**, Dectris, Ltd, was scheduled to speak on *High data rate processing – a puzzle of metadata, compression and software*, but was unable to attend, so Herbert Bernstein presented the slides for him. Nicholas Sauter, LBL, then moderated a discussion on *What gaps remain for serial crystallography?* In particular, still-shot data as presently processed apparently require far higher multiplicity to obtain equivalent maps compared with rotation data, and the optimal algorithms for still-shot data treatment are not yet a settled matter. Much remains to be done as light sources and data collection techniques are upgraded, and there are unique issues for synchrotrons as there are for XFELs, but there is common ground and room for sharing the lessons learned.

Nicholas Sauter
Herbert Bernstein

2.1.3: Porous Materials

L-R: Paul Forster, Len Barbour (at rear), Laura McCormack, Michael Zaworotko (at rear), Peter Wood, John MacDonald (at rear), Wenqian Xu. Photo by ACA Meeting student volunteer.

Porous materials represent an important area of science where crystallography has much to offer, but application of crystallographic techniques can remain far from routine. Many of the most attractive features of metal organic frameworks (MOFs) relate to the behavior of guests inside the pores. While crystallography on the frameworks themselves is not always routine, interpreting the much weaker and more diffuse signal associated with guests within pores may be even more challenging. However, to understand processes such as gas storage and separations and catalysis, this is precisely what must be accomplished.

Michael Zaworotko and his teams at U Southern Florida (1999-2013) and Ireland's U Limerick (2013-present) have been instrumental in the development of MOF chemistry and the closely related field of crystal engineering. His talk entitled *Crystal engineering of hybrid ultramicroporous materials* presented their work in the field. One of their emphases in the field of MOF synthesis has been the preparation of materials with increasingly larger and larger pores extending well into the nanometer scale. While there is certainly scope for utilizing such compounds for molecules too large to fit into conventional crystalline nanoporous materials, such pores are also less useful for many separations processes involving small molecules. A key theme, which he backed up with plenty of examples, is the importance of engineering the right pores for the right behavior.

Next, **Len Barbour**, Stellenbosch U, RSA, provided an excellent complementary talk focusing on the importance of structural flexibility in porous applications. His teams' unique combination of high-quality crystallographic and calorimetric analysis under practical conditions has led to a number of compounds with promise for advanced separations and storage applications. Additional speakers in this morning session included **Travis Mitchell**, U Buffalo, *Development, synthesis, and characterization of dithienylethenes and their incorporation into crystalline solids*, **Laura McCormick**, U St. Andrews, UK, and Lawrence Berkeley National Laboratory, *Nitric oxide and the Kagome lattice*, **John MacDonald**, Worcester Polytechnic Institute, *MOFs as porous hosts for generating singlet oxygen*, and **Peter Wood**, CCDC, UK, *Metal-organics: A rich seam of data for knowledge mining*.

Paul Forster

2.1.4: NMR Crystallography

Session 2.1.4 inaugurated the topic of NMR Crystallography to ACA Annual Meeting Sessions. The session was chaired by Manish Mehta, Oberlin College, and Tomislav Friščić, McGill U, Canada, and involved five speakers who formed a compelling and complementary set, presenting a good cross-section of this growing field. The session was very well attended, with a strong audience of at least 50 throughout all the talks. **Manish Meta** gave the opening remarks on the emerging importance and current state-of-the art in NMR Crystallography. He was followed by **James Harper**, U Central Florida, with his presentation, *Developing accurate crystallography without diffraction*, focusing on the use of theoretical techniques including crystal structure prediction (CSP) and density functional theory (DFT) modeling, for understanding and resolving solid-state crystal structures of organic compounds. An example of James's work is found in *J. Phys. Chem. A*, **2013**, *117*, 5534-5541, focusing on use of solid-state NMR in resolving the dynamics in the disordered crystal structure of methyl α-L-rhamnofuranoside. His lecture was followed by that of **Mihails Arhangelskis**, McGill U. In his lecture entitled *Combined use of solid-state NMR spectroscopy and theoretical modelling as a method of structure determination*, Mihails provided a number of increasingly complex examples of solid-state NMR studies facilitating structural characterization of organic solids. Some of that work can be found in his paper *Chem. Eur. J.* **2016**, *22*, 10065-10073.

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2.1.4: NMR Crystallography, ctd

Following a brief coffee break (during which the audience did not disperse!), the session continued with a presentation of **Kenneth Harris**, Cardiff U, UK, on *"NMR Crystallization": New in situ NMR techniques for time-resolved monitoring of crystallization processes*. In his lecture, Kenneth presented a truly exciting methodology for simultaneous observation of crystallization processes through solution-based and solid-state NMR spectroscopy, in that way providing an extremely and surprisingly clear insight into the processes of nucleation, crystal growth and polymorph selection. More information on the **CLASSIC NMR** pulse sequence that enables these measurements can be found in: *Acta Crystallogr*. **2017**, *C73*, 137-148. One note for non-experts regarding "**CLASSIC**" – the NMR community loves acronyms! A major chemical shift in topic followed, with the lecture *NMR Crystallography in the enzyme active site of tryptophan synthase* by **Leonard Mueller**, U California Riverside. His lecture addressed the world of protein structures, and in particular the active site of the pyridoxal phosphate (PLP)-requiring tryptophan synthase enzyme, where the combined use of X-ray crystallographic and solid-state NMR data, all tied together through theoretical modeling, enabled the identification of the protonation state in a reaction intermediate. More on this use of NMR Crystallography can be found in the recent paper: *J. Am. Chem. Soc.* **2016**, *138*, 15214-15226.

(a) Manish Mehta opening the NMR Crystallography session at the New Orleans 2017 ACA Annual Meeting; (b) James Harper talks on crystallography without diffraction; (c) Mihails Arhangelskis illustrating benefits of solid-state NMR in solid-state structure solution; (d) Kenneth Harris describes the CLASSIC NMR approach to monitoring crystallization in situ; (e) Leonard Mueller discusses understanding protonation in enzyme active sites using NMR Crystallography; (f) Darren Brouwer with his legendary zeolite structure solved by NMR Crystallography.

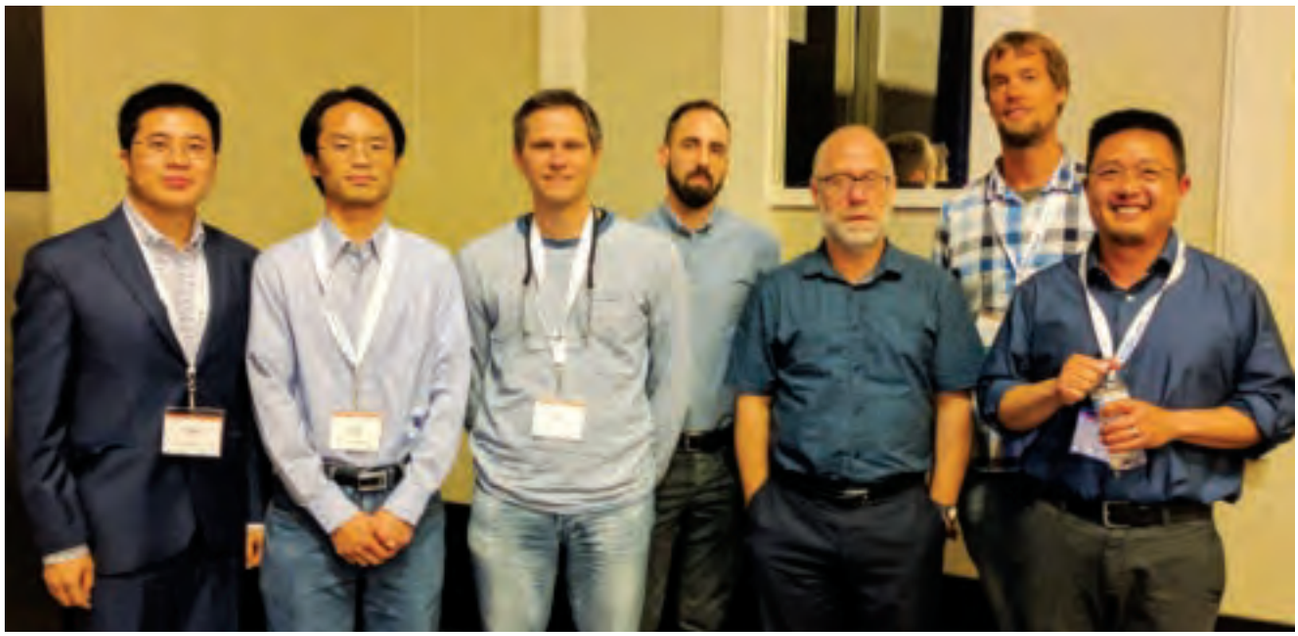
The final talk of the session was by **Darren Brouwer**, Redeemer U, Canada, who gave a clear and compelling illustration of the power of NMR spectroscopy in the solid state for resolution of complex structures. His pioneering work in zeolite structure determination by NMR can be found in: *J. Am. Chem. Soc.* **2005**, *127*, 10365-10366, and more recent work is here: *Acta Crystallogr.* **2017**, *C73*, 184-190. Just like the noted paper from Kenneth Harris, this one has also been published in the special issue of *Acta Crystallographica C*, dedicated to NMR Crystallography and co-edited by David Bryce, University of Ottawa, Canada, and Francis Taulelle, Université de Versailles Saint Quentin en Yvelines, France. The publication of this special issue of *Acta C*, just like this very first NMR Crystallography session at an ACA Annual Meeting, is an excellent demonstration of the acceptance and utility of nuclear magnetic resonance in structural solid-state science and crystallography. This very successful session in New Orleans was aimed to bolster further mixing and discussions of the NMR and crystallography communities, and we believe this was both fun and accomplished in full. Therefore, we would like to invite you to the upcoming **second ever** NMR Crystallography session at the 2018 ACA Annual Meeting in Toronto!

Tomislav Friščić

ACA RefleXions Co-Editor Tom Koetzle (at left) with participants of the first ever NMR Crystallography Session at an ACA Annual Meeting, L-R: Manish Mehta, Mihails Arhangelskis, Darren Brouwer, Kenneth Harris, Tomislav Friščić, James Harper, Leonard Mueller

The not-so-official part of the session took place at the Bombay Club restaurant in the New Orleans French Quarter. Photo courtesy of restaurant staff.

Session 2.2.1: Enzymes of Posttranslational Modification



L-R: Shukun Luo, Danny Huang, Frank Sicheri, Cameron Noland, Roland Dunbrack, Bernhard Lechtenberg, Hua Su. Absent: Carrie Wilmot.

The **Enzymes of Posttranslational Modification** session was dedicated to enzymes (and pseudo-enzymes) that regulate a diverse set of posttranslational modifications including phosphorylation, ubiquitination, lipidation and proteolytic cleavage. The first half of the session firmly focused on kinases. **Frank Sicheri**, U Toronto, Canada, presented work on RNase L. RNase L contains an inactive kinase domain, a pseudokinase, that functions as a regulatory unit to control its RNase activity. Frank explained how the sensory domain of RNase L recognizes the viral second messenger 2-5A in infected cells, while the kinase domain binds ATP. Both events are necessary for RNase L dimerization and activation of its C-terminal RNase domain to degrade viral RNA.

In the second presentation, **Roland Dunbrack**, Fox Chase Cancer Center, explained how it is often worthwhile to take a second look. Roland and his group developed a bioinformatics approach to analyze all possible protein-protein interactions in a crystal structure. He applied his tool to identify novel auto-phosphorylation complexes in published crystal structures. Excitingly, some of these auto-phosphorylation interactions were not identified in the original publications and thus described novel enzyme-substrate complexes.

In the final presentation on kinases, **Hua Su** from Merck presented his work on the identification of a novel inhibitor against the kinase TrkA, a target to treat chronic pain. Unexpectedly, the inhibitor does not bind to the active site, but to an adjacent site that includes a region outside the kinase domain, the juxtamembrane domain.

Following the coffee break, **Shukun Luo**, Columbia U, shared his insights on the structure of the yeast separase/securin complex. Separase is a protease that cleaves the cohesin complex to allow chromosomal segregation during cell division. The inhibitor securin regulates its activity. The structure shows how securin wraps around the whole length of separase to stabilize the complex. Importantly, the structure also reveals securin's mechanism of inhibition by binding and blocking the separase active site.

Cameron Noland, Genentech, discussed his approach to develop much-needed novel antibiotics. His research focused on the structural analysis of the bacterial acyltransferase Lnt, which is required in the last step of lipoprotein biosynthesis and is critical for bacterial infections in a clinical setting. Cameron's work provides novel insights into the catalytic mechanism of this enzyme and lays the foundation for drug development approaches.

Finally, **Danny Huang**, Cancer Research UK Beatson Institute, presented an elegant approach to suppress the p53 transcription factor in cancer. The activity of p53 is controlled by the E3 ubiquitin ligase complex of MDM2/MDMX that targets p53 for proteasomal degradation. Based on a crystal structure of the MDM2/MDMX/E2-ubiquitin complex, Danny's group designed MDM2 mutants that lack E3 ligase activity but retain p53 binding capability. In cells these mutants do not decrease p53 levels but rather reduce expression of p53 target genes, in this way rendering cells hypersensitive to stress. Thus, these mutants point the way to new therapeutic approaches in cancer to inhibit MDM2 E3 ligase activity without affecting its p53 binding ability, which may reduce side effects in healthy cells.

Bernhard Lechtenberg
Carrie Wilmot

2.2.2: Home-Built Software

L-R: Bruce Foxman, Horst Puschmann, Paul Sanschagrin, Paul Boyle, Larry Falvello, Len Barbour, Ken Littrell, Marshall McDonnell, Victor Young. Photo by Brandon Mercado, courtesy of Victor Young.

Considering the ample scope of the software described by the eight speakers in the **Home-Built Software** session, it would appear that the session title encompasses just about all aspects of crystallographic programming. "Home-Built Software" as a topic does cover a large swath of the programming efforts that have taken place to date, since much crystallographic software, from the most extensively used to the most obscure, has been developed by practicing crystallographers, usually in the context of their own laboratories and very often without specific funding for software development.

The session began and ended with talks about well-known and widely used software. **Len Barbour**, Stellenbosch U, RSA, opened the session with a history and description of his program XSeed, a Shelx-PovRay interface written in Pascal beginning in 1984-1985 [*J. Supramol. Chem.* (2001) *1*, 189-191]. The history of XSeed serves as a good example of how a program can develop from a modest beginning to become a powerful tool in the crystallographer's repertoire. Len also described and demonstrated a second program that he has written, a diffractometer simulator that is highly useful in an educational setting. For information on downloading this software, contact Len by e-mail at ***ljb@sun.ac.za***.

The other famous program described in the session is Olex2, the topic of **Horst Puschmann**'s (OlexSys Ltd., UK) closing talk. Unlike essentially all of the other software described in the session, the well known and widely used Olex2 did benefit in its infancy from dedicated funding for software development. One of the key aims of Olex2 is to bridge the gap between difficult concepts and usability. A vast store of information regarding Olex2 can be found at the OlexSys web site, ***http://www.olexsys.org/Software***.

The recently released Python application-programming interface to the Cambridge Structural Database was the subject of a talk by **Paul Sanschagrin**, CCDC. This API permits the home programmer, using Python, to prepare what amounts to extensions of the functionality of the CSD. While there may be something of a learning curve for its use, the potential added value and flexibility that this API adds to the utility of the database make it well worth exploring seriously. More information: ***https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd-python-api/***.

Home-built software has a critical role to play at large facilities. At neutron sources such as SNS and HFIR at Oak Ridge National Laboratory, as described by speakers **Marshall McDonnell** and **Ken Littrell**, the custom-made instruments and the need for flexibility imposed by the diversity of user projects make it essential that customizable but stable, purpose-built software be available. Marshall talked about ADDIE, for processing TOF data for PDF analysis. Ken described in some detail the procedures that he has written, both at IPNS and at Oak Ridge. The software, dedicated to processing SANS data, is largely developed within Igor Pro (a commercial product from Wavemetrics). These modular, extensible procedures have contributed significantly to the user program, figuring in some 90% of the 350+ publications to date from the CG2 and CG3 instruments.

The home lab can benefit in at least two principal ways from the development of home-built software. As described by **Paul Boyle**, U Western Ontario, Canada, the need for efficiency and some degree of quality control and standardization in a productive structure-determination laboratory calls for the use of custom software to achieve desirable results, such as the standardization of file-name structures, the insertion of local information and experimental data into the CIF produced by a refinement program, and the archiving of results in final form in a sustainable and easily utilized manner. Paul described how some readily available tools from the Linux world can aid greatly in automating tasks. The web site of the Chemistry X-ray facility at UWO (***http://xray.chem.uwo.ca/***) has more information on Paul's software.

Larry Falvello, U Zaragoza, Spain, used a programming example involving the analysis of displacement parameters to illustrate some general principles involved in deciding whether to undertake a specific programing project and how to carry it out without going off course. Following Larry's talk, Horst Puschmann commented that useful subroutines are available for use in home programming projects.

A high point of the program was an informative talk by **Bruce Foxman**, Brandeis U, about software that he has written over a half-century, including a recently written program for determining twin obliquity. The talk was dedicated to Howard Flack, and touched on a number of programs that Bruce has written. Full information can be found at Bruce's web site, ***http://people.brandeis.edu/~foxman1/***.

The near-capacity audience in Celestin A hall engaged the speakers in lively discussion. Sponsored by the Small Molecule SIG and organized by Victor Young and Larry Falvello, this session provided a good survey of the diversity of form and function that can be found in home-built software. The great success of this half-day session suggests that ACA should consider similar themed sessions in years to come.

Larry Falvello
Victor Young

2.2.3: General Interest I

L-R: John Rose, Carla Slebodnick, Igor Nederlof, Bi-Cheng Wang, Oleg Borbulevych, Madushani Dharmarwardana, Gerald Audette, Gloria Borgstahl, Bill Duax, Andrey Kovalevsky. Photo by Vicky Doan-Nguyen.

This session focused on topics of broader interest to the macromolecular crystallography community, including historical overviews, recent scientific results, and new or improved software and instrumental techniques. The session started with **John Rose**, U Georgia, presenting a historical overview of the first structure solved by ISIR methods. **Bill Duax**, Hauptman-Woodward Medical Research Institute, followed with a thorough analysis of the importance of glycine conservation toward conservation of structure in different families of ribosomal proteins.

Bi-Cheng Wang, U Georgia, gave an overview of a pilot program at the SER-CAT facility involving collecting complete datasets on a metalloprotein crystal at multiple wavelengths across the metal's absorption edge, giving simultaneous crystallographic and spectroscopic data.

Igor Nederlof, Amsterdam Scientific Instruments B.V., The Netherlands, outlined possibilities, limitations, and recent advances in solving protein structures on nanocrystals using electron crystallography. **Gerald Audette**, York U, Toronto, Canada, presented recent progress toward determining the structure of TraF, a component protein of the *Escherichia coli* F-plasmid type IV secretion system. **Gloria Borgstahl,** U Nebraska Medical Center, provided an introduction to incommensurately modulated protein crystals, superspace groups, and recent software advances toward processing the complex datasets from these systems. **Andrey Kovalevsky**, Oak Ridge National Laboratory, presented the structure of the PLP-dependent enzyme aspartate aminotransferase (AAT) and highlighted the power of neutron crystallography by identifying different protonation states of both the ground and substrate-bound states of the protein. **Eric Zhou**, Formulatrix, outlined advances in macromolecular crystal screening and growth optimization through use of Second Order Nonlinear Imaging of Chiral Crystals (SONICC) to differentiate between chiral protein, RNA, and achiral salts on crystals as small as submicron size. The session concluded with **Oleg Borbulevych**, QuantumBio Inc., explaining the use of the DivCon plugin to complete mixed-QM/MM computation during structure refinement to give lower residual electron densities and better refinement statistics than traditional stereochemical restraints.

Madushani Dharmarwardana
Carla Slebodnick

2.2.4 Integrative Approaches to Structural Biology (NMR, cryo-EM, SAS)

L-R: Michal Hammel, Yuba Bhandari, Gabriel Valez, John Tanner, Sangita Sinha, Greg Hura, Kushol Gupta, Daniel Saltzberg, John Tainer. Photo by Kushol Gupta.

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2.2.4 Integrative Approaches to Structural Biology (NMR, cryo-EM, SAS), ctd.

Cutting-edge insights into structural biology require comprehensive approaches to the determination of structure and dynamics in macromolecular assemblies to elucidate their complex macromolecular structures and function. This session featured a breadth of experience across these areas and highlighted integrative approaches to challenging questions in structural biology, with a focus on small-angle scattering. Small-angle X-ray and neutron scattering (SAXS/SANS) provides information that is highly complementary to other well-established structural approaches including NMR, cryo-EM, and X-ray crystallography.

Invited speaker, **John Tainer**, MD Anderson Cancer Center, U Texas, presented an overview of the state-of-the-art in biological small-angle X-ray scattering (BioSAXS), using ongoing studies of dynamics complexes acting in DNA replication and repair as examples of how SAXS can be applied to distinguish different conformational states, intrinsic flexibility, and as a screen in high-throughput under most solution conditions. Our next invited speaker **Yuba Bhandari**, NIH, presented general methods for high-throughput topological structure determination of RNAs, guided by SAXS-based rigid-body modeling, secondary structure constraints, and additional long-range interaction information. He also demonstrated the applicability and feasibility of the approach to derive low-resolution topological structures of relatively large multi-domain RNAs. **Greg Hura**, Lawrence Berkeley National Laboratory, presented current methods development at the ALS SIBYLS beamline with the focus on describing dynamic solution states of macromolecules using an integrative structural approach combining crystallography and SAXS. **Gabriel Valez**, U Iowa, presented a new crystal structure of the catalytic core domain of human Calpain-5. In comparison to the calcium-bound state observed in the crystal, SAXS and molecular dynamics revealed a highly open conformation of the domain in solution. This in turn provided insight into the molecular mechanisms that regulate this family of proteins and inform the design of specific inhibitors. **Sangita Sinha**, North Dakota State U, presented an integrative approach to the study of structure and function in BECN and ATG/BARKOR, key components of the autophagy nucleation complex. X-ray crystallography, SAXS, isothermal titration calorimetry, and site-directed mutagenesis revealed possible mechanistic differences among the BECN paralogs that enable dynamic exchange between diverse coiled-coil containing partners within the cell. **John Tanner**, U Missouri, demonstrated the integration of SAXS, crystallography, hot-spot mutagenesis, and analytical ultracentrifugation, which provide the tools to understand the role of oligomerization in the function of enzymes of the aldehyde dehydrogenase (ALDH) superfamily. **Kushol Gupta**, U Pennsylvania, presented the crystal structure of allosteric inhibitors of integrase (ALLINI) bound to viral-encoded integrase (IN). The structure reveals for the first time the complete ALLINI-binding interface, comprised of both IN C-terminal and catalytic core domains. Our last invited speaker for the session, **Daniel Saltzberg**, U California San Francisco, presented structural modeling using Integrative Modeling Platform (IMP) with particular focus on development and implementation of structural restraints for hydrogen-deuterium exchange data.

Kushol Gupta
Michal Hammel

2.2.5: Electron Diffraction of Solid-state Materials

This symposium, supported jointly by the Powder Diffraction, Materials, and Neutron Scattering SIGs, was the first in several years dedicated to the use of electron scattering to understand the structure and crystallography of solids with materials science applications. The goal of the symposium was to represent a broad range of topics at the state of the art of electron scattering in both real and reciprocal space applied to problems in nanoscience, spanning timescales from static to ultrafast, and in crystallography from bulk defects in crystalline materials through surfaces and amorphous structures.

To begin the symposium, **Laurence Marks**, Northwestern U, presented an overview of the competing driving forces controlling the surface crystallography in single- and multi-element nanoparticles with ample historical perspective on the use of electron scattering to study nanoparticle surfaces and growth. An important growth area in electron scattering involves the collection of full 2D diffraction patterns from a 2D map of rastered electron probe positions, producing very large 4D or 5D (*in-situ*) datasets ripe for many and varied analyses. **Paul Voyles**, U Wisconsin – Madison, reported on the efforts of his group to determine the differences in local medium-range order in metallic glasses through fluctuation electron microscopy and the effect of slight composition variations on glass-forming ability. The use of scanning diffraction data to recover the full electron phase at atomic resolution through ptychographic methods was presented by **Hao Yang**, Lawrence Berkeley National Laboratory (LBL). These methods were applied by **Roberto dos Reis**, also from LBL, to determine local nanoscale variations in space-group symmetry of beam-sensitive $CsPbBr_3$ and $CsPbCl_3$ halide perovskite materials, revealing the mosaic nature of octahedral disorder. 4D scanning diffraction data was also analyzed by **Yu-Tsun Shao**, U Illinois Urbana-Champaign, to uncover the local symmetry breaking at nanoscale resolution in the vicinity of relaxor ferroelectric domain boundaries $(1-x)Pb(Zn_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$, elucidating the interaction of 1D and 2D topological defects through lattice rotation vortices in these materials. To conclude the symposium, **Jing Tao**, Brookhaven National Laboratory, outlined the challenges and early results using megavolt ultrafast electron diffraction to study metastable charge-density waves in transition-metal dichalcogenide materials.

This year's symposium received positive feedback from the community, and there is momentum to organize a similarly focused symposium at ACA 2018.

Jim Ciston
Olaf Borkiewicz

2.3.1: Evening Session on Diversity and Inclusion

L-R: Krystle McLaughlin, Cheryl Stevens, Bernard Santarsiero, Oluwatoyin Asojo

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

The first talk was by **Bernard Santarsiero**, U Illinois at Chicago (UIC), who described the L@S GANAS program at UIC. Funded by the U.S. Department of Education, the L@S GANAS program aims to improve outcomes for Latino STEM students, including academic performance as well as persistence and graduation rates. L@S GANAS targets Latinos and low-income undergraduate students, and aims to support the whole student through strong ties to their heritage. For this holistic support approach, the program places students in a structured, intensive, and intrusive environment, including a special fall-term course to improve their academic and professional skills, while providing an emphasis on creating supportive diverse networks to improve students' sense of belonging and develop "social capital." Participants also receive active and collaborative learning opportunities to improve their success in gateway courses. Additionally, significant financial support is provided to students in the program in the form of research fellowships, to sustain interest and to assist with "unmet needs." Often these "unmet needs" can derail students, and addressing them can improve outcomes. Santarsiero also described another project that involved community members and the underrepresented STEM students, bringing them together to promote citizen-science. The UIC administration has given its full support to the program, and this emerged throughout the rest of the session as a common theme: To tackle diversity and inclusion issues, you need "buy-in" from your administration!

The next talk by **Oluwatoyin Asojo**, addressed some strategies to do this, and how to communicate the significance of diversity and inclusion issues. She noted that one of the main questions you may get when trying to start any discourse on diversity and inclusion or any programs targeting underrepresented scientists is, "Why do we need to do this?" Asojo provided several resources, including published papers to help answer this question.

https://www.scientificamerican.com/article/how-diversity-makes-us-smarter/

https://psmag.com/news/here-are-four-myths-about-diversity-in-science

Lu Hong and Scott E. Page, *Groups of diverse problem solvers can outperform groups of high-ability problem solvers, Proc. Natl. Acad. Sci. U. S. A.* **2004**, *101(46)*, 16385–16389 ***http://www.pnas.org/content/101/46/16385.full***

Hannah A. Valantine and Francis S. Collins, *National Institutes of Health addresses the science of diversity*, *Proc. Natl. Acad. Sci. U. S. A.* **2015**, *112(40)*, 12240–12242 ***http://www.pnas.org/cgi/doi/10.1073/pnas.1515612112***

Asojo discussed methods used since 2001 to engage high-school and undergraduate students in crystallographic research in her laboratory and identified successes and failures involved in the process of fully integrating these pre-baccalaureate students in crystallography research. The need for "buy-in" from the host-institutions, strategies for recruiting and retaining students, and major barriers to operating these summer research programs were also discussed. Additionally, Asojo identified potential funding sources such as NSF, NIH, ACS, and foundation grants.

In the third talk of the session, *Diversity and inclusion – steady progress by degrees*, **Cheryl Stevens**, Western Kentucky U (WKU), shared her experience addressing the issue of diversity in the faculty through her position as the Dean of the Ogden College of Science and Engineering at WKU. Stevens described the strategy she took, adapted from Wittenberg-Cox, *How Women Mean Business* (2010): (1) Take a look at where we are, and be aware of the problems; (2) Collect data to actually prove there is a problem, and (3) Develop a plan to address the problem. Addressing the problem, for example, might include strategies to address campus attitudes, processes/procedures, financial challenges, and culture. When Stevens arrived in 2012 at WKU from Xavier University, an HBCU in New Orleans, she was surprised at the low diversity in her environment. For example, out of 90 tenured Associate Professors in her college, there were only 14 women and few people of color overall. First, Ogden College defined overall goals that included diversity and inclusion. These became a core value for the college, providing the necessary institutional "buy-in." Some strategies they undertook to address the problems were refining the search committee process for new faculty hires, recruiting underrepresented faculty candidates at conferences, and creating a college level Task Force on Diversity. They also introduced strategies for increasing faculty retention, including a welcome reception for new faculty and spouses, meetings 2-3 times during the academic year, faculty mentors, research mentoring for setting up labs and proposal writing, a luncheon for international female junior faculty, and the initiation of a Women in Science and Engineering group. Together, these strategies have enabled a positive increase in diversity and inclusion for faculty in the Ogden College at WKU. With the implementation, the aim is to focus on sustainability, making sure there is long-term success, to keep making positive progress. Hiring diverse faculty, said Stevens, is the short-term goal, but culture change and longevity is the long-term objective.

Krystle McLaughlin
Oluwatoyin Asojo

3.1.1: Materials for a Sustainable Future

L-R: Sofia Antal, Kamila Wianderek, Ryan Hadt, Andrea Bruck, Alfred French, Vicky Doan-Ngyen, Cheng Wang, Craig Bridges

The **Materials for a Sustainable Future** session focused on innovative characterization techniques and materials development for energy production and storage. Research areas covered included scattering studies done on materials for energy-related technologies such as batteries, solar conversion, hydrogen storage, and carbon capture. **Cheng Wang**, Advanced Light Source, opened the session with a presentation of resonant soft X-ray scattering (RSoXS) as an important complementary tool for studying polymeric and biological materials. **Sofia Antal**, New Mexico Highlands U, reported on investigating crystalline products of CO_2 capture by carboxyamines. **Ryan Hadt**, Argonne National Laboratory, pivoted the topic to energy conversion by cobalt and nickel oxygen-evolving catalysts and their role in O–O bond formation for oxygen evolution reaction. **Craig Bridges**, Oak Ridge National Laboratory, discussed computational design and development of ion-conducting oxides for solid oxide fuel cells. **Albert French**, U. S. Department of Agriculture, continued the discussion of sustainability with the topic of crystallography and computed charge density of aged cellulose chromaphores. The session's final speaker, **Andrea Bruck**, Stony Brook U, received the **Margaret C. Etter Student Lecturer Award** from the Materials SIG. Andrea presented on the roles of composite electrode constituents in the electrochemistry of $Li/Ag_2VO_2PO_4$ batteries.

Vicky Doan-Nguyen

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

This session considered innovative ways to obtain crystallographic data using standard methods and tools. A wide range of non-standard protocols was discussed, tackling topics from K-edge mass absorption coefficients to centering samples. **Michael Ruf**, Bruker AXS, described enhancements in hardware and software to increase the completeness in high-pressure experiments using multiple samples in a Diamond Anvil Cell. **Arturas Vailionis**, Stanford U, discussed grazing incidence diffraction using a single-crystal diffractometer with a kappa goniometer. **Randy Alkire**, Argonne National Laboratory, described a method developed for determining the near K-edge mass absorption coefficients for Ni, which shows good agreement at the 1% error level. **Martin Adam**, Bruker AXS, focused on optimizing sample centering through automation, while **Milan Gembicky**, U California San Diego, demonstrated ingenuity by customizing a multi-purpose diffractometer to analyze biological calcification. Finally, **Cary Bauer**, Bruker AXS, demonstrated how powder diffraction could be investigated with a single-crystal diffractometer.

Tiffany Kinnibrugh

Session 3.2.2: Complementary Methods

L-R: Craig Bridges, Avni Bhatt, Haydyn Mertens, Leiah Carey, Leighton Coates. Photo by ACA Meeting student volunteer.

This session focused on the need to combine multiple advanced analytical methods to properly understand complex materials and phenomena. The initial concept was found to be relevant for both the biological and materials tracks of the ACA meeting, and thus it was constructed as an interdisciplinary session. The session therefore attracted wide-ranging talks, from proteins to inorganic materials. The session was well attended, with good discussions following each talk, and the mix of subject matter was useful in promoting the sharing of ideas across different fields. The opening talk of the session was given by **Edward Snell**, U at Buffalo

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and Hauptman-Woodward Medical Research Institute, in which he showed that a combination of particle induced X-ray emission (PIXE) and comprehensive analysis of crystallization screening outcome can identify erroneous metals that would otherwise compromise the study of metalloprotein structure. The second talk by **Haydyn Mertens**, European Molecular Biology Laboratory, Germany, focused on membrane proteins and discussed the wide range of methods used to uncover structural information in these complex systems, with a particular focus on the complementarity of SAXS and SANS. Next, **Leighton Coates**, Spallation Neutron Source (SNS), Oak Ridge National Laboratory, discussed the current state of neutron protein crystallography at SNS, with the application to structure-derived information on enzyme mechanisms, and how neutrons can be used with X-ray scattering to determine both heavy atom and light atom positions.

After the break, **Luke Daemen**, also of SNS, discussed how neutron vibrational spectroscopy could be used to derive structural information that can be combined with diffraction studies, and the advantages of the high intensity of the VISION beamline in performing studies of small samples or weak scatterers that were not previously possible. **Leiah Carey**, North Carolina State U, then discussed the first neutron diffraction structure of a multifunctional heme protein, in particular the heme reactive center of the enzyme dehaloperoxidase (DHP) from the marine worm *Amphitrite ornata*; this structural information is combined with spectroscopic analysis of substrate binding to better understand the differing functionalities that exist on the heme active site. Finally, the Etter award-winning talk of **Daniel Olds**, SNS, was presented by **Matt Tucker**. This talk ended the session on a high note by showing how new analysis of data collected with total scattering and pair-distribution function (PDF) methods at time-of-flight neutron sources can improve the quality of fit, and allow detailed study of atomic order that is complementary to traditional wide-angle scattering (Rietveld) methods. The session benefited greatly by receiving sponsorship from Douglas Instruments and Art Robbins Instruments.

Craig Bridges
Avni Bhatt

3.2.3: Crystal Structure and Property Prediction

This session, very kindly sponsored by Boehringer-Ingelheim, showcased some of the challenges in the prediction of crystal structures and their properties as well as the interpretation of this structural information.

Our session opened with an entertaining and thought-provoking presentation from **Joel Bernstein**, Ben-Gurion U of the Negev, Israel, on the relationship between chemistry, fuzzy logic and patent law (the true sport of kings!). Chemists, particularly academic ones, often think in terms of exact answers or observations – discussing rules and scientific laws. In practice, a lot of the structural chemistry questions that come up in patent litigation, such as that around pharmaceutical solid form patents, is concerned with the exceptions to these rules or grey areas where interpretation is required. Joel took us through some intriguing examples of real patent litigation cases where "fuzzy logic" came into play to tackle these grey areas (see also: *Israel Journal of Chemistry*, **2017**, *57*, 124-136).

Angeles Pulido, U Southampton, UK, next introduced us to the design of porous organic molecular crystals using Crystal Structure Prediction (CSP) techniques. Awkwardly shaped molecules that form strongly-directional intermolecular interactions can potentially be arranged into unusually stable porous frameworks. The use of CSP along with energy-structure-function maps provided guidance as to which molecules can actually form these surprisingly stable honeycomb-like frameworks (see also: *Nature*, **2017**, *543*, 657-664).

Juan Manuel German Acacio, National Autonomous U of Mexico, then shared with us some recent results illustrating the inclusion of unexpected guests in a series of Pd-complex crystal structures.

The second half of the session started with **Joost van den Ende**, Hoffman-La Roche, who spoke about energy barriers and mechanisms in solid-state transitions. Joost presented several interesting cases of polymorphic transitions, such as DL-norleucine and fatty acids in chocolate. He also discussed the role of predictions, based on various theoretical and semi-empirical tools, to explain and rationalize mechanisms of solid-solid phase transitions (see also: *CrystEngComm*, **2016**, *18*, 4420-4430).

Victoria Soghomonian, Virginia Tech, presented an interesting topic of structural aspects of electrical conductivity as a function of pressure. Victoria discussed a family of mixed vanadium gallium hexafluorides, which undergo a monoclinic to cubic phase transition upon heating or under high pressure. She presented a very interesting case relating structural chemistry with electrochemistry in the context of a highly important research of energy storage.

Our final speaker of the day, **Madushani Dharmawardana**, U Texas at Dallas, was awarded the Industrial SIG **Etter Student Lecturer Award** for her talk on a thermo-mechanical responsive crystalline organic semiconductor. Madushani discussed polymorphic transitions in the context of thermal expansion and thermochromism. She presented several studies of naphthalene diimides and other compounds that exhibit a color change during polymorphic transition, gave structural reasons for color change with temperature, and discussed cases of unusual thermal expansion.

Peter Wood
Mariusz Krawiec

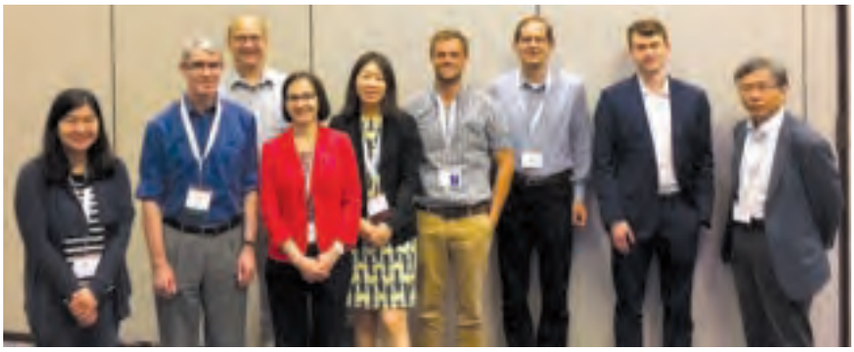
Neela and Hemant Yennawar. Photo by Richard Bromund.

3.2.4: Hot Structures

The **Hot Structures** Session was co-chaired by Elizabeth Goldsmith, U Texas Southwestern Medical Center, and Sangita Sinha, North Dakota State U. Several speakers presented breakthrough research. **Nicholas Noinaj**, Purdue U, presented data on how bacteria load proteins into their outer membranes. **Kerry Goodman**, Columbia U, presented new data on how cadherins mediate neuronal self-vs.-nonself-discrimination. **Diana Tomchick**, U Texas Southwestern Medical Center, presented the structure of the long-sought multi-domain vesicle fusion protein MUNC13. **John Tainer**, U Texas MD Anderson Cancer Center, spoke about higher-order oligomerization of AIF, and how AIF sites of allostery link to the NADH-binding site. Talks on enzymology and drug discovery were presented by **Andrzej Joachimiak**, U Chicago, and **Margarita Tararina**, Boston U, while session co-chair **Elizabeth Goldsmith** described conformational regulation in WNK protein kinases by environmental factors. All-in-all, brain-food for a structural biologist!

Elizabeth Goldsmith
Sangita Sinha

3.2.5: Crystal Growth



L-R: Miki Senda, Kenneth Harris, Tom Friedlander, Magdalena Owczarek, Yi-Yeoun Kim, Benjamin Palmer, Travis Gallagher, Daniel Wrapp, Rui Tamura

The session on **Crystal Growth**, organized by Kenneth Harris, Cardiff U, UK, covered a range of different aspects of crystallization sciences, including fundamental understanding of crystallization processes in both biological systems (e.g., biomineralization) and laboratory contexts, and developments in experimental techniques for the preparation of high-quality crystals.

Benjamin Palmer, Weizmann Institute of Science, Israel, opened the session with a beautifully illustrated lecture on biologically controlled crystal growth, focusing on the image-forming mirror in the eye of the scallop. He demonstrated that each eye of the *Pecten* scallop contains a concave mirror to focus light onto a retina, operating on principles similar to a reflecting telescope. The hierarchical organization of the multi-layered mirror is exquisitely controlled for image formation, both with regard to the structure of the component guanine crystals at the nanoscale and the complex morphology of the crystals at the millimeter level. Amazingly, each layer of the mirror is formed from a tiling of regular square guanine crystals. The ability of the scallop to form almost perfectly square crystals for a monoclinic crystal structure is believed to be achieved by controlling crystal twinning and by carrying out crystallization inside a confined environment.

Yi-Yeoun Kim, U Leeds, UK, then gave a very enthusiastic presentation of her research to develop bio-inspired strategies aimed at incorporating organic components within crystals of calcite (calcium carbonate). The strategy recognizes that the nano-composite structure of biominerals derives from an intimate association of organic molecules with a mineral host. She demonstrated that the strategy has been applied successfully to prepare single crystals of calcite as a host mineral, precipitated in the presence of a wide range of guest species, encompassing commercial latex particles, organic/inorganic nanoparticles functionalized with block copolymers, and small molecules such as amino acids. Using several experimental techniques for rigorous characterization of the composite systems, she revealed insights into the mechanism of occlusion within the host crystals, and the relationships between macroscopic physical properties and the microscopic structure of the composite materials.

Over several years, **Rui Tamura**, Kyoto U, Japan, has pioneered a strategy – named "*preferential enrichment*" – for spontaneous enantiomeric resolution, which relies on two processes: (i) a solvent-assisted polymorphic transition, and (ii) subsequent selective dissolution of the excess of one enantiomer from the transformed disordered crystals into the mother liquor. Rui's lecture described the latest developments in this fascinating process, including *in-situ* XRD and microscopic observations of the polymorphic transition, as well as kinetic and thermodynamic studies to understand the chiral symmetry breaking. His research has applied the preferential enrichment concept to a range of co-crystal systems, including those containing chiral drugs.

Magdalena Owczarek, Northwestern U, gave a very enthusiastic presentation of some remarkable recent results on crystals formed from derivatives of imidazole (containing at least one halogen substituent), selected on the expectation that they may exhibit desirable properties such as ferroelectric or piezoelectric behavior. Magdalena discovered that several materials in this class have a strong propensity to form curved crystals, and demonstrated through rigorous experimental studies that halogen bonding may play a key role in the tendency for the crystals to exhibit curved morphologies. Furthermore, by extending this idea, she has shown that co-crystallization of different haloimidazoles gives rise to flexible crystals, many of which do indeed exhibit ferroelectric and piezoelectric properties.

The remaining talks in the session covered different aspects of protein crystallization. **Miki Senda**, Photon Factory, Japan, focused on improving the reproducibility of producing high-quality crystals for protein crystallography. She

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demonstrated that carrying out crystallization under anaerobic conditions in carefully designed apparatus could have significant advantages, including the reproducible formation of crystals of larger size and higher quality than under aerobic conditions. Next, recognizing that vapor diffusion is the most commonly used method for protein crystal growth, **Tom Friedlander**, Formulatrix, described systematic studies of the effects of humidity on the rate of drop evaporation, demonstrating that precise humidity control is a significant advantage in ensuring reproducibility of protein crystallization processes. On a related theme, **Daniel Wrapp**, Dartmouth College, described an automated strategy for iterative optimization of protein crystallization screens. His method takes the results from an initial set of crystallization trials, and then iteratively adjusts the conditions (e.g., precipitant concentrations) to be used in the next crystallization trials. Repetition of this iterative optimization process was shown to lead to a substantial increase in the probability of achieving successful crystallization of a protein from a limited set of reagents. Finally, **Travis Gallagher**, NIST, concluded the session by describing a model for the crystallization of proteins based on concepts of helical pseudosymmetry.

Kenneth Harris

Session 3.3.1: How Do I Get My Data? (Beamlines and Their Capabilities)

L-R: Sanjit Ghose, Tiffany Kinnibrugh, Allen Orville, Marian Szebenyi, Christian Feiler (at rear), Randall Winans, Ashfia Huq. Not shown: Christine Beavers. Photo courtesy of Ashfia Huq.

Facilities that host synchrotrons, neutron sources and free-electron lasers are extremely useful resources for the crystallography community. This evening session hosted several speakers from various facilities to provide information about proposal process, access mode and also beamline description that enables a wide range of materials research from macromolecular crystallography to materials diffraction and studying large-scale structures using small-angle scattering.

First speaker of the session **Marian Szebenyi** from MacChess, Cornell High Energy Synchrotron Source (CHESS), described the NIH-funded resource that provides support for structural biologists collecting data at CHESS, one of the five high-energy synchrotron sources in the United States. State-of-the-art support is provided for macromolecular crystallography (MX) and BioSAXS. The next speaker **Randall Winans** is a Senior Scientist and the leader of the Chemical and Materials Science Group in the X-ray Science Division of the Advanced Photon Source (APS) at Argonne National Laboratory. He is responsible for the beamlines in Sector 12 and the USAXS beamline at 9-ID. Recently, Winans was interim head of the Structural Sciences group, Sector 11 and 17-BM. He went over a wealth of information regarding APS. **Christine Beavers** covered the resources available at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory, followed by **Christian Feiler** who described three MX beamlines at the electron storage ring BESSY II operated by Helmholtz-Zentrum Berlin (HZB), Germany. **Allen Orville**, the Principal Scientist of the UK XFEL Hub, described the mode of operation for larger collaborations mode at the free-electron laser facilities. The last two speakers **Sanjit Ghose** and **Ashfia Huq** gave brief descriptions of beamlines available for crystallography and small-angle scattering at NSLS II, the new synchrotron source located at Brookhaven National Laboratory, and the two neutron facilities Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR) located at Oak Ridge National Laboratory. More detailed information from all these facilities can be downloaded from the ACA New Orleans program website: ***http://www.amercrystalassn.org/documents/2017%20Meeting/HowToGetMyData.pdf***

The session organizers are thankful to CHESS and ORNL for providing funding to serve snacks at this evening session.

Ashfia Huq
Tiffany Kinnibrugh

3.3.2: Would You Publish This?

This ever-popular session was held for the 7th year (originally held in 2009) and was generously supported by Crystallographic Resources, Inc. The session began with **Victor Young**, U Minnesota, presenting compounds that undergo temperature-dependent phase transitions between 'better' and 'poorer' quality structures. Discussion centered on the trade-off between the commitment of time and resources to obtain the structures of both phases vs. the value to the crystallographic community in reporting both phases. **Laura McCormick**, U St Andrews, UK and Advanced Light Source, presented a conundrum where attempts to hone in on reaction scale-up conditions produced five different phases! All but one of the phases were structurally characterized. The 5th phase gives clean diffraction, but a poor structure model. To what extent should the 5th phase be reported, if at all? **Carl Schwalbe**, Aston U, UK, provided examples relating to publication practices. Carl discussed eliminating weak high-angle data to improve statistics. Although truncating data might be interpreted as 'trying to satisfy ones vanity' by improving data and refinement statistics, there can also be real consequence, for example fewer flags in *CheckCIF* or meeting the R-factor < 0.05 filter to achieve more hits in *CSD Conquest*. **Danielle Gray**, U Illinois Urbana-Champaign, presented a trend in her lab of obtaining quick datasets as part of the screening process. The datasets provide enough information to identify the substance and refine isotropically – i.e., enough to satisfy the scientist. The

3.3.2: Would You Publish This?, ctd.

L-R: Laura McCormick, Carl Schwalbe, Christine Beavers, Carla Slebodnick, Danielle Gray, Victor Young. Photo courtesy of Victor Young.

ramifications of this new trend are both local (e.g., lab not bringing in data collection fees) and broader (structures never being published). **Carla Slebodnick**, Virginia Tech, presented a system with space group ambiguity between *I*4/*m* and *I*-4. *I*4/*m* introduces disorder into a significant portion of the molecule, but no disorder is present when refining in the lower symmetry space group, *I*-4. Unfortunately, in *I*-4, the remainder of the molecule is related by mirror symmetry and strong correlation between atoms required heavy restraints to stabilize the refinement. Opinions differ on best choice of space group. The session concluded with **Christine Beavers**, Advanced Light Source and U California, Santa Cruz, presenting the 'low resolution' structure of a single-molecule magnet. The structure model allows identification of the geometry at the Ni_{18} core of the molecule, but not the coordinated ligands. When publishing such structures, what compromises are acceptable?

Carla Slebodnick
Danielle Gray

4.1.1: Etter Symposium for Young Scientists

L-R: back row – Nico Giordano, Justin Kurian, Matthew McLeod, Avni Bhatt, Zhelong Xiang; front row – Roberto dos Reis, Kyle Stiers, Stanislav Stoyko, Anastasiya Vinokur, Daniel Mast, Thomas Bohl, Margarita Tararina. Photo courtesy of Roberto dos Reis.

This half-day session, following the **Margaret C. Etter Early Career Award** presentation, brought together young scientists to present their works for a broad audience at ACA. The session provided a platform of discussion for graduate, postdoctoral fellow, and early career scientists who want to pursue their careers as part of the crystallographic community. The session featured ten exceptional speakers covering a range of subjects from X-Ray crystallography to cryo-electron microscopy (cryo-EM), exhibiting the diversity of the crystallographic sciences. The session started with work presented by **Zhelong Jiang**, U Illinois Urbana-Champaign, on the application of *in-situ* X-ray diffraction to analyze the progress of reactions leading to the formation of inorganic crystal Fe_2SiS_4, followed by **Anastasiya Vinokur**, U Wisconsin – Madison, who presented a combination of X-ray

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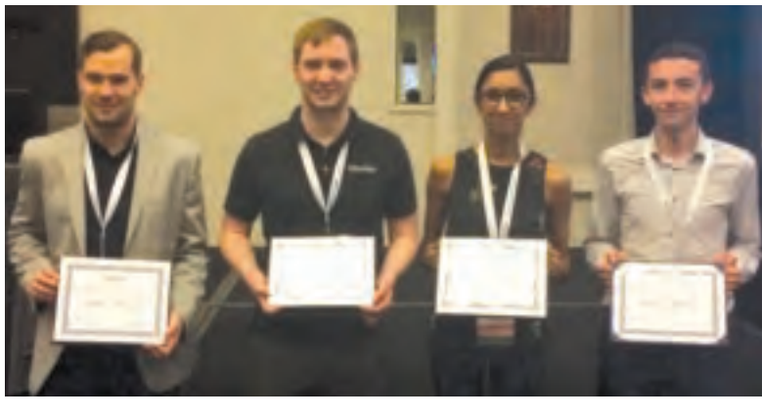
diffraction, NMR, and mass spectrometry data to elucidate molecular structure of natural products extracted from *Millettia versicolor*. An excellent example of combining both theory and experimental methods was given by **Daniel Mast**, U Nevada Las Vegas, who was able to model the negative thermal bond expansion in Tc_2O_7 using variable temperature single-crystal diffraction and Langevin molecular dynamics. Cryo-EM was a highlighted topic at this years' ACA meeting and was represented in the Etter Symposium by exceptional talks from **Justin Kurian** and **Avni Bhatt**, both of U Florida.

In this symposium, ACA has honored students with awards for their outstanding work. The awards were sponsored by the ACA SIGs: Biological SIG award to



2017 Etter Student Lecturer Award Winners honored at this session, L-R: Matthew McLeod, Kyle Stiers, Avni Bhatt, Nico Giordano. For the complete list of 2017 Etter Award winners, turn to p. 44. Photo courtesy of Roberto dos Reis.

Avni Bhatt for her abstract entitled *Crystallographic insight into enhanced catalytic activity of carbonic anhydrase II using "activating" ligands*; Service Crystallography SIG award to **Nico Giordano**, U Edinburgh, UK, for *A pressure induced phase transition of 4-iodobenzonitrile*; Young Scientist SIG award to **Kyle Stiers**, U Missouri, for *Personalized biophysics of human PGM1 deficiency*; and Canadian Division award to **Matthew McLeod**, U Waterloo, Canada, for *Anion inhibition of PEPCK manifested as substrate inhibition; Using crystallographic methods to determine thermodynamic data*.

The YSIG is pleased to have opened this excellent opportunity for young scientists and looks forward to next year's meeting.

Roberto Dos Reis
Margarita Tararina

4.1.3: Conformational Dynamics of Ligand Binding

Session 4.1.3 was organized by Michael James, U Alberta, Canada, and Barry Finzel, U Minnesota, to provide a forum for discussion of the effects of conformational change induced by ligand binding by proteins. Speakers included **Gyanendra Kumar,** St Jude Research Hospital, **Denis Kudlinski**, DKFZ, Heidelberg, Germany, and **Suzanne Mays**, Emory U. **Henry Tang**'s (Lawrence Berkeley National Laboratory) studies with phosphoenolpyruvate kinase combining single-crystal work and HT-SAXS provided a nice example of how point mutations can influence protein dynamics and ligand selectivity. **Michael James** presented a comprehensive summary of published work that enabled the precise quantification of the entropic penalty paid in binding a peptide inhibitor of penicillopepsin with rotational degrees of freedom. Conformational restriction of each rotamer accounts for 0.9 Kcal/mol of binding affinity. **Emil Pai**, U Toronto, Canada, presented some fascinating observations made regarding the conformational dynamics of fluoroacetate dehydrogenase. These confirm the existence of a dynamic cooperativity between subunits of the homodimer that seems to allow the entropic cost of ligand binding in one subunit to be distributed and offset by increasing the conformational dynamics of the other subunit. It will be interesting to see if this turns out to be a more generalizable feature exploited by many homodimeric enzymes.

Barry Finzel

4.1.4: In situ and Operando Measurements

This half-day session covered cutting-edge applications of *in situ* and operando techniques in the areas of chemistry, material sciences and solid-state physics. A total of eight speakers presented their research. **John Parise** from Stony Brook U and Brookhaven National Laboratory led with the opening talk, on combining *in situ* diffraction-DSC experiments with theoretical predictions and data mining to guide the search or synthesis of metal-organic frameworks (MOFs) promising for gas sorption and separation usage. **Tao Sun**, Argonne National Laboratory, introduced the audience to the ultrafast diffraction and imaging applications on his beamline, which pushed the temporal resolution to the microsecond range and opened a door to study very fast transformation processes. Following Tao, **Amy Marschilok**, Stony Brook U, talked about mesoscale to nanoscale investigations of battery materials using both energy and angle dispersive XRD. Amy examined how silver formed and localized in the vanadium phosphate framework upon fast or slow charge and discharge cycles, and the impact on battery capacity and lifetime.

After the coffee break, **Anna Plonka** from Yeshiva U presented her study of Zr-based MOFs for filtrating and degrading simulants of nerve-agent materials. Anna used multiple *in situ* methods including XRD, XAFS and infrared spectroscopy to probe the capturing and degradation of the simulants within the MOFs. The next three talks were about *in situ* synthesis, but with different scattering techniques and for different types of materials. **Michael Campos**, Columbia U, used both small-angle and wide-angle X-ray scattering to understand the nucleation and growth of colloidal quantum dots in the PbS and PbSe systems. Michael's talk was particularly well received by the audience, with four questions about the experimental details and alternative oxide precursors for the synthesis. **Ashfia Huq**, Oak Ridge National Laboratory, talked about her study on solid-state synthesis of lanthanum molybdenum oxide with neutron diffraction, which yielded crucial information on the intermediate phases

and formation temperatures that could only be obtained with the *in situ* measurements. Following Ashfia, **Chunhua Hu** from New York U showed his research on determining the crystal structure of a glycine polymorph that might exist on extraterrestrial bodies. Chunhua applied a flash-cooling method with *in situ* synchrotron XRD to obtain the powder profile of the target phase that led to the structure. **Scott McCormack** from U Illinois Urbana-Champaign gave the final talk of the session, on negative thermal expansion materials. Scott illustrated an *in situ* diffraction setup with a quadrupole lamp that could supply heat to 2000 °C, which he used to study hafnium titanium oxide. He analyzed the evolution of the sample's zero thermal expansion directions with 3D plot and pole figures.

Wenqian Xu
Sanjit Ghose

Session 4.1.5: Enabling New Science with Light Sources and Hybrid Methods

L-R: Alke Meents, Jeney Wierman, Alexey Rozov, Lois Pollack, Seth Cory, Chelsy Chesterman, Armin Wagner, Steve Meisburger

At this year's annual meeting, **Session 4.1.5** was made possible by generous support from Dectris, Xenocs/SAXSLAB, ACA, MiTeGen, and Rigaku. The session was organized by Nozomi Ando and Armin Wagner, and chaired by Armin and Steve Meisburger. Talks ranged over topics from enzyme structure to novel X-ray methods. Highlights included **Lois Pollack**, Cornell U, who spoke about the use of time-resolved SAXS to study nucleosomes. **Seth Cory**, Texas A&M U, winner of the Light Source SIG's **Etter Student Lecturer Award**, gave an excellent talk on the structure of the human cysteine desulferase complex. Two talks addressed aspects of the emerging field of serial protein microcrystallography at synchrotrons. **Jeney Wierman**, Cornell U, a veteran speaker at the ACA, reported on latest results from CHESS using monochromatic X-rays, while **Alke Meents**, DESY, Germany, spoke about recent low-background pink beam experiments at BioCARS.

Armin Wagner
Nozomi Ando Steve Meisburger

4.2.1: Communicating Science to the Public

As Ambassadors for Crystallography we must convey the utility and excitement of our scientific advances to friends, family, funding agencies, legislators, and the general public. This session, organized by Katrina Forest, U Wisconsin – Madison, and Jim Fettinger, U California Davis, and sponsored by the ACA Communications Committee and the Young Scientist SIG, provided enabling advice for connecting with the public audience. The broad appeal of the topic was evident from the 76-attendee crowd.

The session opened with the introduction of **James O'Brien**, Missouri State U, the 2017 winner of ACA's **Wood Science Writing Award**. O'Brien was gearing up for his speech at the Tuesday evening banquet and was not a scheduled speaker for our session, but came as a guest. Moreover, in a last-minute surprise gesture, he provided a copy of his hot-off-the-presses book, *The Scientific Sherlock Holmes*, officially released in paperback on June 1st. This treasure may have been one reason 59 intrepid souls remained spellbound until the session close, when prizewinner Randy Alkire was drawn. O'Brien had explained to the organizers that his winding path to book authorship was not necessarily one that would be easy to follow. He was asked to speak at an ACS symposium on chemistry and science fiction, which led to writing a book chapter, which was nicely contemporaneous with the "flap" about Sherlock as the eponymous BBC series took off, which lead a publisher to invite him to write *The Scientific Sherlock Holmes*. The lesson was to be ready to take advantage when opportunity presents itself.

Coming off a very busy week as co-organizer of the EM **Transactions Symposium**, **Stephen Burley**, RCSB Protein Data Bank, Rutgers U, *Demonstrating the value of 3D macromolecular structures*, described the history of the PDB, the pioneering organization for open-access science. Beginning with seven structures in 1971, the PDB has over 130,000 structures today and grows a little over 10% a year. With 1.5 million hits per day, PDB public access serves as validation, as consumers can readily see the quality of the product. From blind methods development challenges at the cutting edge of research, to outreach and education such as David Goodsell's wildly popular PDB-101 series, the PDB has become essential to biomedical research and education. Major pharmaceutical companies use the PDB databases for structure-based drug design, with a sterling example being the treatment of leukemia, with such drugs as Gleevec (2001), Sprycel (2006), and Tasigna (2007) playing a role in the doubling of patient survival rates since their discoveries. The annual cost of maintaining the PDB is $6.9 million, mere pennies per download, as the institution approaches its 10-year funding renewal in 2018.

Brian McMahon, IUCr, Chester, UK, *Showing that crystallography matters*, described numerous public resources created by the IUCr Outreach group to, "increase public awareness, inspire young people and promote the universality of science" for the occasion of the

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International Year of Crystallography in 2014. A moving video "Welcome to the World of Crystallography" (***http://www.iycr2014.org/about/video***) was spearheaded by Juan Manual Garcia-Ruiz; remarkably the YouTube version has now been subtitled into 29 languages! A short film starring young Johanna as she learns about discoveries in crystallography (***https://www.youtube.com/watch?v=AlBPajICFIU***) is promoting crystallography to children. The IUCr makes available shareable PDF posters, organizes photo competitions, and manages worldwide outreach such as crystal growth contests. An interactive time line in which one can map one's own events onto crystallographic landmarks (***http://www.iycr2014.org/timeline***) provides a personal link to crystallographic milestones. Recognizable and breathtaking stamp collections from nations worldwide broadcast the beauty of crystals and crystallography.

Beamline scientist, ACA member, author of the banquet review in the Fall 2016 *Reflexions*, and major proponent of social media **Christine Beavers**, Advanced Light Source and U California Santa Cruz, gave a juicy, engaging talk, *Using social media for #SciComm: An interactive tutorial*, in which she encouraged members of the ACA to take full advantage of social media and provided a real-time lesson for audience members to become Twitter users. As Beavers advised, think of these as 140 character microblogs and boil down the essence of your message. Take advantage of searchable hashtag links (like #ACANOLA). Remember that Tweets are dynamic messages and that the time and even time zone you are in when tweeting will impact your readership. Case in point, there were multiple tweets within our session including this one from Camelia Stan, "Learning about Twitter by listening to @XtalGrrl talk about Twitter at #ACANOLA is a bit meta." Was it coincidence that there were 41 new @ACAXtal followers in May and 49 in June compared to 8.5 per month the previous 6 months?

Diane Dickie, Brandeis U and Sandia National Laboratory, *From magic show to crime scene analysis – getting kids interested in science with hands-on investigations*, described her 12 year-long and still-going-strong project at Sandia designed as a collaborative (not competitive) "CSI Dognapping" case to engage children from Title I schools to experience the thrill of laboratory science. As described in a recent *Chemical & Engineering News* article, this program recognizes that "we decide early what we do not want to be when we grow up." Dickie and her colleagues, knowing that kids choose to pursue what they know, show them science is a real future career option so that they may keep it in mind. Knowing just how to engage kids of this age, the scientists bring the children into a "surprise" case involving broken equipment, a missing dog, ID cards so they feel a sense of belonging, and a good dose of yuck factor along with serious experimental analysis of clues and statistical significance. The team has collected data to demonstrate the impact of their program; the children's knowledge increases and is retained at least 2-3 months later when the post-test is repeated.

As the recipient of an ACA Outreach Grant (did you know about these – apply!), **Katharine Page**, Oak Ridge National Laboratory (ORNL), *Uniqueness and you: How the disorder of atomic structure enables your world*, set out to sell Materials Science to the public. Wanting to avoid old and outdated memes, she focused on three components: Inspiration Through Observation, Hands on Structure Activity, and a Web-Based Simulator to help young students engage in materials science. Kids don't get bored building models! As **Thomas Proffen**, also of ORNL, shared with the audience, tool building for kids can turn into tool building for research. Symmetry and structure are fascinating to children, and the ORNL project has now grown into a traveling science fair with six installations. Check for yourself at ***www.myatomicstructureworld.org*** and ***www.orcsgirls.org***.

Representing the AIP, science journalist **Catherine Meyers** of *Inside Science*, *Talking science with journalists*, provided imminently usable advice for communicating with the public by working with science journalists. In a Pew Research Center survey of Americans in 2015, 59% declared themselves very interested in science, which is a heartening figure until you learn that only 2% of all stories in the paper are science-related. Meyers relayed that writing science is hard for journalists due to the real culture clash between them and scientists. So, as a scientist how can you help these fantastic professionals convey your message? According to Meyers, consider the true essence of your story; what you did and why it matters. Be ready to discuss these points with a journalist in every-day language using creative analogies and metaphors; try your talking points out on a neighbor. Another strong recommendation is to get to know the public information officer at your institution, and go to her or him right away when you know an article will be published, as the clock is ticking. Apropos an earlier talk, Meyers confirmed, journalists do follow Twitter, so tweet. And, show your human side. If the public likes scientists, they will like science.

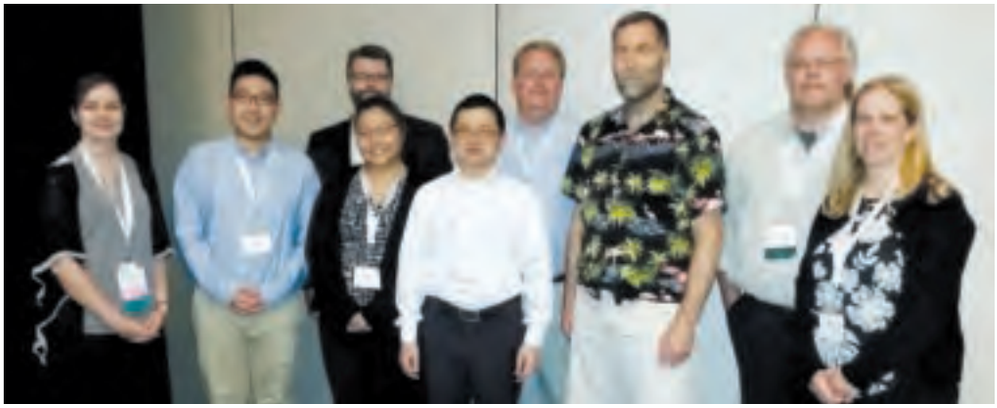
See you at #ACA_TO in 2017!

Katrina Forest
Jim Fettinger

2017 Margaret C. Etter Student Lecturer Awards

Biomac	**Avni Bhatt, U Florida**	**Powder Diffraction**	**Ying Zhang, Brigham Young U**
Canadian	**Matt McLeod, U Waterloo**	**Small Angle Scattering**	**Eric Manley, Northwestern U**
Industrial	**Madushani Dharmarwardana, U Texas**	**Small Molecule**	**Korey Carter, GWU**
Light Sources	**Seth Corey, Texas A&M U**	**Service Crystallography**	**Nico Giordano, U Edinburgh**
Materials Science	**Andrea Bruck, Stony Brook U**	**Young Scientist**	**Kyle Stiers, U Missouri**
Neutron Scattering	**Daniel Olds, ORNL**		

4.2.2: General Interest



L-R: Anastasiya Vinokur, Lawrence Wong, Eric Reinheimer (at rear), Suyin Grass Wang, Shiao-Liang Zheng, Jefffrey Lovelace (at rear), David Schuller, Allen Oliver (at rear), Jennifer Aitken. Absent: Dubravka Jung. Photo by Mark Mashuta.

Despite being one of the final sessions of the ACA conference, the second **General Interest** symposium opened with some 30 audience members in attendance. The session commenced with **Dubravka Jung**, Dectris, who presented advances in the EIGER detector over previous versions of hybrid detectors. **Shao-Liang Zheng**, Harvard U, presented the first of several educational talks, detailing his experiences in developing a course that involves a research visit by undergraduate and graduate students to the Advanced Photon Source. This course is well received by the students and underpins three key philosophies: to encourage and educate students; to incorporate crystallography into chemistry courses; and to develop undergraduate involvement in the science of crystallography. **Jeffrey Lovelace**, Eppley Institute, discussed how one can treat a commensurately-modulated structure as a supercell structure and how to interchange between the two. The discussion on modulation was insightful and clearly explained the underlying features of commensurate vs. incommensurate structures. Prior to the coffee break, **Eric Reinheimer**, Rigaku, gave an enthusiastic talk on how to organize a simple, one laboratory-session experiment involving crystal growth, sample selection and data acquisition. Eric's focus was on an undergraduate laboratory session and how to introduce the topic of crystallography to students. The three key ingredients are: an accessible instrument, software and, most critically, crystals. Eric passionately described how to overcome all three challenges.

The second half of the session was led off by **Lawrence Wong**, Hong Kong U of Science and Technology, who presented his work on using spinols to assist in chiral resolution of a number of new co-crystallant compounds. **Jennifer Aitken**, Duquesne U, followed with a presentation of the emerging classes of lithium chalcogenide materials that her group is synthesizing. These new materials exhibit excellent non-linear optical properties and show promise for their absorption/emission properties. The breadth of resources available at the ChemMatCARS beamline at the APS was detailed by **Suyin Grass Wang**, Argonne National Laboratory. Her talk covered diverse topics such as: extreme conditions (high pressure, extreme cryogenic temperatures), charge density and diffuse diffraction studies, and photocrystallography and time-resolved measurements. In short, the scientists at ChemMatCARS can work with researchers and develop a broad range of crystallographic methodologies to answer the researcher's questions. Rounding out the symposium was **David Schuller**, Cornell U, who discussed the upgrades to the automated mounting hardware at MacCHESS. Upgrades to both the robotic hardware and controlling software have significantly improved automation. The breadth of topics covered in this session demonstrates the scope of the General Interest topics: every field is welcome.

Allen Oliver
Anastasiya Vinokur

4.2.3: Structural Biology of Infectious Diseases

L-R: Erica Ollman Saphire, George Lountos, Oleg Volkov, Christopher Colbert, Marzena Pazgier, Thomas Edwards, Toshiya Senda

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4.2.3: Structural Biology of Infectious Diseases, ctd.

The current status of the contributions of structural biology to the study and development of therapeutic agents against infectious diseases was highlighted at this year's ACA meeting in New Orleans. Erica Ollmann Saphire, Scripps, opened the session with an outstanding talk presenting her lab's ground-breaking work, which required several years of perseverance to solve the crystal structure of the Lassa virus surface glycoprotein bound to a fragment of a neutralizing antibody from a surviving patient. The structure provides the basis for the development of a potential Lassa virus vaccine, for a disease that currently is 50-70% fatal. **Marzena Pazgier**, U Maryland, described crystal structures of a construct of the inner domain of gp120 (HIV-1) complexed with an antibody, and efforts to induce a protective antibody response to HIV-1 with the inner domain of gp120. **Toshiya Senda**, High Energy Accelerator Research Organization, Japan, described the deletion mechanism of SHP2 by CagA from *Helicobacter pylori*, while **Thomas Edwards**, Beryllium Discovery, described the novel crystal structure of acid deoxyribonuclease and insights into its catalytic mechanism. **Oleg Volkov**, UT Southwestern Medical Center, presented crystal structures of *Trypanosoma brucei* S-adenosylmethionine decarboxylase and discussed how allostery activates the enzyme. The mechanism of peptide editing by the TAPBRP/MHC-1 complex, which provides insights into understanding tapasin function, was presented by **Jiansheng Jiang**, NIH. Finally, **Christopher Colbert**, North Dakota State U, presented his laboratory's work on elucidating the structural basis of cell-surface signaling by the sigma-regulator, PupR, in *Pseudomonas putida*. The afternoon's collection of outstanding talks and engaging audience questions demonstrated that structural biology continues to provide major contributions toward our understanding of the molecular basis of infectious diseases and will continue to provide critical information needed for the development of novel therapeutic agents.

George Lountos

4.2.4: Frontiers in SAS

L-R: Youngha Hwang, Soren Skou, Martha Brennich, Thomas Weiss, Timothy Ryan (at rear), Sai Venkatesh Pingali, Volker Urban

This session focused on new developments and latest advances in the experimental protocols and data analysis methods for small-angle scattering. The session was opened by **Martha Brennich**, European Molecular Biology Laboratory, Grenoble Outstation, France, who showed how the idea of online purification of the sample can be carried further from the established size-exclusion chromatography to methods such as ion-exchange and nickel affinity chromatography. She discussed further how, in order for these methods to work, the correct buffer background must be carefully determined before subtraction, and pointed out the advantages and challenges brought about by these new methods. In the following presentation **Volker Urban**, Oak Ridge National Laboratory (ORNL), standing in for Hugh O'Neill, showed how time-resolved neutron scattering helps to elucidate the complex thermochemical processes that take place during pretreatment of biomass. **Youngha Hwang**, Purdue U, presented a numerical analysis on how, e.g., organo-metallic gold clusters attached to icosahedrally-symmetric particles (such as certain viruses) can be used to resolve ambiguities in the radial density function obtained from solution-scattering experiments. Following the coffee break **Soren Skou**, Xenocs, presented the current status of protein solution scattering in a home-lab setting and showed how dedicated instrumentation

combined with a high level of automation facilitates the SAXS data collection and analysis. **Sai Venkatesh Pingali**, ORNL, showed how the increased angular coverage achieved by the recent detector upgrade at the Bio-SANS instrument at HFIR increases the data collection efficiency and enables new scientific capabilities. In the final presentation of the session **Timothy Ryan**, Australian Synchrotron, showed how the use of a novel co-flow sample cell for size-exclusion chromatography coupled solution scattering improved the data quality by eliminating the capillary fouling during the experiment and making it possible to perform the experiment at a higher flux level without significant radiation damage issues on the sample. He further discussed the detail of the flow cell design and its implementation at the SAXS/WAXS beamline at the Australian Synchrotron.

Thomas Weiss

4.2.5: Advances in Structure Solution from Powder Data

This session covered both results and new tools for solving crystal structures using powder diffraction data. **Branton Campbell**, Brigham Young U, gave a brief introduction to group theory and showed how irreducible representations provide the basis for understanding symmetry lowering of a parent space group. Symmetry modes can provide a simplification (smaller number of parameters) of a refinement. In the transformation between the alpha- and beta-$Bi_2Sn_2O_7$ pyrochlore structures, only 13 symmetry modes are important. Characterizing the structures of nanomaterials and systems with significant local distortions requires more information than just the diffraction data, and tools are needed that can accommodate such additional information. **Pavol Juhas**, Brookhaven National Laboratory, described the DiffPy-CMI software toolbox for such complex modeling. Applications of this software included $Au_{144}(p\text{-}SC_6H_4CO_2)_{60}$ metal clusters and CdSe quantum dots. The new hollandite $K_2Sn_3O_7$ was predicted as part of the Materials Project (***materialsproject.org***). **Dan Shoemaker**, U Illinois Urbana-Champaign, described characterization of the structure using both synchrotron and neutron powder data. The neutron data were critical, as the structure falls apart in the 30 keV synchrotron X-ray beam.

Jim Kaduk, North Central College, described the structures of a set of lithium alkali hydrogen citrates, $LiMHC_6H_5O_7$ (M = Li, Na, K, Rb), solved from laboratory X-ray powder data and optimized using DFT techniques. The structures are layered, with metal-oxygen coordination in the center of the layer, and chains of very strong carboxylic acid-carboxylate hydrogen bonds on the surfaces of the layers. **Matt Tucker**, Oak Ridge National Laboratory, showed how the RMCProfile software (*rmcprofile.org*) expands the reverse Monte Carlo (big box) modeling technique to take explicit account of the Bragg intensity from crystalline materials. Matt's example was $SrTiO_3$ at 296 and 5K. He showed how superposition of the RMC results on the average structure gives insight into the local displacements in the structure. **Silvina Pagola**, William & Mary, described the workflow and operation of the new WinPSSP program for applying direct-space methods to crystal structure solution. Her examples included a rigid molecule, a simple co-crystal, and a molecule with a flexible sidechain. The software is freely available at: ***http://users.uoi.gr/nkourkou/winpssp***.

Saul Lapidus
Jim Kaduk

L-R: Benjamin Apker, Garrett Ginell, Krystle McLaughlin. Photo courtesy of Krystle McLaughlin.

Joel Bernstein explaining "fuzzy logic" while addressing the audience in Session 3.2.3. Photo by Peter Müller.

Sue Byram and Ilia Guzei. Photo by Dick Bromund.

Amy Sarjeant presenting the ACA Service Award to retiring ACA RefleXions Co-Editor Tom Koetzle. Photo by Peter Müller.

ACA Summer Course in Chemical Crystallography 2017

ACA Summer Course 2017, L-R: back row – J. Lee, A. Foerster, J. Li, E. Abucayon, M. Imer, B. Bouley, O. Esarte Palomero, G. Díaz de Delgado, R. von Dreele, Y. Liu, J. Kaduk, E. Dolgopolova, A. Peixoto de Abreu Lima, D. Ferreira, C. Lake, M. Crawley, S. Adas, C. Webb, K. Pringouri, J. Sears, S. Antal, H. Munasinghe, E. Eitrheim, D. Gray, K. Storms, N. Henderson, R. Papoular; front row – C. Malliakas, C. Stern, A. Filatov, Y. Kim, M. Ramirez, J. McMahon, E. Reinheimer, A. Sarjeant, A. Oliver, C. Chappell, B. Noll, R. Sommers, C. Powell, V. Sena. Photo by Yuyang Wu.

The University of Notre Dame and Northwestern University have co-hosted the **ACA Summer Course in Chemical Crystallography** since 2012. This year the course was held at Northwestern University from June 25th – July 2nd. Course organizers were: **Charlotte Stern** and **Christos Malliakas** of Northwestern U, **Allen Oliver**, U Notre Dame, and **Amy Sarjeant**, CCDC. For more information, please see the course website: ***http://acasummercourse.net***.

This was the second year we opted to run the course in 7 days instead of 10, which we discovered helps with scheduling. It still remains an intense course with lectures starting at 8:30 am and finishing at 8:30 pm, when everyone is ready for a dinner in town with their new friends. The mornings were devoted to lectures on theory while the afternoons were filled with workshops on the interpretation of the *International Tables*, Symmetry and Space Group analysis, and practical work on sample preparation for both single-crystal and powder-diffraction experiments. Later in the week this practical work included hands-on use of software with students' own data that either they brought with them, or that were collected on Northwestern's single-crystal and powder instruments or on the demo powder units that were on loan for the course. We have noticed that students now have more basic knowledge than in the past, so we divided attendees into groups depending on their ability. We have also incorporated some challenging sample and structural problems that crystallographers might encounter, so that when the students see them in the future they might know where to go or whom to ask for assistance.

Together, students and instructors collected 18 successful single-crystal data sets and a number of powder diffractograms as well. As in past years, we encouraged publication of these data with a request that an acknowledgment to the ACA summer course be included.

This year we had 26 attendees from across the globe, including Canada, South Korea, Uruguay, Venezuela, and the U. S., from academia and industry. Many of the same faculty have continued to be involved, which makes the course run smoothly. We had 18 faculty experts in the field of either or both single-crystal and powder diffraction. This is a wonderful ratio that promotes individual, one-on-one interaction. This has already proven to promote networking among all that are involved.

Overall the course is very well received by both students and instructors. Some remarks given in this year's survey at the end of the course were:

"This community of faculty has been overwhelmingly hospitable. Thank you for taking the time to share your love for crystallography. It's encouraging and inspiring!"

"Is there an ACA summer course part II? After a year of intense practice, I'd love to come back for additional training!"

"The course was an incredible experience that I will carry with me for the rest of my life. Course material and instructors were phenomenal. I'm very thankful for this opportunity."

"This course was a great help in first steps in crystallography. The great team of faculties makes this a great experience."

"The faculty were absolutely amazing and the perfect choices for presenting such difficult materials in such a condensed period of time."

We would like to thank the following vendors and associations for their kind and generous support of the course: The American Crystallographic Association, The U. S. National Committee for Crystallography, Bruker AXS, Cambridge Crystallographic Data Centre, Pittsburgh Diffraction Society, The International Centre for Diffraction Data, MiTeGen, STOE, Olex2, Rigaku Americas, and Dectris. We would especially like to thank all of the Faculty for their time and dedication to the course.

Charlotte Stern

Remembering Philip Coppens

Philip Coppens, SUNY Distinguished Professor Emeritus and Distinguished Research Professor of Chemistry at the University at Buffalo-SUNY, passed away on June 21, 2017, at the age of 86. Chair of Chemistry at UB David Watson said, "Philip was a giant in his field and pioneered the technique of time-resolved X-ray crystallography … He was renowned for promoting the discipline, organizing international meetings and mentoring younger colleagues in his field." A memoir written by Philip can be found in the History Portal of the ACA (***http://www.amercrystalassn.org/h_coppens_memoir***). What follows are the remembrances of several of our crystallographic community who knew him well.

Jane Griffin

I was an older graduate student in the Chemistry Department of SUNY at Buffalo in 1968 when Philip Coppens came to give a seminar for an open position in the Department. It was on his X-N work on triazine. It was exciting to see experimentally produced electron-density maps that showed bonding and lone-pair density. Philip was hired, and I took his first course in X-Ray Crystallography in 1968.

How many professors would take a mother of four young children as their first graduate student? Philip brought the world to Buffalo. He never went to a meeting that he did not return with a new collaborator, post doc, or graduate student. In my time in the lab my mentors included Finn Larsen from Aarhus University; Pierre Becker from France; Dan Jones, South Carolinian fresh out of Lipscomb's lab at Harvard; Niels Hansen, Aarhus; and Bob Blessing from University of Pittsburgh and Lund University in Sweden. Life was never dull in Philip's lab. He was a wonderful teacher, well prepared, clearly explaining the mathematics involved in every aspect of crystallography. He was an expert at using time as efficiently as possible. Every morning he walked into the lab to ask, "How's it going?", and you better be prepared to answer. When you made a presentation in his group meetings, his first question was always, "So what is your major conclusion?" What had you learned?

Philip in his office at UB. Photo by Nancy J. Parisi.

Philip never rested on his previous accomplishments; he was always looking for what new scientific question could be solved by an advance in crystallographic technology. Although recently retired and relocated to be near his sons and grandchildren, he had returned to Buffalo to work on a joint paper when he died.

Finn Krebs Larsen

I came across Philip's seminal *Science* paper entitled *Comparative X-ray and neutron diffraction study of bonding effects in s-triazine* (*Science, vol. 158 (Dec. 22, 1967), 1577-1579*) during studies for my degree in X-ray and neutron diffraction. Subsequently I very much wanted to learn more about what could be achieved by X-N studies. I got in touch with Philip and persuaded him to take me on. I arrived in Buffalo in late 1969 with my wife and small daughter and became one of Philip's first post docs after he moved from Brookhaven National Laboratory to his new chair at SUNY at Buffalo.

It was a tumultuous time there, with student demonstrations against the war in Vietnam and with groups of police patrolling campus; very exciting and a little scary for a small family from peaceful Denmark. Philip and Marguerite were extremely helpful in getting us started. Philip helped us buy a car and Marguerite drove us around town until we found an apartment.

My main project was to help develop low-temperature X-ray equipment and also to go on measuring trips to Brookhaven National Laboratory. Our collaboration continued after I, in 1971, returned to a position in the Department of Chemistry at Aarhus University, Denmark, and it endured right up to my retirement. The most important way I kept close collaborations with Philip was by stationing some of the best of my Ph.D. students in Buffalo for extended stays as part of their education. Some remarkable works and noteworthy theses resulted from these contacts with Philip. It should be mentioned that Niels K. Hansen (sadly, now deceased), during such a stay, tested aspherical atom refinements of small molecules and developed, with Philip, the MOLLY program, which later was extended to the most successful program system XD2006.

Very early on Philip realized the great potential of synchrotron radiation for crystallography. He involved himself deeply by raising funds and building a beamline at the National Synchrotron Light Source at Brookhaven and later at the Advanced Photon Source in Chicago. The very intense synchrotron X-radiation beam with variable wavelength and low-temperature capability opened new and exciting crystallographic research and made the use of such beamlines an irresistible goal for many, including myself. Fortunately it was possible even for an outsider from Denmark to be allocated beam time through application and according to scientific merit. We from the Department of Chemistry, Aarhus University have continued to benefit to this very day.

There is another extremely important side to Philip's impressive achievements that I will laud and praise, namely his never failing willingness to help educate students. Many Nordic students have benefitted greatly from this. The governments of the Nordic countries – Denmark, Sweden, Norway, Finland and Iceland – give substantial sums of money to finance Ph.D. courses, summer schools in advanced subjects. About 10 Ph.D. students

from each of these countries get all expenses paid for taking weeklong courses. I have for many years arranged such Nordic Research Training Courses, every three to four years since 1988. The subject is: *The application of X-ray synchrotron radiation in chemistry, physics and biology*. Lecturers are well-renowned scientists from the Nordic countries, but also some top experts from other parts of the world. Philip was extremely kind and came to lecture whenever I asked. He was a most popular lecturer at every single one of the courses. I want to mention that he did not – like some busy lecturers unfortunately do – just turn up to deliver the lecture and then leave immediately afterwards. In fact, every time Philip spent several days with the students and they appreciated it.

Philip has had a deep impact on my entire professional life – indeed, my life in total. My life would have been completely different had I not seen Philip's *Science* paper on the X-N study of *s*-triazine. This was a defining moment for which I am, Philip, eternally grateful.

Pierre Becker

When doing my Ph.D., I was stymied by the abstract nature of wave-functions until I saw the *Science* paper by Philip Coppens that showed the bonding density observed through X-ray scattering in *s*-triazine: so, the square of a wave-function was a reality! That's why I got in contact with Philip. In 1972-1973 I joined him in Buffalo for six months and brought my family. He immediately exposed me to the reality of scattering experiments: absorption, thermal effects, extinction, the difference between X and N atomic data, optimization of signal/noise ratio. He had me work with his young collaborators (including Bob Blessing and Jane Griffin). We had a weekly meeting where everyone shared his or her work with the whole group. This was when Philip started time-resolved research, since every 15 minutes he came to ask about our progress!

I was always impressed by Philip's chemical intuition. We solved several interesting problems. What a joy to obtain (in cooperation with Fred Ross) the experimental electron density of tetracyanoethylene showing single, double, and triple bonds and lone pairs: this gave sense to LCAO approaches in quantum chemistry.

Such a fantastic time, where we also discovered the strong human qualities of Philip and his wife Marguerite (in particular at the occurrence of two dramatic family events in France).

It was a great pleasure to continue working with Philip and his international collaborators. This strengthened my scientific life immensely. During my whole career, I kept in mind fantastic lessons from Philip: when working with other people find complementary skills and give priority to strengthening their talent, put their name first on publications, and see that they are invited to international lectures. Another valuable point: when publishing a rather theoretical model – which is often complex to read – provide a simple strategy to apply your model. This was the case with our work on extinction. Philip was a man who made his work open to the whole community. He never said or wrote, "I did," but always put emphasis on his co-workers.

And how was he able, starting in 1997, to develop a new field of time-resolved crystallography? He attracted so many young, talented scientists and structured a revolutionary time-dependent crystallography, which let us go from pictures towards molecular movies.

Philip's retirement symposium, organized by Jason Benedict last October, was an unforgettable event where we all felt as if we were members of a family!

Philip Coppens was a fantastic man and scientist. Sadly, he has left us, but his spirit is present in our lives. I personally cannot give a course or work with a scientist without having him present in me. And all my family loved him, Marguerite and their sons.

James Phillips

My professional association with Philip Coppens began when my phone rang in my office at the EMBL Outstation in Hamburg. A woman's voice announced, "United States calling," and Philip came on the line. He offered me a job to coordinate the building of a beam line for SUNY at NSLS (the old one). I had applied for the job, as advertised in the ACA newsletter, but a direct offer amazed me. I asked for an interview and to see NSLS. To say it succinctly, as I found out Philip often did, I went to New York and soon accepted the job. I did have to tell Sir John Kendrew that I was no longer working for him!

Thus began an eight-year period of working closely with Philip Coppens. Many people remember his scientific achievements, but I also saw him as a wise administrator. As part of the SUNY beam line management team, and eventually as its leader, he helped steer the project through the difficult priority decisions necessary for the construction of a facility that would serve the diverse experiments needed for five SUNY campuses. In short, he had my back. I found that he drove me hard but drove himself harder.

Philip's original scientific concept for his synchrotron radiation work was to expand the charge-density field, perhaps with anomalous dispersion techniques. Soon, though, he had the idea of time-resolved crystallography. An NSLS bending magnet line proved inadequate so his vision came to fruition with his work at APS. This illustrates Philip's determination to see his visions through. It also shows his ability to innovate the instrumentation necessary for time-resolved work.

When I moved to industry I saw Philip in a new light, as a customer. Siemens/Bruker salesmen will tell you how tough a bargainer he was. However, he did let us use the SUNY facilities to test some variations on phosphors used in the detectors of the time. Again, he showed wisdom. He knew what improvements in instrumentation would benefit all.

It is said that we all stand on the shoulders of giants. Though Philip is gone, crystallographers of the future will be standing on his shoulders.

Jason Benedict

I joined Philip's research group as a post doc in 2008. In a word, his style as a research supervisor was "demanding." It was not uncommon for Philip to request that you present at

group meeting – with only a few hours' advance notice. The first time this happens, which is often shortly after joining Philip's group, the experience is rather jarring. Only when it's over and you debrief with other group members do the intensity and high expectations of being a Coppens group member become apparent. When I had the opportunity to organize a symposium at the 2011 ACA Annual Meeting, I had the chance to meet Coppens' group members who pre-dated me by decades, all of whom assured me that this older Philip was now a real softy – I had it easy!

While I was fortunate enough to forge countless scientific memories with Philip and crew in his lab at the University at Buffalo and at the APS (he was an active member of the Scientific Advisory Committee of the ChemMatCARS beamline), some of my fondest experiences occurred outside of science, for instance, swimming get-togethers in the Coppens' pool at their Amherst home. Marguerite would prepare an amazing fruit salad and make sure we all departed with a bounty of chives, an herb that overtook much of the free space in their back yard. Many reading this will also recall the group hikes in the serene wilderness just outside of the city.

Much is omitted when my memories of Philip are distilled into a couple of short paragraphs, but the following is absolutely certain: Philip was a great friend and mentor and will be missed dearly.

Connie Rajnak

My first memory of Philip was way back when I was a novice crystallographer and my boss, Dave Duchamp, drove me to hear him speak. Philip's talk was something to do with monopoles, and he made them sound so easy to understand that I imagined I did in fact understand. From then on I admired Philip from afar until I started going to ACA meetings, and, subsequently, IUCr meetings. In 1978 Philip was President of the ACA and from 1993 to 1996 he was President of the IUCr.

We somehow became friends and when I eventually married Stan, in 2007, we put Philip and Marguerite on our Christmas letter list. Marguerite decided Stan must be British or at least have spent a long time in the UK (not true). They wrote, *"Your poem reminded us of the many limericks we heard and read and we enjoyed it equally (no Schadenfreude)."* After another Christmas letter (2011) describing our travels in South Africa they wrote, *"We were in Kruger Park and the Cape Province about 10 years ago, but did not see a quarter of what you people managed to see and photograph. What beautiful pictures. We will follow your trail next time we may get to South Africa!"*

I sent Philip congratulatory notes when he was awarded the Gregori Aminoff Prize in 1996, the Ewald Prize of the IUCr in 2005, and the Kołos Medal in 2013, which he always politely acknowledged. But what I admired most about Philip was that in his talks he always, always showed photos of the people in his lab, and gave them the credit he claimed they deserved.

When I co-edited *ACA RefleXions*, Philip was a frequent contributor so we corresponded often. In 2009 Philip provided a *RefleXions* cover based on his Plenary Lecture at the Toronto ACA meeting on *New developments in X-ray photocrystallography*. Dick van der Helm's obituary appeared in the Fall 2010 issue and Philip helped with that – they were both Dutch and neither of them ever lost the Dutch accent. After the Boston ACA meeting in 2012, I requested and promptly received an image from Philip to include in the *Transactions* report. In the Fall 2013 issue his article *Workshop on dynamic structural photocrystallography in chemistry* appeared.

I was profoundly saddened to hear of Philip's (much too early) death.

Bob Blessing

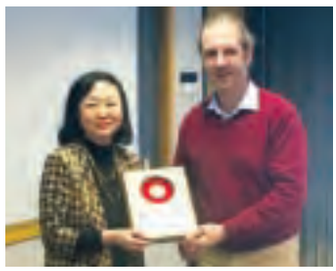
A signal characteristic of Philip Coppens' research career was his uncanny ability to quickly see through to the central questions in a new, emerging field of research on chemical structure and energetics. As a result of an insightful focus or refocus of the work in Philip's laboratory, the lab was consistently an innovative leader at the frontier of new research areas.

Philip's lab at the University at Buffalo (UB) and at his synchrotron beamline stations at Brookhaven and Argonne were for fifty-some years strong attractors for a steady succession of international students, fellows, collaborators, and colleagues. Many in that group became and remain good friends and continuing research collaborators and colleagues. Philip was our nexus for the growth of worldwide friendships and cooperation in ongoing research. Happily, it was the good fortune for many of us to be able to assemble in Buffalo in October 2016 to salute Philip on the occasion of his UB retirement at the fest-symposium organized by Jason Benedict.

Editor's Note: *This remembrance was assembled by Kay Onan.*

News & Awards

ICDD Announces New Distinguished Fellow



Winnie Wong-Ng receiving her Distinguished Fellow Award from ICDD Board of Directors Chairman Matteo Leoni

In March, 2017, the Board of Directors of the International Centre for Diffraction Data (ICDD) awarded **Winnie Wong-Ng**, Research Chemist at the National Institute of Standards and Technology (NIST), the ICDD's **Distinguished Fellow Award**. This award is given to a member, currently recognized as an ICDD Fellow, who has given long and meritorious service to the ICDD. Besides serving the ICDD, Winnie has given sustained and meritorious service to the ACA as indicated by her being named an ACA Fellow in 2014.

"Visionary" Speaker

Majed Chergui, Professor of Chemistry and Physics at the Ecole Polytechnique Fédérale de Lausanne, Switzerland, ACA member and founding Editor-in-Chief of the ACA's flagship journal *Structural Dynamics*, was invited to be one of the visionary speakers at the 2017 Frontiers in Optics + Laser Science conference. Majed was chosen to discuss the future of innovation

Majed Chergui

and to provide insight into cutting-edge advances in optics and photonics. He is most noted for his contribution to the development of new ultrafast spectroscopic techniques with which he addresses fundamental questions in, for instance, the photophysics of transition-metal complexes and the charge-carrier dynamics in semiconductors.

ACA Member Receives ASBMB Award

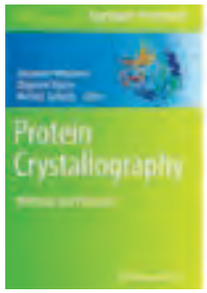
Leemor Joshua-Tor

Leemor Joshua-Tor, Professor and Howard Hughes Medical Institute Investigator at Cold Spring Harbor Laboratory, has won the 2018 **Mildred Cohn Award in Biological Chemistry** from the American Society for Biochemistry and Molecular Biology (ASBMB). The Cohn Award was established to honor the pioneering scientific accomplishments and the spirit of the late Professor Cohn, who was the first female president of the ASBMB. The award recognizes and honors scientists who have made substantial advances in understanding biological chemistry using innovative physical approaches.

Joshua-Tor's lab studies the molecular basis of nucleic acid regulatory processes using the tools of structural biology, biochemistry and biophysics. They study proteins and protein complexes associated with these processes to elucidate how they work. The use of X-ray crystallography, electron microscopy, and other structural techniques enables them to obtain the three-dimensional structures of these molecular machines. Biochemistry, biophysics and molecular biology allow them to study properties that can be correlated to their function and biology.

Kay Onan

Book Reviews



Protein Crystallography: Methods and Protocols: Alexander Wlodawer, Zbigniew Dauter and Mariusz Jaskólski, Eds., Springer Science+Business Media, New York, 2017, 672 pp., ISBN-13: 978-1-4939-6998-2

This book is a compilation of 27 reviews by 50 contributors on current methods in protein crystallography. Each contributor is recognized as a leader in their area of specialization, adding gravitas to each review.

The book starts with a chapter (1) on expression and purification, followed by a chapter (2) on traditional crystallization. The micrographs in this chapter of growth steps are beautiful and instructive. Three more chapters (3-5) cover state-of-the-art processes in crystallizing problem proteins. Another chapter (6) on finding crystals for the diffraction experiment illustrates the problems of selecting an object from the background when there is little contrast.

Once crystals are grown, the next step is data collection. The ensuing five chapters (7-11) cover conventional data collection, microbeam data collection, serial synchrotron data collection and time-resolved data collection. Chapter 12 covers structure determination with X-ray free-electron laser data while Chapter 13 reviews the problems of data processing from XFELs.

Chapters 14-19 cover experimental solutions to phasing with derivatization, anomalous diffraction and long-wavelength data collection, and computational methods via Patterson and direct methods and molecular replacement. Chapter 20 covers the issues of radiation damage and even loops back to experimental phasing using radiation damage.

With an initial model, the book flows through five chapters (21-25) on modeling, refinement and validation before closing with two chapters (26 and 27) on databases in crystallography.

What is missing from this tome are reviews on cryo-techniques and conventional data processing. Nevertheless, I believe this modern volume will replace the venerable Volumes 276 and 277 of *Methods in Enzymology* on many shelves.

Back in January the *1A* podcast did a special on dystopian novels because of the surge in sales of books in that genre since November 2016. *1984* was at the top of the list, but because I've read it once a decade since high school I didn't reread it this year. I picked up two of the novels on the list, *It Can't Happen Here* and *A Handmaid's Tale*, and also found a Great Course titled *Great Utopian and Dystopian Works of Literature*.

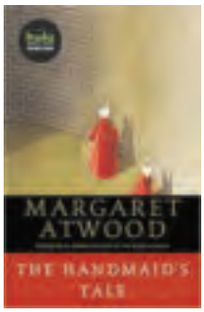
Great Utopian and Dystopian Works of Literature: Pamela Bedore, Ph.D., The Great Courses, Chantilly, VA, 2017

Pamela Bedore is an English professor at the University of Connecticut. She is the recipient of an Excellence in Teaching Award, and when you listen to the course you will understand why. I wish my English teachers in college had been as animated as she is. The course begins with an analysis of Thomas More's *Utopia*. The next few lectures cover the classics by Voltaire, Swift, Hawthorne, Alcott, Butler and Bellamy. For me, things began to get interesting with the analysis of H.G. Welles' *The Time Machine*. Here is where I realized one being's utopia is another's dystopia, a fact Bedore points out in a later lecture. The mid-20th century classics are included for analysis: Huxley's *Brave New World*, Orwell's *1984*, one of my favorites, Dick's *Minority Report*, and Burgess' *A Clockwork Orange*. Here Bedore begins

the analysis of movie versions of the studied novels. More recent classics are also studied: Atwood's *A Handmaid's Tale*, Collins' *The Hunger Games* trilogy and McCarthy's *The Road*. I found this a fascinating and rewarding series of lectures and highly recommend it as a diversion from current events.

It Can't Happen Here: Sinclair Lewis, Signet Classics, New York, 1935-2014, 416 pp., ISBN: 978-0451465641

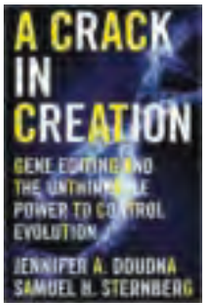
The novel is set in the 1930s and is based on the premise that Franklin Delano Roosevelt loses the 1936 election to a fictional character, Buzz Windrip, modeled on Huey Long (who was assassinated just before the election). Dystopia arises from Windrip's destruction of American democracy and imposition of totalitarian rule through a paramilitary force created from unemployed workers. The hero is Doremus Jessup, a journalist, who fights Windrip throughput the novel. I don't want to spoil the ending, but I really enjoyed the book.



A Handmaid's Tale: Margaret Atwood, Houghton Mifflin Harcourt, New York, 1986, 320 pp., ISBN: 978-0385490818

The novel is a first-person narrative provided by the protagonist, a woman renamed Offred, who has been forced to become a handmaid (surrogate for infertile wives) in an America that has become a theocracy called Gilead based on the Old Testament. Since women have been relegated to subservient tasks throughout society, one wonders how Offred manages to write the account. You will find out in the last chapter; to provide any more information will spoil the ending. Hulu has produced a miniseries based on the novel, which has received a lot of positive press, at least in the periodicals I read; however, I always recommend reading the book before seeing any screen adaptations.

Joseph Ferrara



A Crack in Creation: Gene Editing and the Unthinkable Power to Control Evolution: Jennifer Doudna and Samuel H. Sternberg, Houghton Mifflin Harcourt, New York, 2017, 282 pp., ISBN-13: 978-0544716940

CRISPR is one of the hottest buzzwords in the biotech world right now. The ability to edit genes directly in living things – plants, animals, and even maybe one day soon humans – is here. And Jennifer Doudna is one of CRISPR's foremost pioneers. In her lab at Berkeley, she helped start the CRISPR revolution. Sternberg is one of her fellow researchers, and their book (according to the jacket cover, a favorite of *Star Wars'* creator George Lucas) reads a bit like "CRISPR for Dummies" – but in the best way possible.

Doudna and Sternberg break down CRISPR – which stands for Clustered Regularly Interspaced Short Palindromic Repeats – into plain, simple English. Even someone without a strong science background could probably understand the basic principle behind CRISPR. It allows scientists to edit DNA – remove bad genes or add good genes. It can help us make cows more muscular so that more meat comes from each animal, or make plants less susceptible to fungal outbreaks.

But the most interesting part of Doudna and Sternberg's book wasn't the specifics of CRISPR and how it works. It was the dissection of the ethical and moral implications of direct germline editing. They detail the obvious possible pitfalls of the process – like eugenics – and even detail a Chinese experiment where attempts were made to edit the germline in embryos – an experiment that failed.

CRISPR represents a tremendous breakthrough – but the most important lesson in the book isn't about what it can do, it is about what we choose to do with it.

Jeanette Ferrara

Editor's Note: *Joe Ferrara has pointed out to us that the reviews of The Glass Universe and Shoot Like a Girl in our summer issue were actually authored by Jeanette, rather than by Joe himself as we erroneously indicated in the by-line. Our apologies to Jeanette!*

10 Reasons Why ACA Partners with the American Institute of Physics (AIP)

In the early 1930s amid the Great Depression, five scientific societies banded together to amplify efforts at a time when resources were scarce and to leverage economies of scale for scholarly publishing. The societies served a diversity of communities – physics, optics, acoustics and rheology. They settled on the name American Institute of Physics, as Physics was widely understood as the foundational science from which all other physical sciences emerge. Over the years, AIP has grown its services for its Member Societies, and for the greater good. The ACA became a member in 1966, and several others joined in the ensuing years. AIP now has 10 Member Societies with a collective 120,000 members.

Membership in AIP allows the ACA to extend our influence beyond our membership, to connect with the broader physical sciences community, to support programs that raise the profile of the physical sciences to policy makers and the public, and to

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strengthen our voice and capacity to address mutual concerns.

Below are a few ways in which ACA benefits from belonging to AIP:

1. To be a part of a bigger physical sciences community

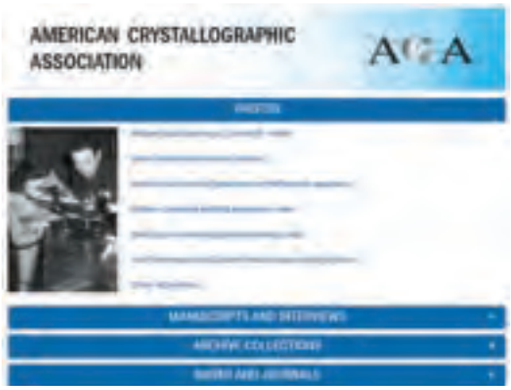
We share a common mission with AIP and their Member Societies to inspire and improve human lives through the knowledge of the physical sciences and their applications to human welfare. Through leadership meetings and committees, we routinely exchange information and expertise on areas of common interest. Thus, we are better equipped to serve our own communities and to partner as needs and opportunities arise.

2. To keep current about other areas of research

Physics Today keeps all 120K Member Society members informed about technological advances and ground-breaking research across the physical sciences, including crystallography. See the July 2017 editorial, *Electron cryomicroscopy comes of age* (***http://dx.doi.org/10.1063/1.882609***). ACA members receive *Physics Today*, AIP's flagship magazine, in print or electronic format each month, at no extra charge.

3. To preserve our history and make it available to thousands of researchers

The Niels Bohr Library & Archives is the collecting repository of AIP and its Member Societies with over 30 collections connected to ACA. To learn more about the treasures the Library holds for ACA, see AIP's archives portal online (***http://history.aip.org/society-portals/aca/aca.html***). See the article on page 5 for news on the ACA History Project.



4. To promote increased diversity and inclusion in the physical sciences

The ACA serves on the AIP Liaison Committee for Underrepresented Minorities (LCURM), which fosters collaboration to increase these groups' representation in the physical sciences. This year, LCURM helped to launch a national task force to increase the number of bachelor's degrees in physics and astronomy among African Americans.

AIP's Statistical Research Center also produces data-driven reports on the representation of women and minority populations in the physical sciences, and is conducting a membership survey for the ACA in the fall.

5. To engage in public policy

AIP offers the ACA an opportunity to advance science policy campaigns, increasing visibility and representation through Executive Branch and Congressional visits, to sign on to statements for endorsement, and to enhance other policy efforts. Only Member Society members may apply for AIP science policy fellowships offered each year. ACA members, Caitlin Murphy, Christopher Cahill and Matthew McGrath are a few of the most recent beneficiaries of this program (***https://www.aip.org/policy/fellowships/overview***).

6. To educate the public and raise awareness

As a Member Society, ACA supports programs that promote the physical sciences, inform the public, and illustrate how scientific advancements influence our way of life. *Inside Science* (***www.insidescience.org/***) brings science news into mainstream media. AIP has also promoted compelling research presented at ACA meetings, writing press releases and pitching them to the media. *FYI science policy news* (***www.aip.org/fyi***) helps researchers, policy makers, and the public keep current on policy and funding developments in Washington, DC that affect the physical sciences.

7. To attain funding for innovative, collaborative projects

This year, AIP launched a new program to encourage partnerships with its Member Societies. Next year, the *Venture Partnership Program* (***www.aip.org/aip/member-benefits/venture-partnership-fund***) will increase the total award amount to ~$250K for strategy- and growth-driven innovation. Submissions for this program were due this year on September 25.

8. To extend our ability to reach students

The Society of Physics Students' (SPS) (***www.spsnational.org***) joint membership program introduced 200 undergraduate physics majors to ACA in 2016. The year of free membership gives the ACA the opportunity to engage these prospective crystallographers and attract new members among the best and brightest. SPS works with the ACA's Young Scientists Interest Group to hold student-focused sessions and awards at ACA meetings.

9. To bring in exhibit revenue

AIP Publishing manages the ACA's meeting exhibits. This not only yields ~$60K in revenue, it also enables the ACA to focus on meeting content.

10. To leverage publishing expertise

AIP Publishing worked closely with the ACA to launch our flagship journal – *Structural Dynamics* – in January 2014. In just a few years, the journal has reached an impact factor 2.968 putting it well within the top third of highest ranking scholarly journals. We are optimistic about its future development. See pp. 7-9 for an update on *Structural Dynamics* (***http://aca.scitation.org/journal/sdy***).

Amy Sarjeant
2017 ACA President

Spotlight on Stamps

A Special Kind of CAT

Daniel Rabinovich

Computer-assisted tomography (CAT) is a medical diagnostic technique in which X-ray scans taken from multiple angles are used to generate cross-sectional images of the bones and a variety of soft tissues inside the body, including the brain, heart, lungs, and the gastrointestinal tract, which cannot be visualized with conventional X-ray techniques.

The original ideas behind computed tomography were conceived in 1967 by Godfrey Hounsfield (1919-2004), a British engineer at Electric and Musical Industries (EMI), where he had also worked on research projects ranging from guided weapon systems and radar to the UK's first all-transistor computer, the EMIDEC 1100. Hounsfield, an expert on pattern recognition problems, designed and built several prototypes of head scanners during the next four years and, on October 1, 1971, CT scanning was introduced into medical practice when the first image of a patient with a potential brain tumor was obtained at Atkinson Morley Hospital in London. Remarkably, Hounsfield was not aware at the time that South African physicist Allan Cormack (1924-1998) had devised a mathematical method in the late 1950s and early 1960s for measuring different tissue densities within the body and, in fact, had predicted that such calculations could be used to create X-ray images of cross-sections or "slices" of organs like the brain.

Hounsfield and Cormack shared the 1979 Nobel Prize in Physiology or Medicine "for the development of computer-assisted tomography," the same year that H.C. Brown and G. Wittig were recognized with the Chemistry Prize and Mother Teresa was honored with the one for Peace. Interestingly, Hounsfield and Cormack not only worked independently from one another to bring about CAT, but also had never met in person until they attended the Nobel presentation ceremony in Stockholm in December of that year. During his Nobel Banquet speech, Cormack also stressed the irony of the award since neither he nor Hounsfield were physicians, and proclaimed that Alfred Nobel himself would have been pleased that an electrical engineer and a physicist had contributed in their own way to the advancement of medicine.

Although CAT gets some serious competition these days from Magnetic Resonance Imaging (MRI) in medical diagnostics, it has a number of noteworthy applications in other fields, including precision metrology, reverse engineering, failure analysis, airport security, and art conservation.

Daniel Rabinovich

Puzzle Corner

For this issue, we have a word-search puzzle by **Guest Puzzler Joe Ferrara**, a new **Crystal Connections** and solution to the previous one, mention of those who provided solutions to previous puzzles, the solution to the baseball-themed **DISORDERED** puzzle, and a few comments about it.

You'll find Joe's word-search puzzle right here in the adjoining column. It contains names of Nobel laureates associated with crystallography. There are 51. How many can you find?

Turn the page for the new **Crystal Connections** and the solutions to previous puzzles.

Turn to p. 56

Crystal Connections #12

What do the answers to these clues have in common?

1) Deck _____: for transmitting natural light below deck in sailing ships

2) Full-page illustration; scute

3) "Well I headed for Las Vegas, Only made it out to _____"

4) Highest symmetry hexahedron

5) _____ of the Moon, Teotihuacan

6) A one-person hot air balloon; type of rail car

7) The Doric temple at Segesta is thought to have never been completed, since these are not fluted

8) _____ Runner: 1982 movie based on *Do Androids Dream of Electric Sheep?*

9) The _____: *Prelude and Fugue in E Minor*, J.S. Bach; a golf club

10) A 3-ball in the Manhattan L_1 Metric, taxicab geometry

Solution to Crystal Connections #11 - Names of diffractometers

1) Banjo player or gleaner – Picker (FACS-1)

2) Polar rhombohedral space group lacking glides – R3 (Nicolet, then Siemens)

3) To abstain from food; very sensitive film – Fast (Nonius)

4) Second most common Sohncke space group – $P2_1$ (Syntex)

5) Acronym for engineering software, followed by space group number for 4) - CAD4 (Enraf-Nonius)

6) Smart Museum of Art, at the University of Chicago - (Bruker)

7) Major source of elements heavier than oxygen – SuperNova (Rigaku/Oxford)

8) Lies on the ecliptic. *Castor*, *Pollux* and *Alhena* are its brightest – Gemini (Oxford)

9) The Italian *tarantella* dance is thought to have origins in the bite of this animal – Spider (Rigaku R-axis)

Marian Szebenyi, Cornell U, submitted the correct solution for Crystal Connections #11.

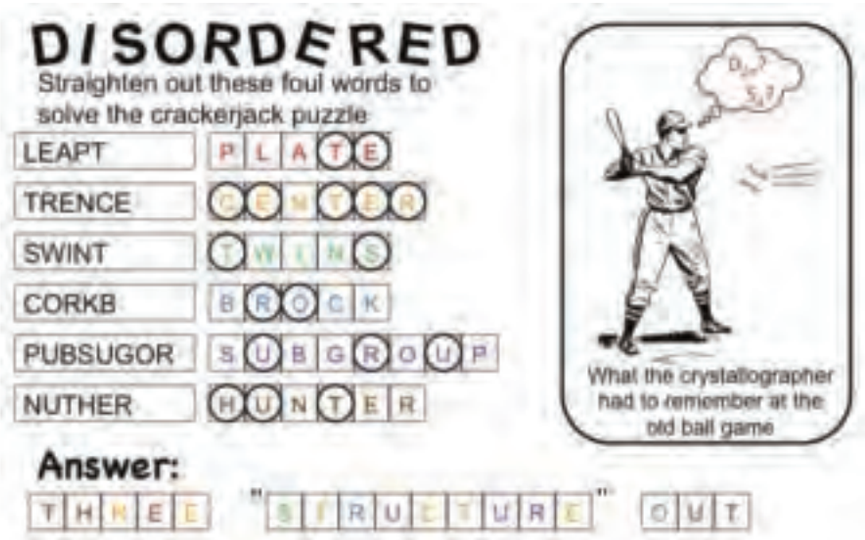
Tim Royappa, U West Florida, provided the solution to the baseball **DISORDERED** puzzle, shown at left below.

Notes on the answers: **PLATE** is a bad habit or home base; **CENTER** is a field or a symmetry element; **TWINS** are a Minnesota baseball team or a crystallographic nuisance; Lou **BROCK** and Jim (Catfish) **HUNTER** are baseball Hall-of-Famers, Carol Brock, Allen Hunter and Bill Hunter are not; point group S_4 is a **SUBGROUP** of D_{2d}. Concerning the latter, a favorite point symmetry question for students is to assign the point group of a tennis ball or *baseball*, including the seams, and the accepted answer is D_{2d}. However, note that the stitching makes the seams of a baseball *directional*, as seen at right below, viewed down the direction of one of the potential dihedral twofolds.

The directionality destroys not only these twofolds, but also the vertical mirrors, and only the S_4 remains, as is being contemplated by the batter.

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

Frank Fronczek
ffroncz@lsu.edu



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ACA TORONTO

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Abstract Deadline: March 31, 2018
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Abstracts accepted online only
at least 40% of all talks will be from contributed abstracts

http://www.amercrystalassn.org

Abstract submission - Meeting registration - Full call for papers
Sponsorship opportunities
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Program Chair - Gerald Audette
audette@yorku.ca

Program Chair - Tiffany Kinnibrugh
kinnibrught@gmail.com

Posters Chair - Louise Dawe
ldawe@wlu.ca

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

OPENING SESSION KEYNOTE SPEAKER

John Polanyi - 1986 Nobel Laureate in Chemistry

WORKSHOPS

Cryo-EM – A Guide to High-Resolution Structure Determination
Molecular Art and Animation in 3D
X-Ray Crystallography: Structure Preparation, Electron Density and Solvent Analysis
Applications of Small Angle Scattering to Structural Biology: An Introduction
Rietveld Refinement and pdf Analyses of in situ X-ray Scattering Data within GSAS-II

EDUCATIONAL SESSIONS & YSIG EVENTS

3-Minute Thesis Session
YSIG Orientation and Networking Mixer
Career Development Session
Engaging Undergraduates with Crystallographic Research
Diversity & Inclusivity Session

ACA AWARDS

Buerger Award honoring Frank Hawthorne
Warren Award honoring Simon Billinge
Margaret C. Etter Early Career Award honoring Jason McLellan

SESSIONS

Transactions Symposium – Shining a Light on Structure-Based Drug Design
Structural Dynamics – in Honor of Philip Coppens
Special Sessions in Honor of Dick Marsh
Crystallography on the International Space Station
Advances in Biological Cryo Electron Microscopy
Structural Biology of Pathogens
NMR Crystallography
Neutron and X-ray Scattering of Correlated and Quantum Materials
Dynamic Crystals as Molecular Materials
Mineralogical Crystallography

Transactions Symposium – Shining a Light on Structure-Based Drug Design

Organizers: **Stephen Soisson** (Merck; *stephen_soisson@merck.com*) and **Vincent Stoll** (AbbVie, *Vincent.Stoll@abbvie.com*)

Meeting participants working in the area of protein crystallography, cryo-electron microscopy, and with an interest in drug discovery will have an opportunity to learn from experts how cutting-edge technologies are being applied to next-generation drug discovery. Unique facets of industrial structural biology will be highlighted in the course of discussing small-molecule hit-finding efforts, such as fragment-based drug discovery, and the integration of structural and computational approaches to facilitate structure-based drug design. The role of structural information in "new" modality discovery such as vaccines, biologics and peptides will also be discussed. Unique opportunities to increase the breadth and scope of structural impact in drug discovery will be presented in context of new methods to access traditionally challenging targets such as ion channels and GPCRs, and how next generation synchrotrons, XFELs, and serial data collection techniques could play key roles in the future.

General Meeting Information

As the 2018 ACA Meeting is taking place outside of the United States, advanced planning by US and foreign travelers is critical. Thorough research should be completed on the documentation needed to access Canada and what is needed to return to your country of origin.

The following links may be helpful:

US Department of State: US Passports & International Travel (https://travel.state.gov/content/passports/en/country/canada.html)

US Customs & Border Protection: Travel to Canada & Mexico (https://www.cbp.gov/travel/us-citizens/canada-mexico-travel)

Government of Canada: Traveling to Canada (https://travel.gc.ca/returning/travelling-to-canada)

Government of Canada: Visa Information (http://www.cic.gc.ca/english/visit/apply-who.asp)

Canadian Tourism Commission (http://caen-keepexploring.canada.travel/)

To request a letter of participation from ACA contact the Meeting Registrar at ***aca@hwi.buffalo.edu.***

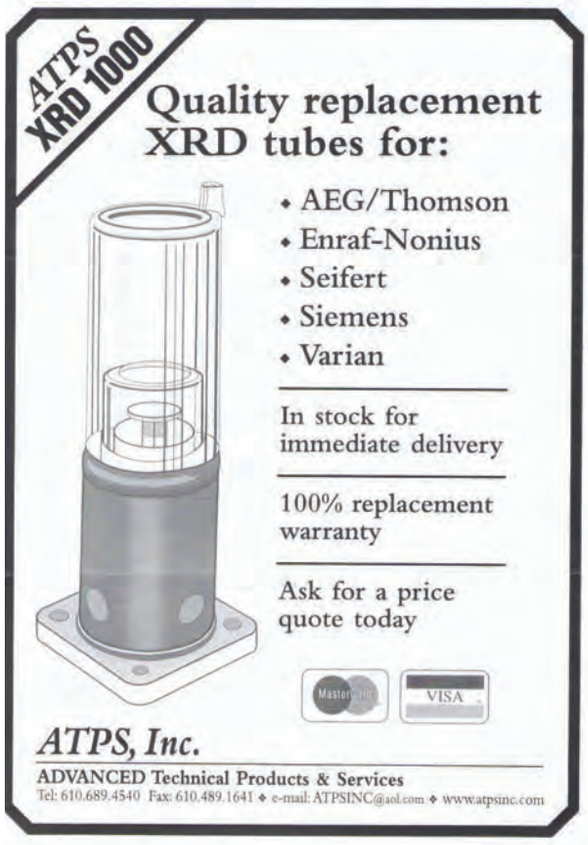
Staying Green: All attendees will receive a hardcopy of the ***Program Book***, but the full set of abstracts will only be available online. We are not planning to have a meeting bag, so if you would like one you should remember to bring your favorite from an earlier meeting.

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

Room rates, in Canadian dollars, are $199 CAN for one or two people, per night and plus taxes. A special rate of $169 CAN has been negotiated **for students and post docs only**. Room sharing can make these rates even more reasonable – use the e-mail ***Room Sharing*** feature under accommodations on the meeting web site at ***http://www.amercrystalassn.org/2018-accommodations***.

Financial Support: Travel support will be available for young scientists. Applications for travel support should be made by March 31, 2018. For additional information see ***http://www.amercrystalassn.org/2018-young-scientists***.

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



FEBRUARY 2018

13-15 **5th BioXFEL International Conference**. New Orleans, LA
https://bioxfel.org/events/details/1155

17-21 **Biophysical Society. 62nd Annual Meeting**. San Francisco, CA
https://www.biophysics.org/2018meeting

MARCH 2018

1-14 **Cryoelectron Microscopy**. Cold Spring Harbor, NY
https://meetings.cshl.edu

APRIL 2018

2-6 **MRS Spring Meeting & Exhibit**. Phoenix, AZ
http://www.mrs.org/fall2018

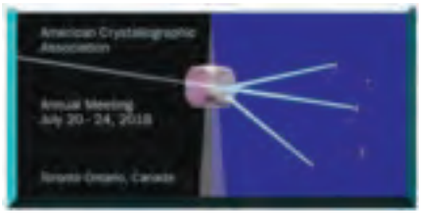
10-13 **BCA Spring Meeting**. University of Warwick, UK
http://ww.bcaspringmeetings.org.uk

22-27 **RapiData 2018**. Menlo Park, CA
http://smb.slac.stanford.edu/rapidata/rapidata-2018

JUNE 2018

1-10 **51st Erice Course: Electron Crystallography** &
52nd Erice Course: Quantum Crystallography. Erice, Italy
http://crystalerice.org

JULY 2018



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

24-28 **ACNS-2018**. College Park, MD
https://www.mrs.org/acns-2018

AUGUST 2018

19-24 **XXVII International Materials Research Congress**. Cancun, Mexico
http://www.mrs.org/imrc-2018

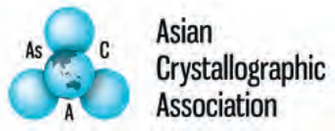
22-27 **31st European Crystallographic Meeting**. Oviedo, Spain
http://ecm31.ecanews.org

OCTOBER 2018

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

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

DECEMBER 2018



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

JULY 2019

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

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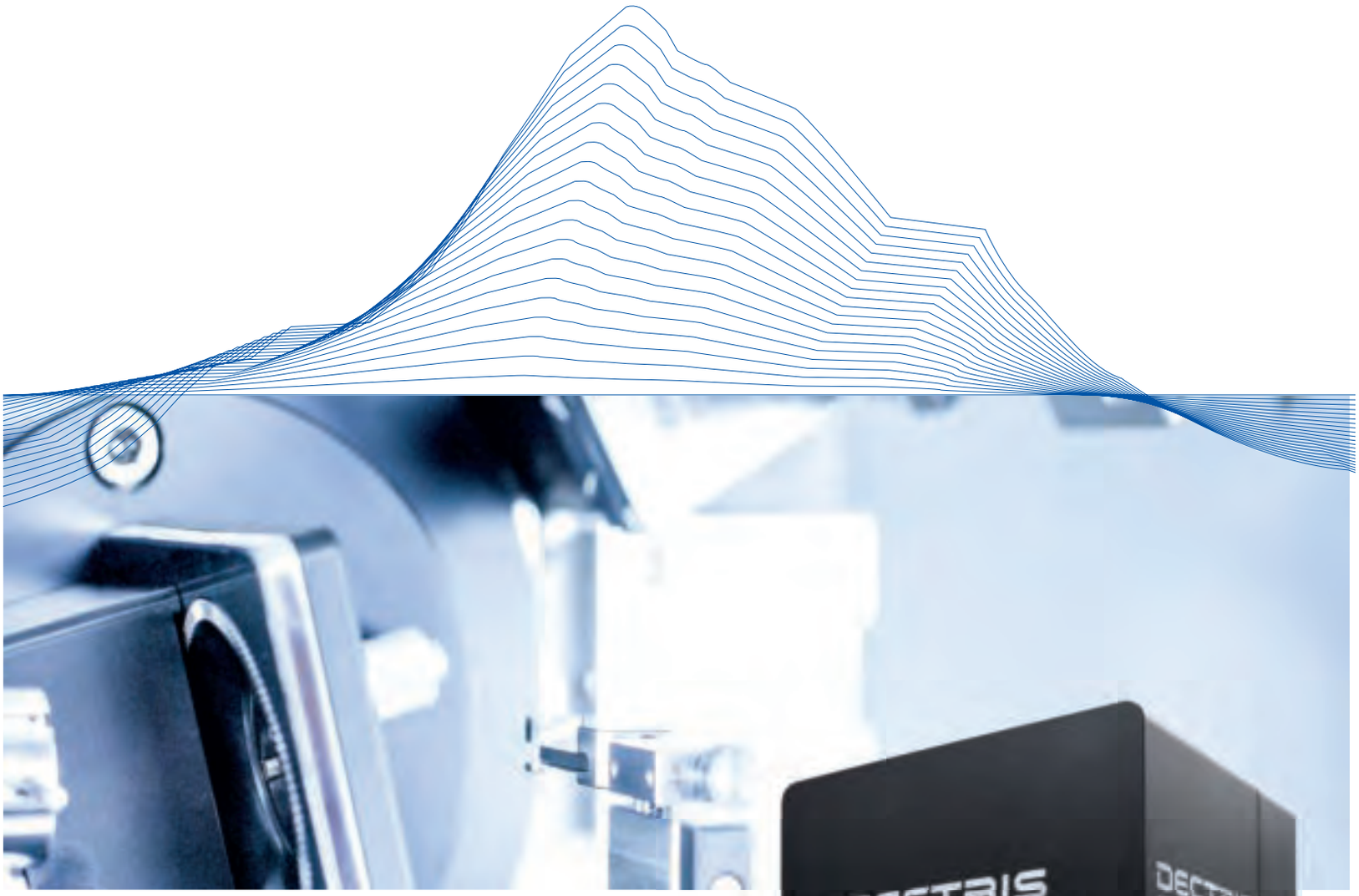

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