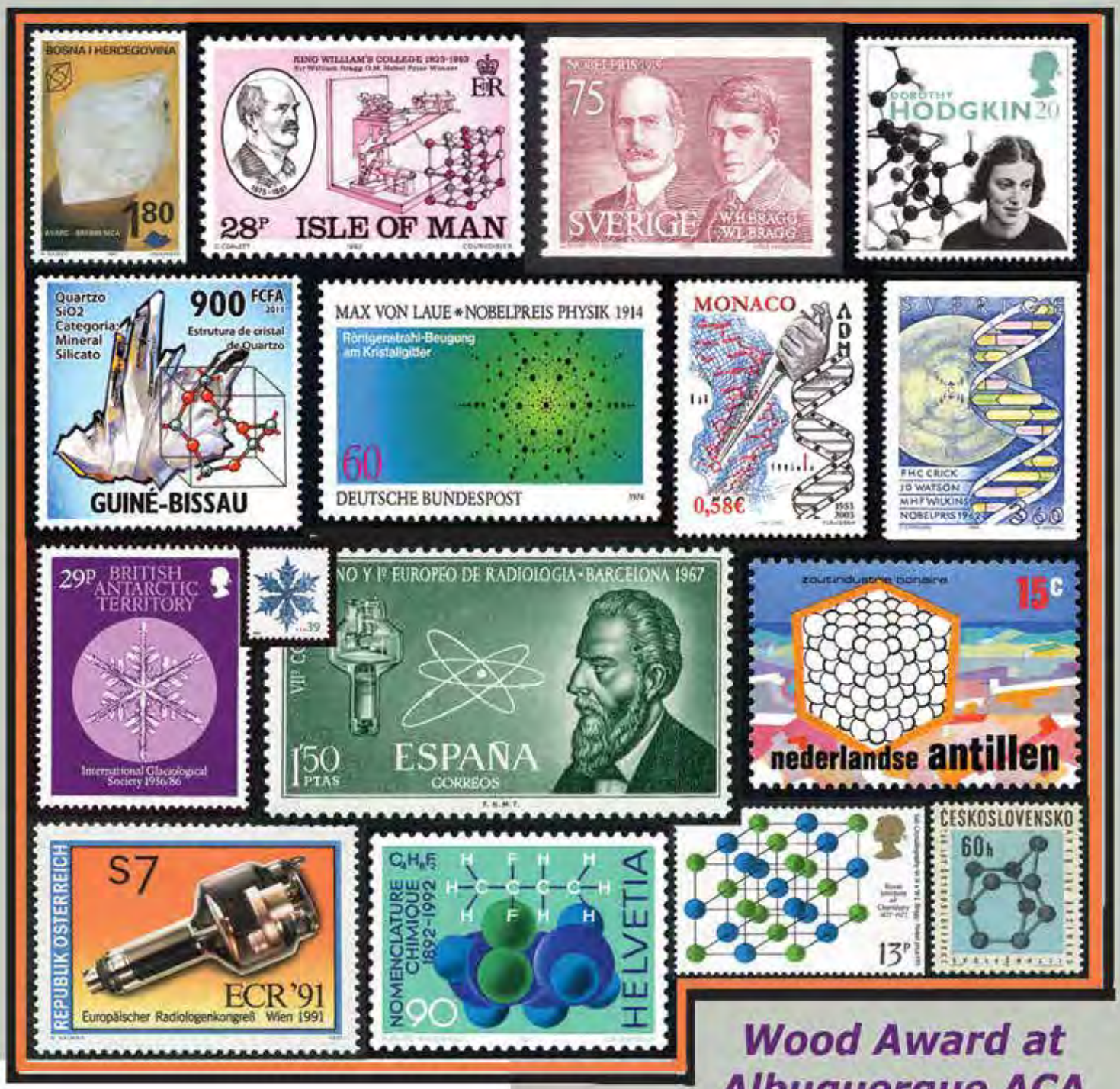
ACA RefleXions

ACA
Structure Matters

Number 3

Fall 2014



Wood Award at Albuquerque ACA

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On the Cover

A sampling of stamps from the collection of E. A. Wood Awardee Dan Rabinovich.
See page 5.

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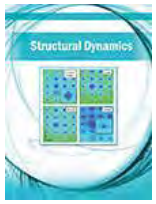

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President's Column

The International Year of Crystallography (IYCr) 2014 is more than half over. But there are still many outreach successes and opportunities to report in North America. Five I know of in particular come to mind. At the recent IUCr 2014 Congress in Montreal, I learned of two exciting events, one last spring and one in mid September, that can inspire us and can serve as model crystal outreach activities for us. The first event is a school program unit in crystallography from North Dakota, while the second is an outreach initiative and symposium at the Canadian Light Source in Saskatoon. The three upcoming fall events are the US and the Canada Crystal Growing Contests and the US/Canada Video Contest.

Angel Ugrinov & Christopher Colbert

A talk at the Hawaii ACA meeting in July 2013 recounted a core science hands-on lesson in crystallization and diffraction for 5th grade. The Hawaii talk showed that after the lesson students had a significant improvement in science skills. That impressed many of us working on IYCr and also caught the attention of Angel Ugrinov, staff scientist and crystallographer at North Dakota State University (NDSU). Last fall, Angel attended an open house at his son Alex's Longfellow Elementary School. Alex's teacher, K. DeLa Pointe, asked if any parent was a scientist, and Angel replied that he was one. He then wrote to Colleen Lopez, one of the Hawaii presenters, and got activity ideas from her.

Then this spring, together with Christopher Colbert, NDSU assistant professor and crystallographer, Angel gave the children in his son's 5th grade class a hands-on crystallographic experience. Such activities are at the heart of Next Generation Science Standards, developed through the National Academy of Sciences as a science core. On the first two days, Angel had one-hour long classes where the 5th graders discussed what is science, chemistry, crystallography, and what is their influence in our every day life. Kids learned crystallography vocabulary like atoms, molecules, order, disorder, crystallinity, amorphous materials, *etc*. The 3rd day of the activity was the most exiting for the kids. Angel, Christopher, and graduate student Karen Preskay showed them crystals under the microscope and how to see structures in stereo. They then built a diamond molecular model. Finally, they prepared saturated solutions of alum colored with food dye and grew crystals that they shared.

Now, after this successful hands-on demonstration in his son Alex's classroom, several teachers from different schools are asking Angel to have the demonstration in their classrooms. So, from one seed can grow many opportunities!

I hope all of you will approach your children's teachers, or those of children of scientists in your group, and offer them this type of activity for their classes. Out of such visits can come crystal growing or video contest entries (see below). I'll be presenting crystallographic demonstrations such as this at the joint Long Beach (CA) National Science Teachers Association regional meeting and CA Science Teacher's Association meeting in early December. Your teachers may even be learning about crystallography there!

The fall outreach initiative that I mentioned above is a Canadian Light Source event for local high-school students and teachers followed by a symposium for the general public on September 15, 2014, planned by Pawel Grochulski and Mirek Cygler. The high-school outreach included a tour of the light source, demonstration of diffraction using diffraction grating slides and a laser, a demo of data collection at a macromolecular crystallography beam line, crystal growth, and visualization of structural results. The symposium featured Alex Wlodawer talking about 100 years of crystallography and also about the accomplishments of crystallography in HIV and AIDS research.

Synchrotrons are very important to our crystallographic data collection as a community. An outreach and symposium event like the one I've described above would be excellent for synchrotron sites with crystallographic beam lines to replicate, both to celebrate IYCr 2014 and also the International Year of Light 2015. A synchrotron has a high cost and a large presence in a community, and it's up to researchers like us to talk to the public, to fellow professionals and to politicians about the importance of scientific accomplishments. There were many rich examples at IUCr 2014. In Britain, the young crystallographers in the British Crystallographic Association take part in synchrotron outreach annually, as well as other science fairs (like the Big Bang Fair).

The last three ACA events that I've mentioned are contests this fall for school children. There are the Canadian and the US (first ever) Crystal Growing Contests, modeled on the successful Canadian contest. Also, there is a Video Contest for US and Canada together. These provide a wonderful opportunity for crystallographers to interact with school children and excite them about science through crystals, crystallographers and their accomplishments. Please check details at ***www.iycr2014.org/aca/contests***.

I hope everyone will take an opportunity to 1) grow your own crystals of borax at home (see Crystal Jars at ***www.iycr2014.org/aca/education***), 2) approach a school teacher with an introduction to crystallography, 3) promote one of our contests, or 4) tell your neighbor or a local politician about why crystallography is important. If we are to survive and thrive as a discipline, we need to share the impact of our field with others. We need to tell people about the value of what we do and excite the next generation about science through crystals and crystallography.

Martha Teeter

From the Editor's Desk

This issue of *RefleXions* features reports from the ACA's Annual Meeting, held in Albuquerque, New Mexico, in late May.

Connie Rajnak assembled the meeting reports and also produced the layout of the meeting pages. We are deeply indebted to Connie for volunteering her time, and for stepping in to act in my place, when at the last minute I was unable to travel to Albuquerque due to a family medical emergency.

RefleXion's comprehensive coverage of the Annual Meeting would, of course, not be possible without the efforts of many people, including our poster prize judges and session chairs who drafted reports, and our staff photographer Peter Müller who took many of the photos. Our thanks go out to everyone who contributed and especially for putting up with those ever-present 'reminders' from Connie and me to get their pieces in!

This issue also has our usual features including an extensive *News & Awards* piece assembled by Chiara Pastore. Enjoy!

Tom Koetzle

Highlights from the 2014 Spring/Summer ACA Council Meeting

The Spring/Summer ACA Council meeting kicked off with a presentation from Fred Dylla, CEO of the American Institute of Physics (AIP) who discussed current ACA / AIP interactions and described several additional ways in which AIP could be of service to our organization.

Considerable discussion was devoted to the International Year of Crystallography (IYCr) 2014, focusing on the various initiatives that had been (or will be) undertaken by ACA members in honor of IYCr. An amazing amount of work has gone into IYCr-related outreach activities, with important contributions being made from all parts of the ACA.

Council welcomed the new representatives from the Canadian Division and the YSSIG, Michael James and Eric Montemayor, respectively. In response to a request from Montemayor, Council approved a change in the mechanism by which the YSSIG representative will be chosen. Going forward, the YSSIG members will choose their Council representative (rather than have that representative be appointed by Council). This will happen on a yearly basis, rather than every three years, in order to spread the experience among YSSIG members and bring new ideas to Council.

A recurring topic of conversation during the Council meeting was the steady decline in ACA membership, which, if unchecked, has serious ramifications for the future health of the organization. Ideas covered during this discussion included ways to increase both the value of membership and the perceived value of membership; one suggestion was to increase the educational component of the annual meeting, which many believe would attract attendees and hence boost membership.

The 2015 meeting has been scheduled in Philadelphia, the City of Brotherly Love. As venues for future meetings were discussed, Council noted that many members were concerned about expensive meeting sites and wondered if it would be possible to locate meetings at, for example, university campuses. While noting that this issue is complex, and the meeting must accommodate a wide variety of needs, council agreed this topic warrants further investigation and deputized several individuals to look into it.

Finally, an update was presented on the strategic planning process. Broad objectives have been identified, and the challenge going forward will be to flesh these out and identify specific courses of actions. Stay tuned.

Patrick Loll

Report of Canadian Division Representative

The big crystallographic event in Canada this year was the 23rd Congress and General Assembly of the International Union of Crystallography (Montreal, Quebec, August 5-12, 2014). There were ~2,100 attendees (including 205 registrants from Canada). The co-chairs for the Congress were Mirek Cygler (University of Saskatchewan) and Albert Berghuis (McGill University). It was fortuitous that the Congress was held during the UN sanctioned International Year of Crystallography, 2014. There were 31 members on the International Program Committee, chaired by Jim Britten (McMaster University). Those people worked tirelessly with the local organizing committee of 20 members to put together an excellent and comprehensive program consisting of 112 microsymposia (held in 8 parallel sessions both morning and afternoon), 4 plenary Lectures, 34 keynote lectures, and 2 Gjonnes Lectures (given by the recipients of the Gjonnes Medal in Electron Crystallography and named in honor of the first recipient, Jon Gjonnes of the University of Oslo in 2008). The plenary and keynote lectures that I managed to attend all were excellent and were presented by leaders in the numerous fields.

There were two very well attended microsymposia dedicated to the memory of Louis Delbaere. These microsymposia, *Enzymes and macromolecular machines*, covered topics of special interest to Louis. Two of Louis' students, Zongchao Jia and Gerald Audette, were invited speakers: Zongchao (Queen's University) spoke on the molecular structure and enzymatic mechanisms of a novel oxygenase, PhnZ, that is involved in the cleavage of carbon phosphorous bonds, whereas Gerald's (York University) lab is tackling the structures and the mechanisms of bacterial F-plasmid proteins in the T4 secretion system (T4SS). Gerald presented the structures of several of these proteins, some of which crystallized in spite of predictions that they would not do so.

The audience for these microsymposia also heard from Bill Furey (University of Pittsburgh) about the advances made in the structural

studies of pyruvate kinase. This is a huge complex existing in two forms, an octahedral complex consisting of 60 subunits (24E1, 24E2 and 12E3) and five cofactors that are required for the conversion of pyruvate to acetyl CoA via an acetyl transferase involving lipoamide. Several groups have been working on these structures for many years. Mirek Cygler (University of Saskatchewan) discussed his group's work on the bacterial kinases that are secreted through the syringe-like secretion systems T3SS and T4SS. Several of these kinase molecules have large unstructured N- terminal domains of ~100 amino acid residues. Mirek's work showed that many of the phosphorylation sites in NleH1 and NleH2 are found in the unstructured regions but that the catalytic domains adopt a similar fold to the core of PKA.

In addition to organizing several demonstrations and poster sessions celebrating the International Year of Crystallography, Louise Dawe (Wilfred Laurier University) was an invited speaker in microsymposium 92, *Crystallography education and training in the 21st century: New pedagogies and new paradigms Part II*. In her presentation, entitled *Holistic integration of crystallography in undergraduate chemistry*, Louise discussed the way in which she has integrated a high school senior class in crystallography and enabled them to teach and evaluate the crystallography taught in an introductory undergraduate chemistry class. Louise's methods emphasized active learning rather than passively listening (or sleeping) in lectures.

In general the Canadian contingent, which included the three Canadian delegates to the IUCr General Assembly (Marie Fraser (University of Calgary), Michael James (University of Alberta) and David Rose (University of Waterloo)), made an excellent contribution to the Congress. It was a bit disappointing that only one Canadian was selected to give one of the keynote lectures (*Structural genomics of chromatin regulators for biological discovery & epigenetic therapy* by Cheryl Arrowsmith, University of Toronto). I was also disappointed by the fact that the Canadian National Committee for Crystallography (CNCCr) had a booth reserved, but no one was ever at the booth and there was nothing in the booth that highlighted the outstanding role of crystallographic sciences in Canada. However, on the bright side, many of the 205 Canadian attendees at the Congress are in the early stages of their careers, and we are currently forming a committee (headed by myself and Louise Dawe) that will concentrate on increasing activity of Canadians both on the CNCCr and within the ACA.

Michael James

On the Cover

The **2014 Elizabeth A. Wood Science Writing Award** was given to **Dan Rabinovich** for *bringing science to the attention of a wider audience*, in particular through the use of postage stamp illustrations to enhance publications and oral presentations. Dan is a regular contributor to *Chemistry International*, the IUPAC bimonthly newsmagazine, and (since 2005) is the Editor of *Philatelia Chimica et Physica*, a quarterly periodical dedicated to the study of stamps related to chemistry and physics.

The cover image depicts a sampler of stamps related to the history and applications of x-rays. This is a very timely topic since 2014 is the International Year of Crystallography. Dan's plenary lecture at the ACA annual meeting in Albuquerque featured stamps highlighting the history of x-ray crystallography, from the observation of crystals in nature (*e.g.*, minerals, gemstones, snowflakes) and the discovery of x-rays by Wilhelm Röntgen in 1895, to the key contributions of Max von Laue and the Braggs. Several stamps depict the molecular structures of organic and inorganic compounds, from simple triatomic molecules like water and carbon dioxide to complex biomolecules such as DNA and the ribosome, thereby underscoring the importance of x ray diffraction techniques to chemistry, biochemistry, mineralogy, medicine, physics and related fields.

On March 16th Dan gave a very well received talk, *Philatelic tribute to the IYCr: Crystallography on stamps* at the 247th ACS National Meeting in Dallas. That talk was in the ACS Division of the History of Chemistry – Dan also was author or co-author on several presentations in the Division of Inorganic Chemistry.

See Amy Sarjeant's report on Dan's Wood Award lecture on page 15. An audiovisual recording was made by Ilia Guzei; all materials will be available from the ACA's history portal (***www.amercrystalassn.org/history_home***).

IUCr Election Results

The triennial IUCr Congresses are major international scientific events for crystallographers worldwide. Each Congress includes sessions of the General Assembly, which drafts the policy lines within the Union. Two of the main functions occurring during these sessions are selecting the site for a future Congress and electing members of the Executive Committee. It was decided at the Congress in Madrid (2011) that the 2017 Congress will be held in Hyderabad (India). At the most recent Congress in Montreal, which ended on August 12, 2014, it was decided that Prague (Czech Republic) will be the site of the 2020 Congress and General Assembly. The results of the elections for the members of the Executive Committee are as follows:

Terms ending in 2017:

President: Marvin Hackert (USA) (continues to 2020 as Immediate Past President)

Vice-President: Anthony Glazer (UK)

Immediate Past President: Gautam Desiraju (India)

Ordinary members (elected in 2011): Hanna Dabkowska (Canada), J. Mitchell Guss (Australia); (*elected in 2014 to fill out the term vacated by M. Hackert*): Masaki Takata (Japan)

Terms ending in 2020:

Ordinary members (elected in 2014): Wulf Depmeier (Germany), Santiago Garcia-Granda (Spain), Radomir Kuzel (Czech Republic)

IUCr Executive Committee 2014-2017

Structural Dynamics

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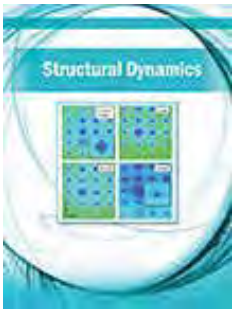


Co-published by ACA and AIP Publishing, Structural Dynamics is a peer-reviewed, open access, and online-only journal entirely devoted to recent development in and research on Methods, Techniques, and/or Science to understand time-resolved changes in chemical, biological and condensed matter systems. The community of scientists and engineers working on structural dynamics in such diverse systems often use similar instrumentation and methods enabled by the emerging new instruments (*e.g.*, XFELs, high harmonic generation, electron sources, *etc*.)

The journal welcomes articles in the following areas:

- *Time-resolved x-ray and electron diffraction and scattering*
- *Coherent diffractive imaging*
- *Time-resolved x-ray spectroscopies (absorption, emission, resonant inelastic scattering, etc.)*
- *Time-resolved electron energy loss spectroscopy (EELS) and electron microscopy*
- *Time-resolved photoelectron spectroscopies (UPS, XPS, ARPES, etc.)*
- *Multidimensional spectroscopies in the infrared, the visible and the ultraviolet*
- *Nonlinear spectroscopies in the VUV, the soft and the hard x-ray domains*
- *Theory and computational methods and algorithms for the analysis and description of structural dynamics and their associated experimental signals.*

These new methods are enabled by new instrumentation such as:

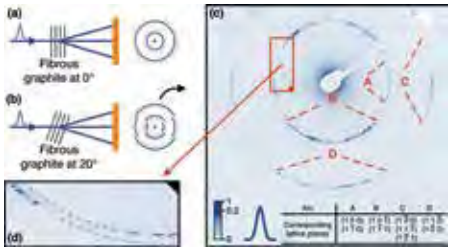
- *X-ray free electron lasers, which provide flux, coherence and time resolution*
- *New sources of ultrashort electron pulses*
- *New sources of ultrashort Vacuum Ultraviolet (VUV) to hard x-ray pulses, such as high harmonic generation (HHG) sources or plasma-based sources*
- *New sources of ultrashort infrared and terahertz (THz) radiation*
- *New detectors for x-rays and electrons*
- *New sample handling and delivery schemes*
- *New computational capabilities*

The journal accepts Short Communications, Topical Reviews and Regular Articles in the following subjects:

- *Experimental Methodologies*
- *Theory and Modelling*
- *Surfaces and Interfaces*
- *Materials*
- *Liquids and Solutions*
- *Biological Systems*

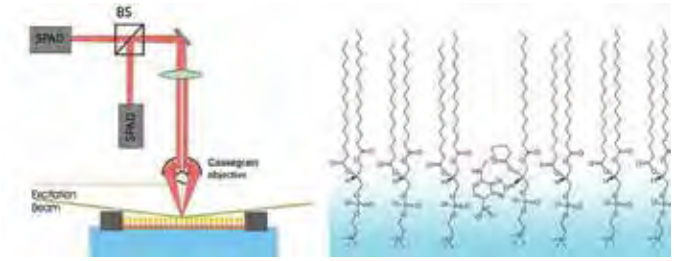
Recently Published

Femtosecond single-electron diffraction, S. Lahme, C. Kealhofer, F. Krausz and P. Baum. Struct. Dyn. 1, 034303 (2014); http://dx.doi.org/10.1063/1.4884937



Abstract: Ultrafast electron diffraction allows the tracking of atomic motion in real time, but space charge effects within dense electron packets are a problem for temporal resolution. Here, we report on time-resolved pump-probe diffraction using femtosecond single-electron pulses that are free from intra-pulse Coulomb interactions over the entire trajectory from the source to the detector. Sufficient average electron current is achieved at repetition rates of hundreds of kHz. Thermal load on the sample is avoided by minimizing the pump-probe area and by maximizing heat diffusion. Time-resolved diffraction from fibrous graphite polycrystals reveals coherent acoustic phonons in a nanometer-thick grain ensemble with a signal-to-noise level comparable to conventional multi-electron experiments. These results demonstrate the feasibility of pump-probe diffraction in the single-electron regime, where simulations indicate compressibility of the pulses down to few-femtosecond and attosecond duration.

Heterogeneous Rotational Diffusion of a Fluorescent Probe in Lipid Monolayers: N. Dadashvand, L. A. Williams, and C. M. Othon Struct. Dyn. 1, 054701 (2014); http://dx.doi.org/10.1063/1.4894379



Abstract: The rotational correlation time of the lipid probe 1-palmitoyl-2-{6-[(7-nitro-2-1,3-benzoxadiazol-4-yl)amino] hexanoyl}-sn-glycero-3-phosphocholine (NBD-PC) is measured using fluorescence anisotropy for two lipid species. We measure the rotational diffusion in a monolayer of 1,2-Didecanoyl-sn-glycero-3-phosphocholine (DPPC) which displays a phase transition at room temperature from the liquid-expanded to the liquid-condensed phase. The constant rotational diffusion of the probe throughout the phase transition reflects the measurement of dynamics in only the liquid-expanded phase. We contrast the dynamic changes during this phase coexistence to the continuous density increase observed in 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) at room temperature. We observe a non-exponential decay of the probe diffusion consistent with heterogeneity of the orientational dynamics.

Articles coming soon

Dynamics of the OH group and the chemical state of alcohols in the liquid phase: S. Schreck, A.Pietzsch, K. Kunnus, B. Kennedy, W. Quevedo, P. S. Miedema, P. Wernet, and A. Föhlisch

pH-Induced Equilibrium Shift Between Closed And Open E. coli β-sliding Clamp Revealed: F. Tondnevis, L. G. Douma, R. E. Gillilan, L. Bloom and R. McKenna

Upcoming special topic issues:

BioXFEL 2nd International Conference --- This issue will highlight primary areas of discovery in femtosecond nanocrystallography; time-resolved imaging and specgroscopy; single particles; and instrumentation and algorithms.

Soft X-ray in Energy and Time (SXET) – This issue will have reports on the current status and new developments in soft x-ray absorption and emission spectroscopy as well as its resonant processes towards the Heisenberg limit (time versus energy limit). It will feature technical and methodological developments for high energy resolution or ultrafast time-resolved approaches addressing new scientific questions for solid, liquids, gases and interfaces.

Meet our editors at the following upcoming conferences:

October 26-31, 2014: 12th International Conference on X-ray Microscopy, Melbourne, Australia.

November 30 - December 5, 2014: MRS Fall Meeting, Boston, MA.

BioXFEL 2ND INTERNATIONAL CONFERENCE

January 13-14, 2015 : 2nd International BioXfel Conference, Ponce, Puerto Rico.

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Waivers may be available for certain authors. The ability to pay does not influence whether or not a manuscript is accepted for publication. Please check the journal website for more details: ***scitation.aip.org/content/aca/journal/sdy/info/about/Publication Charges & Open Access Fees.***

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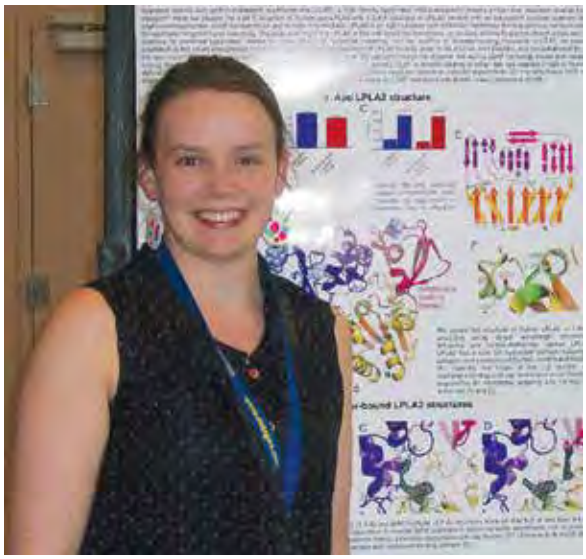
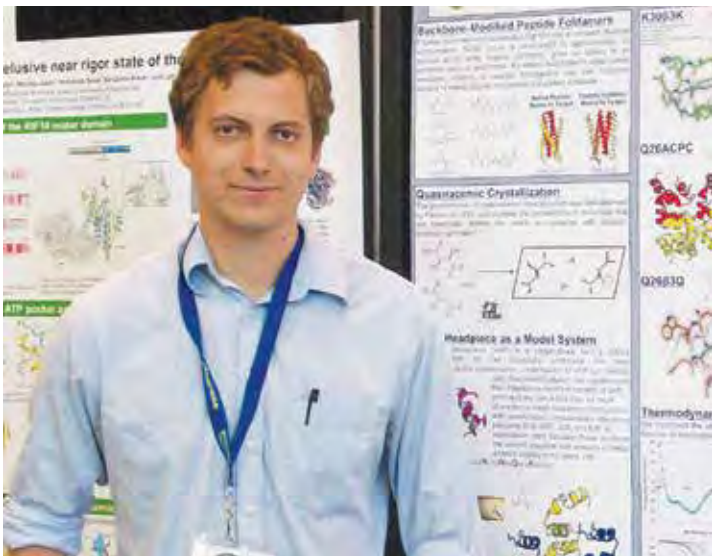
The 2014 poster prize winners. L to R: Sergiu Draguta, Nikita Ussin, Raul Castanada, Farzaneh Tondnevis, Dale Kreitler, Kimberly Stanek, Brian Dolinar, Alisa Glukhova, Robert Evans, Kritica Arora, Eileen Brady.

The **Pauling Poster Prizes,** established to honor Linus Pauling, a pioneer in structural chemistry and biology, are given to students who present outstanding posters at the annual ACA meeting. There are seven Pauling Prizes; five are funded by contributions from ACA members; the **IUCr Pauling** is funded by the IUCr; and the **Louis Delbaere Pauling,** which is given to a Canadian graduate or undergraduate student, is funded by the Canadian Division of the ACA and the Canadian National Committee for Crystallography.



At right, **Alisa Glukhova**, University of Michigan, won the no-special-requirements **Pauling Prize** for **S-27:** *Structural and functional analysis of lysosomal phospholipase A2: a close homolog of lecithin-cholesterol acyltransferase*, by Alisa Glukhova, James Shayman, and John Tesmer. The structures Alisa's poster showed: a 1.83 Å structure of human apo-LPLA2 and a 2.3 Å structure of LPLA2 after treatment with an irreversible inhibitor, along with the position of disease-causing mutations in LCAT, which were important in the group's substrate modeling studies towards explaining the specificity of LPLA2 for fatty acids. They modelled the structure of LCAT and mapped genetic mutations leading to either fish eye disease (FED) or familial LCAT deficiency (FLD), and were able to propose that total loss of enzyme activity in most FLD cases is caused by mutations in particular residues. FED mutations, which mostly cluster on the surface of the enzyme, presumably affect its activation by HDL particles.

The 2014 judges for the Pauling Prizes were: **Rob McKenna, Paul Davies**, and **Marvin Hackert.**



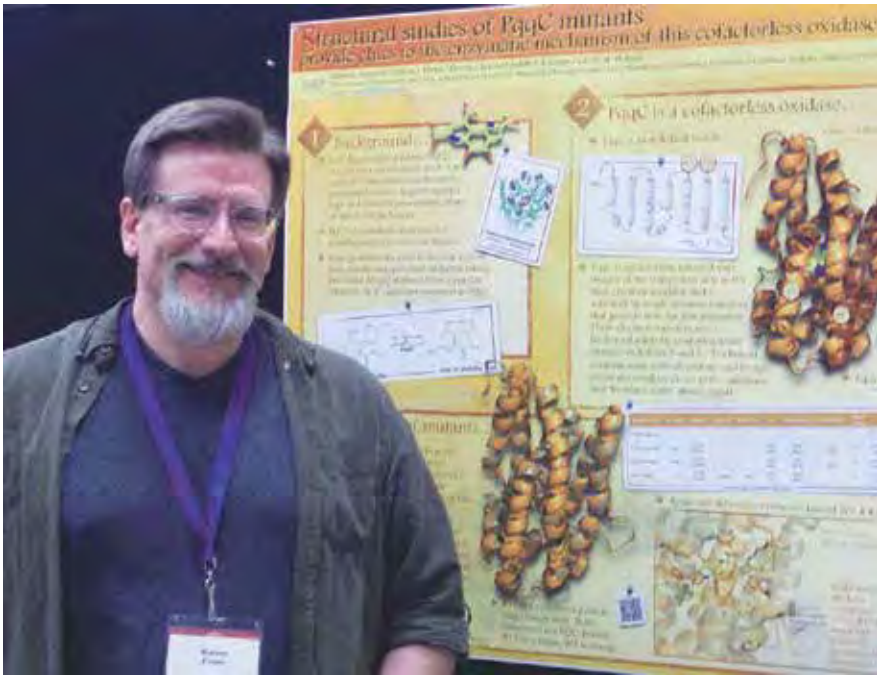
The Muttaiya Sundaralingam Pauling Prize, which honors pioneering work on the stereochemistry of nucleotides and nucleic acids, was presented to **Dale Kreitler,** University of Wisconsin, for his poster **S-24:** *Quasi-racemic crystallization of backbone modified proteins: Not quite centrosymmetric*, by Dale Kreitler, David Mortenson, Katrina Forest, and Samuel Gellman. Short, model peptides are normally reluctant to crystallize by conventional techniques. Dale and his coworkers managed to grow, in hanging drops, three backbone-modified variants of the 35 residue Villin Headpiece (VHP) subdomain. Each quasi-racemic crystal contained the D-enantiomer of the unmodified VHP sequence and a backbone-modified VHP peptide, in a 1:1 ratio. This accomplishment will point the way for efforts to characterize the structural effects of modifications on native protein folds.

Louis Delbaere Pauling Prize

Kritica Arora, from Queen's University, Kingston, ON, was awarded the **Louis Delbaere Pauling Prize** for **S-21:** *Mitotic kinesin structure displays elusive near rigor state of the motor domain,* by Kritica Arora, Parker Anderson, Ana Assenjo, Lama Taije, Monika Joshi, Hernando Sosa, Benjamin Kwok, and John Allingham. Kif14 is a kinesin that creates a structural network of microtubules enabling alignment and separation of chromosomes when the cell divides (it functions in mitosis and cytokinesis). Kritica and her colleagues superimposed the P-loop motif of Kif14 onto available kinesin structures, showing that the ATP binding pocket is open, as if ready to exchange its bound ADP for MgATP, a phenomenon only seen during the transition between ATP-bound and nucleotide-free states of myosins – known as the **near rigor state**. Kif14's inclination to crystallize in this state could explain its microtubule binding affinity, and propensity for futile ATP hydrolysis.

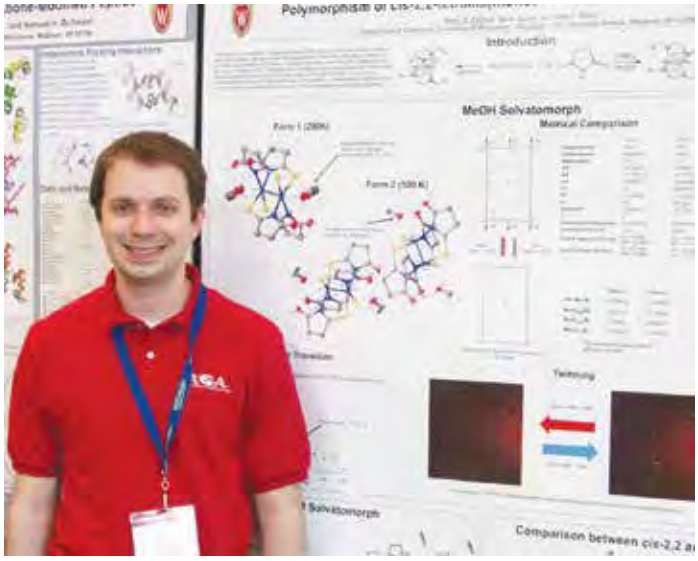
IUCr Pauling Prize

Robert Evans III, University of Minnesota, was given the **IUCr Pauling Prize** for **S-33:** *Structural studies of PqqC mutants provide clues to the enzymatic mechanism of this cofactorless oxidase,* by Robert Evans III, Valerie Klema, Florence Bonnot, Judith Klinman, and Carrie Wilmot. Pyrroloquinoline quinone (PQQ) is the cofactor for bacterial dehydrogenases that play roles in bacterial metabolism, and neither this class of dehydrogenases nor PQQ biosynthesis genes are found in eukaryotes. It is also a member of a group of proteinaceous quinone cofactors (*e.g.* tryptophan tryptophylquinone (TTQ) and topaquinone (TPQ)), but is unique in that it is the only one of these that is synthesized from a stand-alone peptide to create an exogenous cofactor. PQQ's biosynthetic pathway is a potential target for antibiotics development.



Herman R. Branson Pauling Prize

Nikita Ussin, University of South Carolina, won the **Herman R. Branson Pauling Prize** for **S-30:** *Structural characterization of 1-deoxy-D-xylulose-5-phosphate reductoisomerase from Vibrio vulnifcus*, by Nikita Ussin, Makenzie Perdue, Lesa Offerman, and Maksymilian Chruszcz. D-xylulose-reductoisomerase, Dxr, is one of the 5 metabolites essential to the survival of *V. vulnifcus*; it is responsible for converting the poster structure, DX5P, into 2-C-methyl-D-erythritol-4-phosphate (MEP) in the terpenoid backbone synthesis pathway, via cofactor NADPH. In *E. coli*, NADPH binds to the N-terminal end of Dxr. Fosmidomycin is an antibiotic known to inhibit Dxr activity through slow, tight binding inhibition. This inhibition occurs only after the Dxr-NADPH complex has been formed. Structural analysis, as well as biochemical characterization of VvDxr and its interaction with inhibitors, will not only allow for a detailed view of the enzyme's mechanism, but also allow for the potential development of antimicrobial agents against bacteria for which the MEP pathway of terpenoid synthesis is critical for survival.



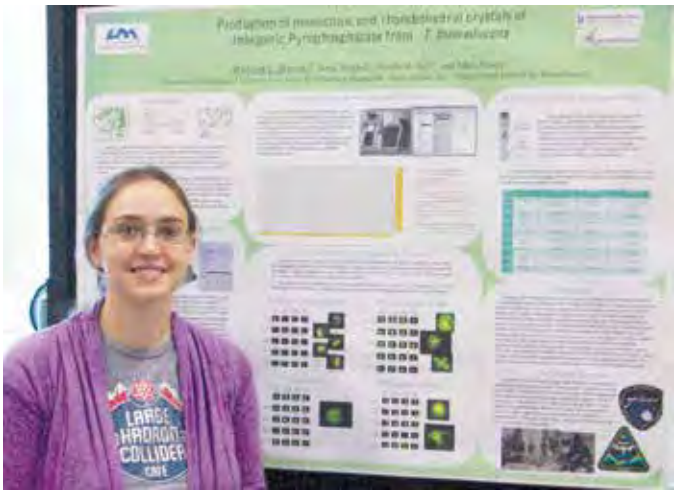
Oxford Cryosystems Low-Temperature Prize

This prize, sponsored by **Oxford Cryosystems, Inc.**, is open to all participants. The 2014 winner for the best poster describing work done at low temperature was poster **M-41**: *Yes, solvent molecules do matter: Solvatomorphism and polymorphism of cis-22-tetrakis(monothiosuccinimidato)dimolybdenum(II),* by **Brian S. Dolinar**, **Ilia A. Guzei**, and **John F. Berry**. The poster describes a quadruple-bonded Mo---Mo system with the paddlewheel shape characteristic of such compounds. The title compound, the *cis*-isomer (C2h symmetry) of a compound that can exist in this form or as a *trans*-isomer (D2d symmetry), or others, depending on the relative dispositions of the four polar ligands, crystallizes with different structures depending upon whether methanol or dichloromethane is used as the solvent. Further, the MeOH solvate undergoes a conservative phase transition from monoclinic to twinned triclinic when the temperature is lowered. The attractive, well executed poster gave the context of the study, the structures of the solvatomorphs, and a succinct description of the temperature-provoked phase transition suffered by the methanol solvate. The judges were **Doletha Szebenyi** and **Larry Falvello**.

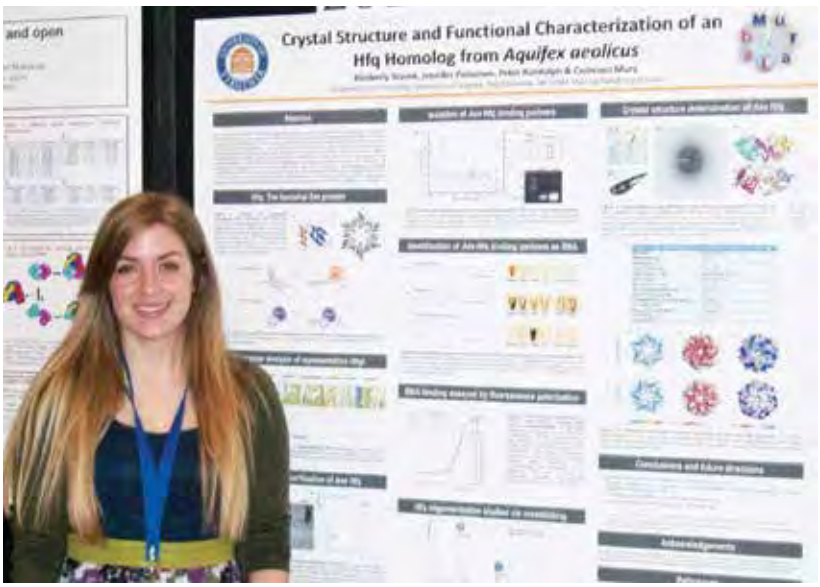
Larry Falvello

Taylor & Francis Biomolecular Crystallography Poster Prize

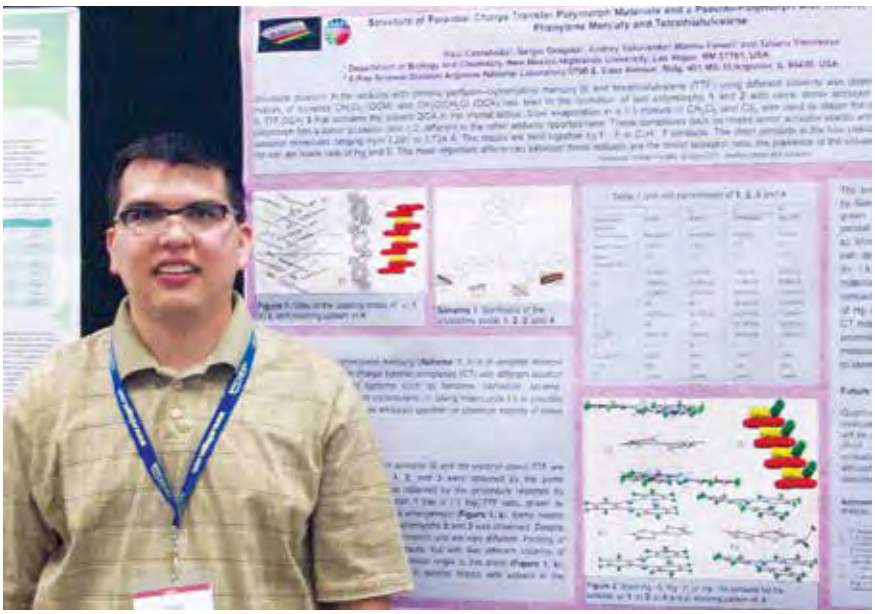
This prize, established in 2012, is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The 2014 judges were **L. Wayne Schultz** and **Thayumanasamy Somasundaram**. They selected **Michelle Morris**, University of Alabama to receive the prize for her poster **M-19**: *Monoclinic and rhombohedral crystals of inorganic pyrophosphatase from T. thioreducens*. Poster Chair Ilia Guzei presented Michelle with Bernhard Rupp's book *Biomolecular Crystallography*, which was donated by the Taylor & Francis Group.



RCSB PDB Poster Prize



The **RCSB PDB Poster Prize** recognizes a student (*graduate or undergraduate*) poster presentation involving macromolecular crystallography. The award consists of two educational books and an announcement on the **Research Consortium for Structural Biology - Protein Data Bank** website and newsletter. The 2014 RCSB PDB judges were: **Esko Oksanen**, **Michael Sawaya**, and **Barry Finzel**, and they selected **Kimberly Stanek,** U of Virginia, for **S-06**: *Crystal structure and functional characterization of an Hfq homolog from Aquifex aeolicus*.



The CrystEngComm Prize

The **CrystEngComm Prize**, sponsored by the **Royal Society of Chemistry**, is awarded to the best graduate or undergraduate poster in the field of crystal engineering/supramolecular chemistry. The 2014 judges were **David Grossie** and **Judy Gallucci**.

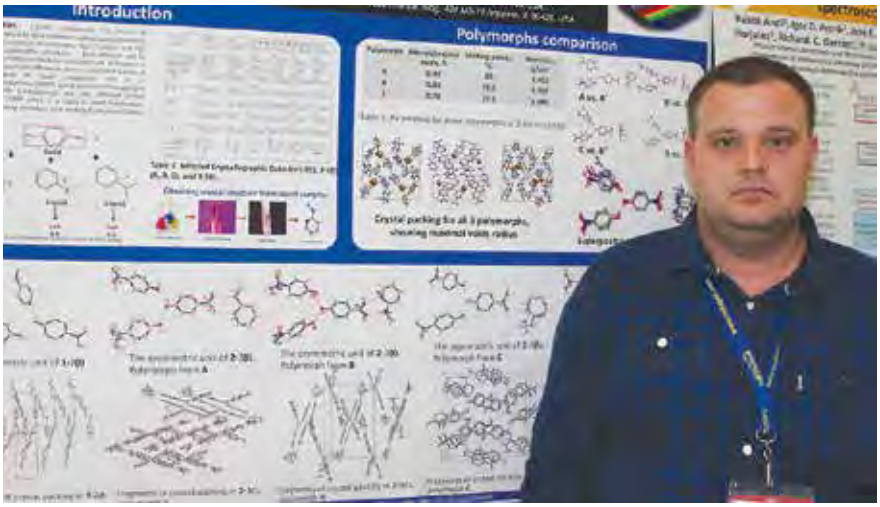
Raúl Castañeda from New Mexico Highlands University was given an RSC book voucher for his winning poster **M-31**: *Structures of potential charge transfer polymorph materials and a pseudo-polymorph with trimeric perfluoro-o-phenylene mercury and tetrathiafulvalene*. An announcement of Raúl's award will be posted on the *CrystEngComm* website.

Judith Gallucci

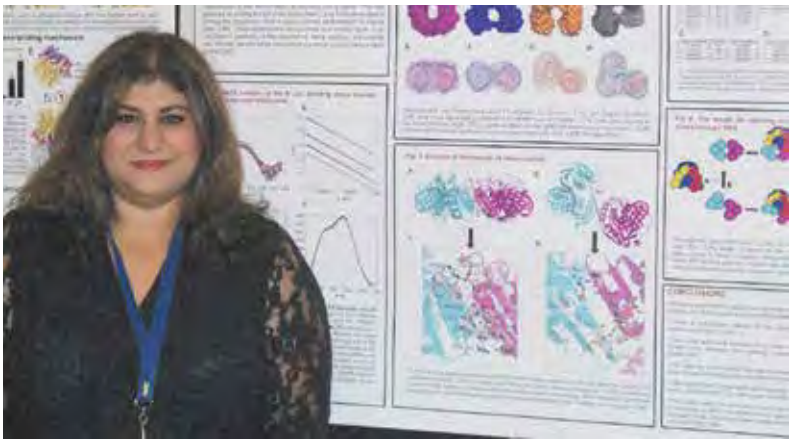
Journal of Chemical Crystallography Prize

This prize, sponsored by **Springer's** *Journal of Chemical Crystallography*, is given to the best student *(graduate or undergraduate)* poster presentation in the area of chemical crystallography or small molecule structure determination and analysis. **Sergiu Draguta**, New Mexico Highlands University, is this year's recipient. Sergiu's winning poster **M-40**, *X-ray structural analysis of liquids compounds and their predisposal to polymorphism*, reported several structures of compounds that are ordinarily liquids, but form crystalline salts when cocrystallized with 4-nitrophenol. When the liquid is 2-(methylamino)pyridine, three polymorphs form. The judges were **Frank Fronczek and Joe Ng**.

Frank Fronczek



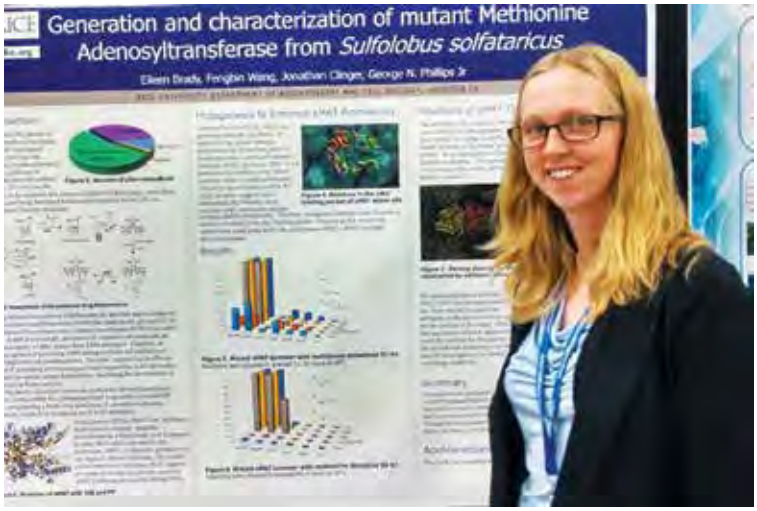
Structural Dynamics Prize



The **Structural Dynamics Prize** of $250, which is sponsored by the new **ACA / AIPP** journal, *Structural Dynamics,* is given 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 and is open to students (*graduate and undergraduate*) and post-docs.

The 2014 prize went to **Farzaneh Tondnevis**, University of Florida, for poster **M-21:** *pH induced equilibrium shift mechanism between closed and open E. coli b-lopjhsliding clamp revealed*. The judges were **Patrick Loll** and **Jan Abendroth.**

MiTeGen-Society of Physics Students Undergraduate Poster Prize



This prize was established through a collaboration with the **Society of Physics Students** (SPS) and the **ACA** to encourage young undergraduate researchers in the field of crystallography and recognizes the best undergraduate poster presentation. **MiTeGen** generously donated a portion of the $250 cash prize. The 2014 judges were **Kraig Wheeler, Roger Rowlett, Yulia Sevryugina, Krystle J. McLaughlin**, and **Toni Sauncy**, the director of SPS. The first recipient was undergraduate **Eileen Brady**, Rice University, for **S-04:** *Characterization of mutant methionine adenosyltransferases from Sulfolobus solfataricus*. Eileen impressed the judges with her firm grasp and understanding of her project, as well as the level of work she presented. We hope this new prize will inspire more undergraduates to join the ACA and attend our meetings.

Krystle J. McLaughlin.

Reception for Undergraduate Students

L to R: Cora Lind-Kovacs, Yulia Sevryugina, Krystal McLaughlin, Toni Sauncy

In collaboration with the **Society of Physics Students** (SPS), there were some new student-centered initiatives at ACA 2014 including a new poster prize for undergraduates (see above) and a lunchtime reception on Sunday that was open to all students, their mentors and anyone else who was interested in learning about SPS. The almost fifty attendees, most of them students, were treated to lunch and a short program. ACA president **Martha Teeter** provided the welcome remarks and then **Toni Sauncy**, Director of the SPS, gave an introduction to the SPS and its activities. Organizers **Krystle J. McLaughlin** and **Yulia Sevryugina** (YSSIG Chair) spoke about the benefits of getting involved with ACA and the activities planned for young scientists during the meeting. Next, **Cora Lind-Kovacs** gave a rousing talk titled *Through the looking glass: A reciprocal space perspective*. Filled with fun demonstrations using diffraction gratings and lasers, the talk engaged and captivated the audience, touching on such topics as 'Why study crystallography?'. After Cora's talk, raffle prizes donated by the SPS were awarded to some lucky attendees. The reception was capped off with the distribution of diffraction glasses to all in attendance!

Krystal J. McLaughlin

Contributors to this Issue

Jessica Addiss, Jonathan Agbenyega, Dan Anderson, Kritica Arora, Eddy Arnold, Gerald Audette, Christine Beavers, Amadeo Biter, Olaf Borkiewicz, Eileen Brady, Richard Bromund, Sue Byram, Chuck Campana, Grace Chik, Ed Collins, Raúl Castañeda, Marcia Colquhoun, Bridget d'Amelio, Paul Davies, Louise Dawe, Jeff Deschamps, Graciela Diaz de Delgado, Brian Dolinar, Antonio dos Santos, Sergiu Draguta, Robert Evans, Jeanette Ferrara, Joseph Ferrara, Zoë Fisher, Frank Fronczek, Judith Gallucci, Stephen Ginell, Alisa Glukhova, Jenny Glusker, Jane Griffin, Colin Groom, Ilia Guzei, Marv Hackert, Gregory Halder, John Helliwell, Fred Hollander, Michael James, Pavol Juhas, Dale Kreitler, Borden Lacy, Cora Lind-Kovacs, Patrick Loll, George Lountos, RamSashank Madhurapantula. Lee Makowski, Robert McKenna, Krystle McLaughlin, Alex McPherson, Jason Mercer, Eric Montemayor, Peter Müller, Allen Oliver, Katharine Page, Chiara Pastore, Dish Patel, Mary Ann Perozzo, Virginia Pett, Patti Potter, Dan Rabinovich, Albert Reger, John Rose, Gerd Rosenbaum, Roger Rowlett, Amy Sarjeant, W. Robert Scheidt, Yulia Sevryugina, Carla Slebodnick, Edward Snell, Kimberly Stanek, Cheryl Stevens, Vivian Stojanoff, Martha Teeter, Tom Terwilliger, Diana Tomchick, Farzaneh Tondnevis, Andrew Torelli, Nikita Ussin, Xiaoping Wang, Suzanna Ward, Kraig Wheeler, Christine Zardecki, Peter Zwart

Many of the speaker photos, the photos in the poster prize pages, and those on pages 13, 24, 35 and 46 were taken by our *RefleXions* staff photographer, Peter Müller.

2014 ACA Meeting - Albuquerque, New Mexico, May 24 - 28

The meeting began with workshops on **Joint Neutron and X-ray Structure Refinement using JointRefine in PHENIX**, on **Grazing Incidence SAXS Theory and Data Analysis**, and on **Reciprocal Space Visualization - MAX3D**. Reports on these and on the **Travel Award** winners will be featured in the winter issue of *RefleXions*.

The **Patterson Award** was presented to **John Helliwell**; **Borden Lacy** received the **Margaret C. Etter Early Career Award**; **Jenny Glusker** gave a plenary lecture on **Women in Crystallography**, and **Dan Rabinovich** received the **Elizabeth A. Wood Science Writing Award**. Dan talked about **The World of Crystallography on Postage Stamps**; see the cover and the **On the Cover** article, page **5.**

The *Transactions* Symposium, **100 Years of Crystallography** took place on the first day of the meeting. **Edward Snell** chaired both the morning and the afternoon sessions. The **Program Chairs** were **Christine Beavers** and **Peter Zwart**; **Ilia Guzei** was the **Posters Chair**; **Jeff Deschamps** managed the **Session Photos**; and **Virginia Pett** and **Richard Bromund** comprised the **Videography Team** that recorded the award and plenary lectures.

Edward Snell

Christine Beavers

Peter Zwart

Ilia Guzei

Jeff Deschamps

Virginia Pett & Richard Bromund

See reports on the *Transactions* Symposium; the awards; and the sessions and posters in the following pages. Scenes from the Opening Reception are below.

L to R in the photo immediately below left: Paul Davie, Colin Groom, Jonathan Agbenyega, Suzanna Ward, Peter Müller; to the right, Philip Martin & Jim Pflugrath.

In the photos at left, L to R: Kunlun Hong; Mary Ann Perozzo & Bi-Cheng Wang; Fred Hollander & ??

John R. Helliwell was presented with the **2014 Patterson Award** by ACA President Martha Teeter for *"his pioneering contributions to the development of instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography."* Established in 1980, the Patterson Award **recognizes and encourages outstanding research in the structure of matter by diffraction methods.** The award is given every three years to outstanding scientists in the field.

John began his talk with the ACA mission statement '*Share your science, change your world*' followed by a quote from ***Patterson and Pattersons*** (J.P. Glusker, ed, Oxford University Press) : *"Patterson obtained a fellowship to go and work with W H Bragg in London. His supervisor said that he should alter his ways and work hard to represent the USA well. When he arrived W H Bragg said: - 'of course besides work do enjoy yourself!'."* Throughout his career John has shared his science and enjoyed himself.

A long-time member of ACA and Professor of Structural Chemistry at the University of Manchester, UK, John received his undergraduate degree in physics from York University, where his studies were guided by Michael Woolfson and Peter Main. He then pursued a PhD in protein crystallography at Oxford under the supervision of Margaret Adams. He was mentored by Charlie Bugg and Guy Dodson in the laboratories of Dorothy Hodgkin and David Phillips and was involved in the first experiments that used synchrotron radiation for macromolecular structural studies.

John thought of himself, as *"… perhaps a rebellious student"* feeling that what was going on in the lab was rather basic. At this time Dorothy Hodgkin shared with him the pre-print of a publication resulting from work led by Keith Hodgson at Stanford, (*Proc. Nat. Acad. Sci.* (1976) **73**:128). The first sentence in the paper stated how controversial it was to consider the use of synchrotron radiation in protein crystallography. (The subject was evidently also controversial in the UK as Ron Mason, in a letter to Dorothy Hodgkin, mentioned his disagreement with the view that the use of synchrotron radiation would not be relevant.) The first reference in Keith's paper was a publication by Rosenbaum, Holmes and Witz (*Nature* (1971) 230:129) where they describe synchrotron radiation as a source for x-ray diffraction. These two papers influenced John to make up his mind; **"There is no controversy; this is really important!"**. John decided to dedicate his career to making synchrotron radiation relevant.

As we celebrate the feats of 100 years of crystallography research, John's role in applying synchrotron radiation to macromolecular crystallography stands out. His book *Macromolecular Crystallography with Synchrotron Radiation*, published by Cambridge University Press in 1992 and available in paperback since 2005, has become a classic and a must read for those entering the field. A protagonist since the very first experiments at SRS, one of John's most lasting contributions to the community is his role with Hassain and Kamitsubo as founding editor of *Journal of Synchrotron Radiation*.

The *Transactions* Symposium at the ACA meeting in Buffalo that John organized with Steve Ealick is in his view his most significant contribution to the ACA and the crystallographic community (*The 1999 ACA Transactions,* **Vol 34**, *Two Decades of Synchrotron Radiation Research*). It was probably around this time that John's attention extended even further into applications of neutrons and electron microscopy to macromolecular crystallography.

John Helliwell & Martha Teeter

It is one thing to be a great scientist, but John has another, very important dimension to his personality and that is his gift to enthuse, inspire and teach others. His former students got to be established researchers in academia, government institutions or industry. He has trained a generation of crystallographers not only through the many students that he supervised but also by being a friend and mentor to many others. John has a very subtle way of mentoring. One of John's former students Edward Snell, Hauptman Woodward Medical Research Institute, said about his time as PhD student in John's group, *"The most fantastic thing was [that he, John allowed you] to follow your own path. He gave you enough rope to potentially hang yourself, but never let you fall."* "John challenges your brain and curiosity,"said Michele Cianci, also a former student of John, now at EMBL Hamburg. "He cares about people and not about how brilliant they are." John became a friend to most of his former students as they got to be established researchers in academia, government institutions or industry. *"John has a warm, generous and approachable personality, and is the best collaborator that you can wish for,"* says Naomi Chayen, Imperial College.

John is recognized for his commitment in advancing women's careers in science, technology, engineering, math's and medicine (STEMM) employment in higher education and research; prior to his arrival in Manchester there were no women among the faculty. In 2013 the School of Chemistry at Manchester University was awarded the Athena SWAN Silver Award in recognition of the school's commitment to advancing women's careers in STEMM.

John always makes time for helping people, and often puts their interests ahead of his own. With his lifelong partner, Madeleine Helliwell, he shares science and family. His wide interests and his essential curiosity about all manner of things ensures that: '*John does not only share his science he shares the fun in it!*'

I am thankful to Edward Snell, Michele Cianci, Naomi Chayen, and Madeleine Helliwell for sharing their personal insights with me.

Vivian Stojanoff

Editor's Note: John's award lecture is now up on the ACA History Portal.

Dan Rabinovich was presented with the **2014 Elizabeth A. Wood Science Writing Award** by ACA President Martha Teeter.

As crystallographers we are keen on finding science in everyday objects. Snowflakes are a winter nightmare to many, but a beautiful essay in symmetry to us. The antibiotics a loved one takes to cure an illness are a medical miracle, but our understanding of their structure shows a different kind of wonder. What of the postage stamps we use to mail our letters? Increasingly stamps have given way to e-mail, text messages and social media – but not for Dan Rabinovich. Just as we find crystallography in the world around us, so does Dan see it in something as simple as a postage stamp.

In his Wood Award lecture entitled *The world of crystallography on postage stamps*, Dan outlined the story of crystallography as told through myriad images found on stamps. From the earliest beginnings with Pliny the Elder's description of crystals to structures of fullerenes and viiiiitamin C, the greatest achievements of our discipline have been affixed to envelopes and curated by philatelists the world over. From Ukraine to Peru, Moldova to Comoros, countries big and small have celebrated crystallography, crystal structures and crystallographers. Each one carries its own story, some not quite accurate, about the wonders of crystallography.

Ilia Guzei with Dan Rabinovich

Dan uses these tales to augment his lectures at UNC-Charlotte. A series of stamps highlighting the rapid advances in understanding x-ray radiation reveals how primed the scientific community was to utilize this new phenomenon. News of this new form of radiation spread around the world almost as fast as the stamps that commemorate it. By showing how widespread these stamps are, students can truly understand how important crystallography is to the world at large. Dan's lecture presented an engaging walk through the world of crystallography as drawn out on something as simple as a postage stamp.

Amy Sarjeant

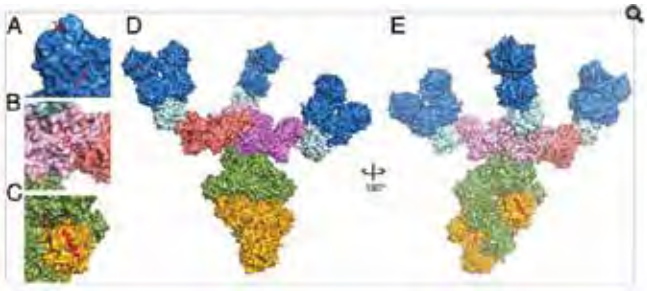
At the Opening Recception: Jessica Addiss & Marcia Colquhoun; RamSashank Madhurapantula

P.03: Margaret C. Etter Early Career Award

The ACA was proud to introduce Professor **Borden Lacy** as this year's Etter Award winner. The **Margaret C. Etter Award** recognizes early career scientists with outstanding achievement and exceptional potential in crystallographic research. Borden Lacy exemplifies these qualities as demonstrated by her record and confirmed by the presentation of one of the top talks at the ACA meeting in Albuquerque. She presented *Exploring the structures of clostridial protein toxins*, where she proceeded to show beautiful connections between her new and previously determined protein crystal structures as well as proposed mechanisms for the effects of bacterial toxins on host cells.

Borden did a masterful job of putting her work in the broader context of bacterial pathogenicity as studied by others, yet showed highly significant contributions of her own, including the new and challenging crystal structures of complexes of toxins and/or receptors solved by her research group that are critical to the field. She went beyond the scope of her title to discuss pathogens other than *clostridium* as a late-breaking bonus for the audience. The insights provided about toxin entry were well explained and quite enlightening. It was easy to see why the award committee chose her for the Etter award. It was an impressive performance.

George N. Phillips, Jr.



16S PCs have multiple sugar binding sites. (A) Two N-acetylgalactosamine binding sites have been identified in the structure of HA1/C (3AH2 and 3AJ6), and the sugars have been superimposed on the BoNT/D (HA1)2-HA2 trimer structure (blue) and depicted as red sticks. (B) The HA3 trimer (pink) was crystallized with alpha 2–3-sialyllactose, which is depicted in red sticks. (C) The GT1b binding site (with GT1b shown in red sticks) is located between BoNT/A1 (gold) and NTNH (green). Superposition of the BoNT/B receptor-binding domain (HCR)-SytII structure (2NM1) onto the BoNT/A1 HCR suggests that the SytII binding site will be accessible in the BoNT/B PC structure (SytII depicted as a red a-helix). (D) Model of a "flat" view BoNT/A1 PC shown with three arms. (E) The BoNT PC rotated 180° to the 'prong' view reveals the accessibility of the GT1b binding site and the SytII binding site. D.A. Benefield, S.K. Dessain, N. Ohi, & D.B. Lacy, Proc Natl Acad Sci U S A. 2013 April 2;110(14):5630-5635.

P04: Plenary Lecture, Women in Crystallography

Jenny Pickworth Glusker

Early Crystallographic Investigations by Nobel Laureate Dorothy Hodgkin. Dorothy Mary Crowfoot was born in Cairo, Egypt on May 12, 1910, the daughter of John Winter Crowfoot, an egyptologist and historian, and Grace Mary Crowfoot née Hood, an expert in ancient textiles. John Crowfoot served with the Egyptian Ministry of Education; he later became the Principal of Gordon College at Khartoum and was Director of Education and Antiquities in the Sudan.

For the first 4 years of her life Dorothy lived in Asia Minor, returning to England with her parents only for a few months each year. She spent the World War I years in the care of relatives in the UK, traveling to visit her parents when they were in Cairo or Khartoum. Encouraged by her mother, she developed a passion for chemistry at an early age – she first attended the Sir John Leman School, Beccles, Suffolk and then, from 1928-1931, Somerville College, Oxford. This was one of the five women's colleges at Oxford, although course work was coeducational. From 1932 until 1934, she studied under the tutelage of John Desmond Bernal at Newnham College, Cambridge, and it was during this time that she learned of the potential of x-ray crystallography to determine the structures of molecules relevant to biological problems.

In 1933 she was appointed a research fellow at Somerville College, and in 1936, when she obtained her PhD, she became a Fellow and Tutor there. She was appointed a University Lecturer in 1946, University Reader in 1955 and Wolfson Research Professor of the Royal Society in 1960, all at Oxford University. Dorothy admired her scientific mentor, J.D.Bernal unreservedly; he influenced her both scientifically and politically (she always referred to him as "Sage," as did many crystallographers).

In 1937 Dorothy married Thomas Lionel Hodgkin, son of Robin H. Hodgkin, provost of Queen's College, Oxford, and a cousin of A. L. Hodgkin, a Nobel Prize winner in 1963. Thomas became an advisor in 1961 to Kwame Nkrumah, President of Ghana, where he remained for extended periods, often visited by Dorothy. They had three children: Luke (born 1938), who became a topologist at King's College, London and also taught at the University of Algiers and Princeton University; Elizabeth (born 1941), who taught at a girl's school in Zambia in 1964 and now works for Amnesty International (she has been very active in Viet Nam and the Sudan); and Tobias (born 1946), who is interested in the conservation and use of genetic diversity and now works for the International Plant Genetic Resources Institute in Rome. Dorothy knew 9 grandchildren and 3 great-grandchildren.


Crystallography group in the OCD laboratory—1954, from left to right
(*standing*) J. H. Robertson, M. Innes, A. Chung, J. Pickworth, B. Oughton, F. Welch;
(*seated*) M. Webster, Dorothy Hodgkin, H. M. Powell, M. Mackay, D. Lawton.

The crystallography group in the OCD lab in 1954. Jenny Pickworth is the 4th from left in back; Dorothy Hodgkin is the 2nd from left in the front.

Dorothy also very much admired Kathleen Yardley Lonsdale (1903-1971). Kathleen was made a Fellow of the Royal Society in 1945; she and Marjory Stephenson were the first women to achieve that honor. Kathleen had many other honors: in 1956 she was named Dame Commander of the Order of the British Empire; in 1966 she became the first woman president of the IUCr; and in 1967 she was the first woman president of the British Association for the Advancement of Science. The crystallographic community knew her because finally, in 1929, she proved by x-ray diffraction methods that the benzene ring was flat. She did this by solving the crystal structure of hexamethylbenzene while in W. H. Bragg's laboratory – this work was published in *Nature* in 1928. In 1936 she published *Simplified Structure Factor and Electron Density Formulae for the 230 Space Groups of Mathematical Crystallography*, G. Bell & Sons, London; her research was used in the preparation of the *International Tables of Crystallography*, first published in 1935.

In a letter to Clifford Frondel, who had named a meteoritic form of diamond after her, Kathleen, who was very petite, wrote: *"It makes me feel both proud and rather humble that it shall be called Lonsdaleite. Certainly the name seems appropriate since the mineral only occurs in very small quantities (perhaps rare would be too flattering), and it is generally rather mixed up!"*

Dorothy said of her, *"There is a sense in which she appeared to own the whole of crystallography in her time."*

Dorothy studied more than 100 steroids in order to show how they packed in the crystalline state. Bernal had shown that the chemical formula for steroids by Wieland and Windaus was unacceptable because the unit cell dimensions and optical properties of crystals indicated that a molecule with their formula could not fit in the unit cell. So Dorothy, back in Oxford, determined the crystal structure of cholesteryl iodide with Harry Carlisle and thus confirmed that the formula that Bernal suggested was correct. Dorothy Hodgkin received the Nobel Prize in Chemistry in 1964 for her determinations by x-ray diffraction of the crystal structures of cholesteryl iodide (which confirmed the chemical skeleton of steroids), penicillin (which showed that it had a beta-lactam ring in its chemical formula), vitamin B_{12} (the largest molecule for which the chemical formula, previously unknown, was established) and, later, the protein hormone insulin.

At right, Dorothy's hand-drawn structure of insulin. Her drawings were very carefully done and required many hours. This one shows the influence of her childhood trips to Khartoum. She presented it as a gift to Helen Megaw, who overlapped with Dorothy in Bernal's lab and in 1957 published a book "Ferroelectricity in Crystals."

Jenny went on to describe to her attentive audience many details about Dorothy's work on penicillin, vitamin B_{12} and insulin. She quoted Jack Dunitz on **Dorothy's Special Contributions to Science** from page 59 of *Structural Studies on Molecules of Biological Interest*, edited by Guy Dodson, Jenny P. Glusker and David Sayre, Clarendon Press, Oxford, 1981.

Jenny also told many amusing stories about the trials and tribulations of the work on penicillin. She was especially gratified when the Google Doodle featured the structure of insulin on May 12, 2014, which was Dorothy's 104th birthday.

Connie Rajnak

TR01 &TR011, The *Transactions* Symposium: 100 Years of Crystallography

L to R: Edward Snell, Cora Lind-Kovacs, Alex McPherson, Martha Teeter, Helen Berman.

Organizers **Stephan Ginell** and **Edward Snell** put together a series of related topics capturing a historical view of the field in this, the **International Year of Crystallography (IYCr). Cora Lind-Kovacs**, U Toledo, began by describing the outreach activities associated with the ACA participation in the IYCr. Her talk, *Fun with crystals, light and symmetry,* included a preview of the new IYCr website and a description of a crystal growing competition open to the public. **Martha Teeter**, UC Davis, followed with *A brief history of women in crystallography*. From very early times crystallography has been one of the scientific fields where women have had a large impact; as examples, Martha mentioned luminaries including Nobel Laureate Dorothy Hodgkin, Helen Megaw, Kate Dornberger-Schiff, Rosalind Franklin and Doris Evans. Martha's talk covered a history of the influence of these women and others and also explored relevant current issues such as balancing family with work. She discussed the results of responses to a survey of ~90 senior female crystallographers.

Cora Lind-Kovacs & Martha Teeter in high spirits.

Alex McPherson talked about protein crystallization in his talk, entitled, *Protein crystallization over 200 years: From art to science*. He noted that the first reports of protein crystals date back almost 200 years. Initially these crystals were an intellectual curiosity and crystallization was used to isolate a protein and demonstrate its homogeneity. Alex showed how these early observations, *e.g.*, the crystallization of urease in 1926 by J. B. Summer, led to many of our modern physical and chemical approaches to crystallizing proteins. Alex took the audience through two centuries of crystallization history with stunning pictures, the 'art' of crystallization.

Helen Berman, Rutgers U, described *Databases in crystallography, past present and future*. Appropriately, the Protein Data Bank (PDB) celebrated its 100,000th entry just before the start of the meeting. Helen told about the very early days when the databank held just a handful of proteins. She covered the rapid development of databases, not just protein, which have mirrored the rapid acceleration of crystallographic techniques and broadened into other structural studies. She brought the audience up to date with the latest and planned future developments, summarizing both the historical and future challenges.

TR011 opened with **Wayne Hendrickson**, Columbia U, who presented *Changing practice in crystallographic phase evaluation for biological macromolecules*. Wayne described the history of phase determination in macromolecular crystallography and how it was initially influenced by methods for phasing small molecules. As more models were deposited in the PDB the method of molecular replacement became more successful and therefore increasingly popular. Noting that these methods were limited experimentally because often no homologous structure was available, he described the development of multiwavelength anomalous diffraction (MAD) and how synchrotron sources and molecular biology techniques made MAD readily available. He then described how single-anomalous diffraction (SAD) experiments were taking over from MAD, with examples of many beautiful structures along the way. Finally, Wayne described the debt that macromolecular crystallography owes to the pioneers in the small molecule world.

L to R: Edward Snell, Robert Sweet, Brian Toby, James Holton, Wayne Hendrickson

James Holton, UCSF, ALS, LBNL, talked about *The dawn of the age of uncertainty,* a journey through the history, geography and interpersonal relations that characterized the development of x-ray crystallography during the past century. He linked the physics of x-rays with the experimental and theoretical developments that have led to structural crystallography as we know it today and described the key developments that enabled the field. The talk by **Bob Sweet**, BNL, *Synchrotron radiation in structural biology, past, present and future* reinforced some of the other talks in its emphasis on personality as a strong element of discovery. He discussed the first synchrotron experiments, current instruments and future sources. Synchrotrons and their associated instrumentation have matured in the 60 or so years they have been part of the century of crystallography but, as Bob made clear, there is still much potential to be harvested.

Brian Toby, APS, ANL, provided balance to this weighted-very-heavily-towards-biology session with his talk *Powder diffraction: 98 years as plan B* noting that powder diffraction is a little younger than single crystal studies, *i.e.*, only 98 years old. Brian covered not only x-ray developments but reminded the audience that neutron diffraction is also a significant tool for the structural crystallographer. He finished his presentation with some exciting glimpses of things to come.

Edward Snell and Stephan Ginell

1.1.2: Instrumentation and Methods for Structure Solution of Nanosized Materials

L to R: Pavol Juhas, Katharine Page, Simon Billinge, Daniel Olds, John Helliwell.

The development and commercialization of nanomaterials critically depends on an accurate knowledge of their atomic structure. Structure determination of nanomaterials is an open problem, as is our capacity to conduct time studies and stability assessment for individual particles. This session highlighted developments in experimental and data analysis methods for nanostructure determination, including diffraction, imaging, spectroscopy, and also theoretical approaches to nanostructure prediction. Different perspectives on the nanostructure problem, including the physical and biological sciences relevant to inorganic, organic and biological nanomaterials were discussed. **John Helliwell**, U Manchester, UK, gave a brief report on IUCr's participation in a CODATA/VAMAS Working Group for standardization of nanomaterials.

Daniel Chateigner, Université de Caen, France, talked about structure analysis of nanopowders using combined x-ray and electron powder diffraction patterns, and their studies of the size, shape and texture of nanoparticle assemblies. He also described the CODATA/VAMAS efforts on standards for definition and characterization of nanomaterials, which added to the general overview of CODATA given by session co-chair John Helliwell.

Simon Billinge, Columbia U and Brookhaven National Laboratory, reported on the development of data-processing techniques, algorithms and software tools for nanostructure determination. The essence of this approach is to use inputs from multiple experimental and theoretical probes (pair distribution function, small angle scattering, bond valence sums, chemical knowledge) to overcome poor resolution and low information content in the diffraction data from nanomaterials.

Next, **Katharine Page**, Lujan Center, Los Alamos National Laboratory, presented studies of nanomaterials using total scattering, mostly neutron PDF, as well as their investigation of structure effects on the electronic properties and catalytic performance of nanomaterials. Finally **Daniel Olds**, also from the Lujan Center, described the development of stroboscopic techniques that greatly enhance the time resolution of measurements with pulsed neutrons, and their employment in studies of transient states in soft materials under harmonic loads.

Significant advances in technique are still needed in order to make nanostructure determination routine; accurate nanostructure descriptions, and development of guidelines for instrumentation and for methods of treating nanostructure data are essential to this effort. Hence IUCr involvement in the CODATA/VAMAS efforts to standardize, not least for defining safe use, is vital.

Pavol Juhas and John R. Helliwell

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1.1.4: Frontier of Structure-Selective Characterization in Complex Soft Matter Materials

Paul Butler, NIST Center for Neutron Research (NCNR), started the session by discussing the study of pore formation on the surface of lipid membrane vesicles in aqueous solutions. He highlighted the importance of using a contrast variation technique, where the D_2O:H_2O ratio is selectively altered in order to observe various structures in complex objects.

Cheng Wang, Lawrence Berkeley National Lab (LBNL), reviewed soft x-ray scattering and cited examples of developments that can greatly benefit this emerging new x-ray technique. Studies of soft matter materials can often reveal unique information about the structure.

In back, L to R: Wei Chen, Cheng Wang, Byeongdu Lee, Xin Li, and Kunlun Hong. Seated in front: Joseph Kline, Paul Butler, Yun Liu, Lilin He.

Kunlun Hong, Oak Ridge National Lab (ORNL), Center For Nanophase Materials Sciences, presented the deuteration capability at CNMS available to research communities in the USA and gave a few examples showing how the selective isotope replacement of hydrogen by deuterium can help identify unique structures of complex materials.

Byeongdu Lee, Argonne National Laboratory (ANL) Advanced Photon Source, discussed a few examples from his research using anomalous small angle x-ray scattering (ASAXS) showing how ASAXS helps to explain complex structures. The use of both SAXS and SANS as complementary tools was shown to be very useful for resolving structures.

Xin Li, ORNL, talked about the way in which his lab has used neutron spin echo and SANS to illustrate the dynamic and structure evolution of soft colloids as a function of concentration. **Lilin He**, ORNL, discussed his research on block copolymer gels using SANS.

Joseph Kline, NIST, reviewed their research effort using soft x-ray scattering and critical-dimension SAXS techniques to characterize block copolymer patterns. This is critically important to the semiconductor industry especially for conventional optical lithography.

Wei Chen and Yun Liu

At left: Melissa Pinard at the Opening Reception.

At right, Farzaneh Tondnevis at the Opening Reception.

1.2.1: Industrial Research from Young Scientists

This session highlighted the invaluable research being performed by young scientists either within an industrial environment or in collaboration with industry.

In back, L to R: Christopher Bianchetti, Jacob Trotta, Peter Wood, George Lountos. In front, L to R: Rajni Bhardwaj, Ghazala Sadiq, Puja Pathuri, Melissa Matthews. Photo taken by Peter Müller.

Rajni Bhardwaj, U Strathclyde, gave us an overview of her work in collaboration with Eli Lilly & Co. on the pharmaceutical compound olanzapine. Rajni's research on the compound revealed a wide range of solid forms; at least three anhydrous polymorphs and more than 50 solvates of olanzapine were found. It is intriguing that some compounds seem to show so much solid form diversity. This work highlighted the importance of using both experimental and computational methods to characterise and understand the diversity.

Jacob Trotta, Villanova U and Alkermes, Inc., the **Etter Student Lecturer** chosen by the **Industrial SIG**, presented his research on polymorphic compounds. Jacob told the fascinating story of aripiprazole and its closely-related cousin dehydro-aripiprazole. These compounds differ only by the swap of a single C–C bond to a C=C double bond, and yet their rich polymorphic behavior (five or more polymorphs each) shows no supramolecular structural similarity so far!

Jacob Trotta accepting the Margaret C. Etter Student Lecturer Award from Session Chair Peter Wood. Photo by Peter Müller.

Ghazala Sadiq, U Manchester, gave us two excellent case studies on tailoring solid forms. The first study highlighted how the morphology (macroscopic shape) of crystals can be modified using suitable solvents to make samples more amenable to industrial processing. Ghazala showed how, by using rationally selected additives, one can even affect whether a chiral compound will form racemic crystals or conglomerates of pure *R* and pure *S* crystals.

Puja Pathuri, Astex Pharmaceuticals, discussed the application of fragment-based drug discovery to develop novel treatments for the Hepatitis C virus with particular focus on designing inhibitors for the HCV-N3S/4a protein. Using an in-house small molecule fragment library, a novel fragment-binding site was discovered at the protease-helicase interface on HCV-N3S/4a that led to the structure-based design of an allosteric inhibitor with low nM potency.

Christopher Bianchetti, U Wisconsin-Madison, presented a multi-faceted approach using bioinformatics, bioassays, and x-ray crystallography to study the multifunctional glycoside hydrolase family 5, which can be used to degrade cellulose enzymatically. A combination of all these techniques may allow the structure-guided engineering of these family 5 enzymes in order to improve their activity in large-scale conversions of plant biomass for renewable energy sources.

Melissa Matthews, U California-Davis, presented crystal structures of several enzymes involved in the production of activated CMP-sialic acid. Knowledge gained from these structures in complex with various substrates and analogues will allow for the engineering of improved enzymes that can be used for the chemoenzymatic synthesis of a variety of natural and synthetic sialic acids that can be used to study complex carbohydrates and glycoconjugates.

Peter A. Wood and George T. Lountos

W. Robert Scheidt, listening attentively.

1.2.3: Disorder and Inhomogeneiety in Complex Materials Probed by PDF

L to R: Daniel Shoemaker, Claire White, James Neilson, Allyson Fry, Kevin Know, Vicky Doan-Nguyen, Ram Seshadri.

Among all these dynamic young speakers, the emphasis was on employing and advancing synchrotron x-ray and neutron pair distribution function (PDF) methods that could be used on functional inorganic materials. **James R. Neilson,** Colorado State U, described how symmetry analysis can help to better digest total scattering data on materials, using as an example some Colorado State neutron PDF studies of barium titanate.

Claire White, Princeton U, explained how electronic structure calculations help to make sense of PDF studies of geopolymers. **Kevin Knox**, BNL and Columbia U, introduced the fascinating idea of *emphanisis* and showed evidence for its occurrence in tin and lead chalcogenides.

1.2.4: General Interest I

Jeffrey Deschamps, NRL, and his coworker Damon Parrish examined 28 nitro-aromatics, including triaminotrinitrobenzene (TATB) and three previously unpublished structures in order to identify forces that stabilize this high explosive. Jeff showed, by summing the energies involved in Van der Waals forces, hydrogen bonds, and other intermolecular interactions, that there is a direct relationship between the estimated energy of stabilization and the sensitivity of nitro-aromatic explosives.

George Lountos, Leidos Biomedical Research, presented his work on the crystal structure of the *Trypanosoma cruzi* protein tyrosine phosphatase, TcPTP1, which has been implicated in Chagas' disease, a prevalent tropical affliction. The structure will be used in structure-based drug design efforts to develop specific TcPTP1 inhibitors.

Sergei Pletnev, NIH, described the x-ray structures of green laGFP and red laRFP from lancelet *Branchiostoma lanceolatum;* Sergei went on to talk about a mystery: the laGFP and laRFP chromophores look structurally identical in the crystal structures, but the spectral properties of laGFP and laRFP are different. It appeared that the chromophore of laRFP has an unusual covalent bond that is highly susceptible to radiation damage, and its degradation is not detectable from data processing statistics. This example of laGFP and laRFP proteins shows how important it is to verify whether the obtained results make sense from the standpoint of chemistry, biology and physics, and not just rely on seemingly good data and clear electron density.

Daniel Shoemaker, U Illinois, presented beautifully detailed scattering studies employed in order to understand what happens in a chalcogenide flux during materials synthesis.

Efrain Rodriguez, U Maryland, presented on magnetic chalcogenides studied by neutron techniques. **Allyson Fry**, Johns Hopkins U, discussed dynamic PDF studies of functional materials. **Vicky Doan-Nguyen**, U Penn, the **Powder Diffraction SIG**'s choice to give the **Margaret C. Etter Student Award Lecture** discussed x-ray PDF studies of nanoparticles, drawing analogies with metallic glasses.

Ram Seshadri

Standing in back: Jeff Deschamps, Lynn Ten Eyck, Sergei Pletnev. In front: Graciela Diaz de Delgado, George Lountos, Zhen Huang.

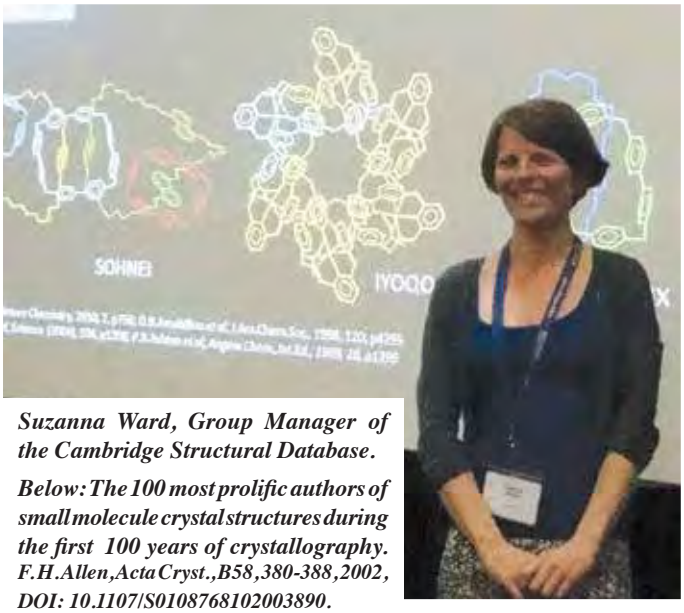
Zhen Huang, Georgia State U, reported the first protein-nucleic acid structure (RNase H/RNA/DNA complex) determined by selenium-derivatized nucleic acids. Their high-resolution crystal structure indicated that Se-replacement resulted in a subtle local unwinding on the RNA/DNA substrate duplex, thereby shifting the RNA scissile phosphate closer to the transition state of the enzyme-catalyzed reaction. They observed that the scissile

phosphate might catalyze its own hydrolysis(!)

Because the refinement process as currently practiced is inherently biased through use of a model to provide phase information, **Lynn Ten Eyck**, UCSD, and his colleagues developed 'model-free' criteria for analysis of crystal structures. Lynn presented preliminary findings from comparisons of high resolution, well-refined structures from the Joint Center for Structural Genomics repository with maps based solely on phases from selenomethionine anomalous scattering. Removal of atoms with little or no support in the 'objective' map reliably improved R_{free}.

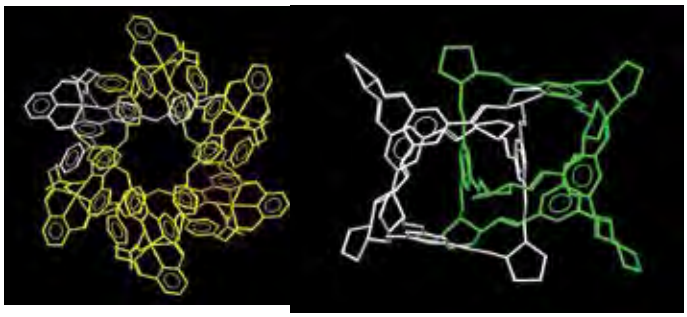
With charming wit, **Suzanna Ward**, CCDC, presented interesting facts extracted from the Cambridge Structural Database: the most prolific authors, the oldest structure, the largest molecules, the molecule with the largest number of different elements, polymorph propensity, and many other features nicely put in her abstract as "extraordinary, curious and bizarre." Case studies of seminal structures such as cholesterol, phthalocyanine, ferrocene and C_{60} were also discussed. See the images below of Suzanna and her work.

Graciela Diaz de Delgado



Suzanna Ward, Group Manager of the Cambridge Structural Database.

Below: The 100 most prolific authors of small molecule crystal structures during the first 100 years of crystallography. F.H.Allen,Acta Cryst.,B58,380-388,2002, DOI: 10.1107/S0108768102003890.



A molecular borromean ring; refcode IYOQOC. F.H.Allen,Acta Cryst.,B58, 380-388,2002,DOI:10.1107/S0108768102003890; K.S. Chichak, S.J.Cantrill, A.R. Pease, Sheng-Hsien Chiu, G.W.V. Cave, J.L. Atwood, J.F.Stoddart, Science, Vol. 304 no. 5675 pp. 1308-1312,(2004),DOI: 10.1126/science.1096914.

Interlocking: One of the more extraordinary small molecule crystal structures in the CSD – A triply interlocked covalent organic cage, with refcode PUZCOL.

F. H. Allen, Acta Cryst., B58, 380-388, 2002, DOI: 10.1107/S0108768102003890; Tom Hasell, Xiaofeng Wu, James T.A. Jones, John Bacsa, Alexander Steiner, Tamoghna Mitra, Abbie Trewin, Dave J. Adams & Andrew I. Cooper, Nature Chemistry, 2, 750–755, (2010) doi:10.1038/nchem.739.

General Interest Posters

S-14: High impact crystallography? - A statistical analysis of crystal structures reported in the CSD (1997 - 2012) by **Amy Sarjeant**, Northwestern U. Many of us who have devoted a lot of effort to making sure that CheckCIF is completely satisfied prior to publishing our results in *Acta Crystallographica*, or to carefully refereeing a paper for *Acta*, have felt that such high-quality structural publications did not have high enough impact. Amy Sarjeant replaced sentiment with solid statistical analysis of small-molecule structures in the Cambridge Structural Database (CSD). Journals were considered if they were in the top 20 by number of structures submitted to the CSD, and/or had one of the top 20 Impact Factors (IFs) for journals in chemical disciplines. From the results she drew 7 conclusions: (1) Before 2005 the journal that published the most structures, usually *Inorg. Chem.*, had an IF around 3; afterwards, this spot was taken by *Acta Cryst E* with its much lower IF. (2) The highest IF of any journal to publish any crystal structures in a given year was generally attained by *Nature* in the range 30-40, but a higher spike for *Acta Cryst. A* in 2009 is attributable to the article about SHELX subsequently cited by every user. (3) Despite improvements in equipment, the average *R*-factor has remained steady at ≈5%. (4) Tolerance of poor data seems to be increasing since the maximum published *R*-factors across the board are trending slightly upwards. (5) The publishers of the most crystal structures on a yearly basis were *Inorg. Chem.*, *Organometallics*, *Dalton Trans.*, and *JACS*, and lately, *Acta Cryst. E*. (6) From 1997 to 2002 there was a positive correlation between IF and *R*-factor, but after 2002 the correlation coefficients became small. (7) The highest IF journals, *Nature* and *Science*, publish small molecule structures in 0.5-1.5% of articles per year. Popular chemical journals have percentages of 20-60%.

Carl Schwalbe

On top, a panorama view of the poster area.

Below that, L to R: Suzanna Ward, Paul Davie, Peter Müller, Colin Groom; Jessica Bruhn with her poster.

At left: Jonathan Agbenyega & Noriko Inoguchi; Allyson Fry.

Below, from the left: Häkon Hope, Marilyn Olmstead, James Fettinger & Kamran Ghiassi; Judy Flippen-Anderson, Mary Ann Perozzo & Jeff Deschamps. Left Corner, Bill Duax; Charles Campana.

1.3.1: Career Odysseys

In the back, L to R: Kevin Bieg, Ilia Guzei, Joseph Orgel. Sitting in front: Claudia Rawn, Jim Pflugrath, Margaret Gordon.

The panel was held on Sunday evening as an educational introduction to the networking/cocktail hour later that night at the YSSIG mixer held at the Hotel Andaluz rooftop bar, Ibiza.

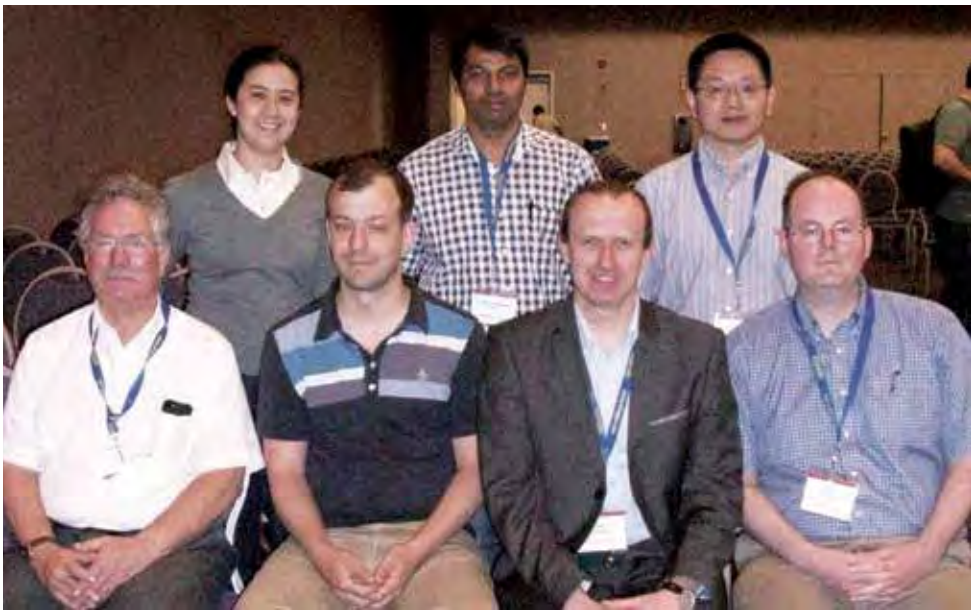
Six panelists were invited from varied career paths. To represent governmental and legal research, we had **Kevin Bieg** and **Margaret Gordon**. Kevin Bieg is a Senior IP official at Sandia National Laboratories and was an AIP Fellow on legislation and policy; as a consequence he was able to share his experience in becoming a chemist who ventured into the legal aspects of research. Margaret Gordon is a researcher at Sandia National Laboratory, and she talked about her research there as well as grant writing and proposal formulation. **Ilia Guzei**, U Wisconsin, and **Jim Pflugrath**, Rigaku, are crystallographers. The professorial career path was represented by **Joseph Orge**l, Illinois Institute of Technology, and **Claudia J. Rawn**, U Tennessee-Knoxville.

The panel began with introductions. This was followed by discussions of the sectors represented: Academia, Industry, and National Laboratories (Research and Legal IP). Questions were then taken from the audience. A summary of the questions and answers can be found at ***http://tinyurl.com/lbfcdoz***. A summary of the speakers' backgrounds can be found at ***http://tinyurl.com/n89q7lk***.

Martin Donakowski

Zbigniew Dauter, Listening.

2.1.1: Scattering and Energy Storage Materials



Standing in back, L to R: Karena Chapman, Jitendra Bahadur Lnu, Lilin He. Sitting in front: Rex Hjelm, Peter Chupas, Olaf Borkiewicz, Paul Forster.

Karena Chapman, Argonne National Laboratory (ANL), discussed their new approaches to decouple mesoscale phenomena. **Paul Forster**, U Nevada, reported how his group used different methods to study the separation of gases.

Rex Hjelm, Los Alamos National Lab, used small angle neutron scattering (SANS) to characterize the morphology of an ionomer, Nafion, in dilute solutions and with different solvents. A combination of SANS and NMR measurements showed that the Nafion structures formed in different solvent types fell into three classes, all well explained by equilibrium and non-equilibrium thermodynamics. There were interesting correlations between Nafion dispersion morphology and the properties of critical membrane electrode assemblies (MEAs). This is consistent with the hypothesis that the properties of the MEAs are dependent on the Nafion morphologys in the ink from which they were cast. The fuel cell industry will use the results of their research to guide the preparation of new Nafion materials which have optimum morphologies and mechanical properties.

Jitendra Bahadur Lnu, Oak Ridge National Laboratory, described their work using SANS to characterize the pores of shales. Shale gas will be a main energy source in the near future in the US, but how the gas is stored in the shale pores and how the gas interacts and moves in the shales remains unclear. SANS with contrast matching technique can provide information about pore structure, pore connectivity, pore accessibility and the unique phase behaviors of gases, all of which is vital for the shale gas industry.

Kamila Wiaderek and **Olaf Borkiewicz**, both from ANL, each talked about the difficulties presented by *in situ* studies of local structure in lithium ion batteries using x-ray powder diffraction and other spectroscopic methods. The impact of such studies could predict new materials for energy storage.

Craig Bridges and Lilin He

2.1.2: Neutrons in Biology: Structural Enzymology

Standing in back, L to R: Matt Challacombe, John Bacik, Oksana Gerlits, Paul Langan. In front, Irene Weber, Andrey Kovalevsky, Zoë Fisher.

The first of two 'Neutrons in Biology' sessions focused on structural enzymology studies using neutron crystallography.

Irene Weber, Georgia State U, presented the neutron structure of perdeuterated HIV-1 protease in complex with the clinical drug amprenavir. The 2.0 Å room-temperature neutron data were collected at the Institut Laue-Langevin (ILL), Grenoble, from a small ~0.2 mm^3 crystal. This is the first study in a series that will attempt to document how protease inhibitors bind to HIV-1 protease and its drug resistant mutant variants. Weber's neutron crystallographic studies revealed novel details about H-bonds between amprenavir, the catalytic Asp residues and other

residues in the active site. Analysis of the enzyme:drug interactions showed that, based on non-H interatomic distances from low-temperature x-ray structures, some H-bonds were weaker than had been assumed.

Paul Langan, Oak Ridge National Laboratory (ORNL), graciously filled in for **Chris Dealwis**, who could not attend the meeting. Paul described joint neutron and x-ray studies of the ternary dihydrofolate reductase (DHFR) complex, comprised of DHFR:Folate:$NADP^+$. This complex represents a pseudo-Michaelis complex and is functionally relevant. DHFR is a very attractive target for a variety of clinical applications, including cancer, malaria, and for the design of novel antibiotic drugs. A proposed hydride shift mechanism based on the neutron structure was presented, along with some practical tips for large crystal growth and a description of the data collection of a 3.6 mm^3 crystal to 2.0 Å resolution at IMAGINE (High Flux Isotope Reactor, ORNL).

John Bacik, Los Alamos National Laboratory (LANL), talked about proposed neutron structural studies of an anhydrosugar kinase, levoglucosan kinase (LGK). LGK is a very interesting target for biofuel research as it has been shown that recombinant expression of LGK in *E. coli* allows the cells to use the abundant levoglucosan as a carbon source. Understanding the catalytic mechanism of this enzyme might help to increase biofuel production from the biomass pyrolysis product levoglucosan. John reported progress toward this goal with initial large crystal growth and test diffraction patterns obtained at the Protein Crystallography Station at the Los Alamos Neutron Science Center, LANL.

Oksana Gerlits, ORNL, presented the first joint neutron and x-ray crystal structure of cyclic guanosine monophosphate (cGMP)-dependent protein kinase (PKG), and reported details about the cGMP binding. This protein plays a role in vasodilation and blood pressure regulation, and hence is a drug target for the development of PKG agonists to treat aneurisms. PKGs are members of the Ser/Thr kinase family and are homologs of cAMP-dependent protein kinases (PKAs). The molecular mechanism by which PKGs are selectively activated by cGMP rather than a structurally similar cAMP is poorly understood. X-ray studies, mutagenesis, and fluorescence polarization assays demonstrated that PKG is highly specific for cGMP binding and revealed 2 specificity mediating residues, Leu296 & Arg297. To study the molecular interactions that mediate selectivity, a neutron structure, at 2.2 Å, of the CNB-B domain of PKG with cGMP bound was determined at the ILL. This structure, along with the CNB-B/cAMP x-ray structure, unambiguously showed which residues and hydrogen bonds are responsible for the regulatory domain's high selectivity towards cGMP.

Matt Challacombe, LANL, presented computational studies of the xylose isomerase (XI) reaction mechanism based on a series of neutron crystal structures. These studies focused on XI complexes with the sugar in the cyclic and linear forms and were carried out with 306 atom, quantum only models at the B3LYP/6-31G** and B3LYP/6-311G** level of theory. The results show very interesting novel features including a proton switch involving a Lys-Asp pair that compensates for the movement of Mg by ~12 kcal/mol. Multiple reaction steps with barriers of ~15-25 kcal/mol each were also observed and, finally, a product state involving the linear isomer sugar and regenerated catalytic water that is significantly lower in energy than the starting (cyclic) state. These results also show the high impact that neutron crystal structure information can have on providing accurate light atom positions for computational studies of reaction trajectories, especially when hydrogen transfer is involved.

Zoë Fisher and Paul Langan

2.2.3: Supermolecular Assemblies

In back, L to R: Eric Montemayor & Gerald Audette. Smita Kakar & Yusong Guo are in front.

Yusong Guo, Rice U, the **Margaret C. Etter Student Lecturer** chosen by the **BioMac SIG**, presented her studies of several proteins, including the viral capsid of a nematode infecting virus. She discussed insights into the assembly of the icosahedral viral capsid, compared the structure of the capsid with other plant and *naroviridae* viruses, and discussed some important protein RNA interactions.

Yusong Guo accepting the Etter Student Lecturer award from Gerald Audette.

Smita Kakar, National Cancer Institute, presented recent structural as well as functional studies into the RapA protein involved in bacterial RNA polymerase recycling. The RapA protein is involved in freeing up multiple transcriptional templates, and Smita used SAXS studies, her crystal structure and enzymatic assays to show that the N-terminal region of the protein was a flexible domain important in the transcript recycling process. **Eric Montemayer**, U Wisconsin, presented structures of U6 snRNA in complex with the tetra RNA Recognition Motif (RRM) protein Prp24. The structures suggest a mechanism by which ATP-independent helicases can chaperone pairing of small nuclear RNA in the spliceosome.

Gerald Audette

2.2.4: Producing and Transporting Energy: Thermoelectrics, Superconductors, Photovoltaics, and Magnets

In back, L to R: Vladimir Antropov, Kirill Kovnir, Huibo Cao. In front: Patrice Kenfack Tsobnang, Michael McGuire, Bryan Chakoumakos.

Kirill Kovnir, U C-Davis, presented a very comprehensive talk about $Ba_8M_{16}P_{30}$ (M= Cu/Zn) clathrates and their phase transformations induced by electron doping. Clathrates are a promising class of thermoelectric materials that convert heat flow into electric current, and vice versa, in cooling and power generation applications. Kirill showed that by combining transition metals and pnictogens in the covalent framework of these compounds, new structure types result. The crystals are likely to be twinned, so powder methods serve best to determine the correct unit cell and symmetry. The high density of twin interfaces may play an important role in reducing the thermal conductivity, which must be low for good thermoelectric performance.

Patrice Kenfack Tsobnang, U Yaoundé I, Cameroon, described the molecular-network-based porous material $Co(C_6H_8N_2)3Cr(C_2O_4)_3•6H_2O$. The molecules are joined by hydrogen bonding, and the hydrated structure contains a unique dodecameric cluster of water molecules. Crystals can be dehydrated and rehydrated reversibly multiple times. During this process, the unit cell volume changes by more than 20%, but the symmetry remains the same. It may be possible to exchange the water with other small molecules. Porous materials such as these have potential applications in gas storage and separation, and fuel cell technologies.

Bryan Chakoumakos, Oak Ridge National Laboratory (ORNL), described results of structural studies from a naturally occurring mineral specimen, stephanite, Ag_5SbS_4. X-ray and neutron diffraction from single crystals were used to examine the temperature dependence of the crystallographic properties, including the atomic displacement parameters. The results indicated the silver ions are loosely bound, and could migrate through the structure, consistent with high ionic conductivity. Ionic conductors, where one species is highly mobile within a rigid framework, are needed for solid-state batteries, supercapacitors and fuel cells.

Vladimir Antropov, Ames Laboratory, pointed out some of the challenges associated with finding new, high-performance permanent magnets, and how to address these problems using first principles calculations. One of the primary challenges is achieving highly anisotropic magnetic properties, the main focus of this presentation. Having a single strongly-preferred direction for magnetization, or easy axis, requires having a uniaxial crystal structure. But that is not enough. Strong spin-orbit coupling or strongly anisotropic magnetic interactions between atoms is also required. The $(Fe_{1-x}Co_x)_2B$ system, which shows both strongly positive and strongly negative anisotropy energies as x varies, was used as an example of the sensitivity of magnetic anisotropy to electron concentration. The unusual increase in anisotropy with increasing temperature in MnBi was emphasized, as was the surprisingly strong orbital moment anisotropy in $Li_2(Li_{1-x}Fe_x)N$. It was noted that close collaboration between experimentalists and theoreticians is key to solving this longstanding problem.

Huibo Cao, ORNL, showed how the application of neutron diffraction to high quality single crystals allowed Huibo and his colleagues to study the complex magnetic structures adopted by intermetallic binary compounds R_5Pb_3 (R=Nd or Tb). It was found that the magnetic order in Nd_5Pb_3 is commensurate with the crystal lattice, unlike the closely related Nd_5Sn_3. In the Pb compound the order develops in two steps upon cooling, with moments on some Nd atoms ordering at 38 K, and others at 10 K. Tb_5Pb_3 was found to undergo a single magnetic ordering transition near 73 K. The data indicated a complicated and incommensurate magnetic structure, with different types of modulated magnetic moments on the two Tb sites.

Michael McGuire

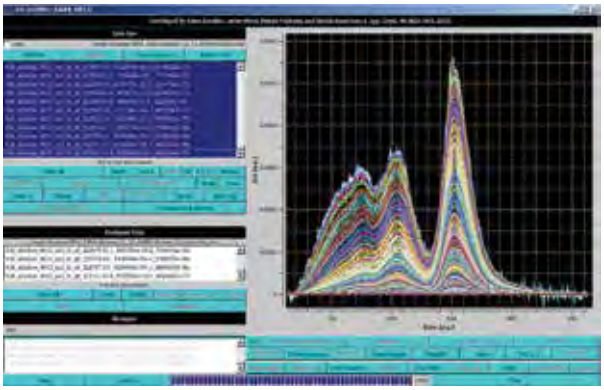
2.2.6: Bio SAS Data Analysis within US-SOMO

This was a special session that covered the SAS capabilities of the UltraScan SOlution MOdeler suite, ***http://somo.uthscsa.edu*** and included a hands-on tutorial working through HPLC-SAXS data analysis on an experimental data set. **Javier Pérez**, Beamline SWING, Synchrotron SOLEIL, Saint Aubin, France, presented a background to SAS and analysis techniques and in particular online SEC-SAXS, commenting on some of the observable problems.

L to R: Mattia Rocco, Emre Brookes, Javier Pérez.

Emre Brookes, U Texas Health Science Center, gave an overview of US-SOMO capabilities, which include multiple hydrodynamic modeling methods, a variety of small angle scattering tools and a discrete molecular dynamics facility for expanding conformational space for subsequent SAS screening. **Mattia Rocco**, Biopolimeri e Proteomica, IRCCS AOU San Martino-IST, Genova, Italy, presented the US-SOMO HPLC-SAXS tools in detail and directed the tutorial while Javier Pérez and Emre Brookes assisted participants in working the examples. The session was attended by several prominent beamline scientists representing the majority of online SEC-SAXS facilities worldwide.

The hands-on tutorial portion began with a look at well-behaved RNase experimental data, to illustrate the basic functionalities of the program, followed by an analysis of noisy and fouled BSA data, and finished off with an analysis of Aldolase data containing multiple overlapping and skewed peaks. The latter two experimental datasets were each decomposed into multiple monodisperse I(q) curves. This involved the transformation of the original I(q) vs. q frames (I(q) being the SAXS intensities as a function of the momentum transfer q) into a series of I(t) vs. t chromatograms (see figure below) for each q value



I(t) vs t chromatograms for Aldolase experimental data as shown in the US-SOMO SAXS HPLC module. Each curve represents an individual q-value. The peaks are not baseline resolved and are skewed likely due to column matrix interactions.

(t being either time elapsed or frame number). The I(t) were then checked for the proper behavior of each chromatogram, *i.e.*, its returning to baseline values after the completion of solute elution. The BSA example [data not shown] did not return to the baseline, a condition most likely indicating that capillary fouling has occurred. While this type of problem should be dealt with primarily at the experimental level, this is not always possible. A novel integral baseline tool, which works on the assumption that fouling by solutes sticking to the capillary is proportional to their relative concentration while under the x-ray beam, was applied to produce a corrected profile. Furthermore, the BSA and especially the Aldolase datasets' chromatograms presented overlapping, not baseline-resolved peaks.

A Single Value Decomposition (SVD) tool demonstrated a method for the estimation of the minimum number of components necessary to fully account for the observed profiles. A Gaussian decomposition procedure, employing either symmetrical or non-symmetrical Gaussian functions (the latter required, for example, for the data shown in the figure), was applied to back-generate single-species intensity curves suitable for further analysis. A concentration profile could be likewise decomposed, allowing, together with data normalization and conversion into absolute units tools, for correct estimation of the molecular weight of each decomposed species. Rapid visualization tools for the evaluation of radii of gyration from Guinier plots from back-generated I(q) vs. q frames and/or their scaling were also demonstrated.

Emre Brookes, Javier Pérez and Mattia Rocco

Philip Martin & Zbigniuw Dauter

L to R: Yi Tian Ting, Brian Mahon, Jaime Jensen, Amadeo Biter, Kimberly Lincoln, Anna Baker, Lagnajeet Pradhan, Eric Reinheimer, Yulia Sevryugina, Katarzyna Jarzembska.

3.1.1: Etter Early Career Award Symposium

Anna W. Baker, U Wisconsin-Madison, presented the structure of Bacteriophytochrome response regulator (Brr), a single domain response regulator (SDRR) from *Ramlibacter tataouinensis* that is implicated in transducing red light signals sensed by a bacteriophytochrome histidine kinase. Anna's structural results show that Brr subunits form homodimers by linking their carboxy-termini in a non-covalent 'arm-in-arm' interaction. The effects of this unusually stable dimer on signaling have yet to be investigated.

Yi Tian Ting, U Auckland, New Zealand, described the 2.2 Å resolution crystal structure of a Type I signal peptidase (SPase) of multi-antibiotics resistant *Staphylococcus aureus*, the first SPase structure for any gram-positive organism. Elucidating this structure is an important step toward the development of drugs for antibiotic-resistant gram-positive bacterial infections.

The Young Scientists SIG chose **Brian Mahon**, U Florida College of Medicine, to be a **Margaret C. Etter Student Lecturer**. Brian discussed the contribution that his research made to the long debate about whether or not the artificial sweetener saccharin is indeed a potential carcinogenic agent. Carbonic anhydrase isoform IX (CA IX) has been shown to be a key modulator of aggressive tumor behavior and established as an anti-cancer target for several types of cancer. A crystal structure of CA IX bound to saccharin could shed light on the debate, but what if the wild-type CA IX does not crystallize? Brian reasoned that since the active site of CA IX differs by only a few amino acids from that of CA II, he could prepare a CA IX mimic to be used as a working model. His successful determination of the 1.6 Å resolution structure of the mimic-CA IX bound to saccharin suggested that saccharin should bind preferentially and with high affinity to CA IX. This would mean that it in fact has a potential as an anti-cancer therapeutic, or at the very least, as a model for the development of structurally homologous therapeutics for several cancer types.

Brian Mahon receiving the Margaret C. Etter Student Lecturer Award from Yulia Sevryugina.

Katarzyna Jarzembska, U at Buffalo, SUNY, presented a method of time-resolved x-ray Laue diffraction for determination of molecular excited state geometries in the solid state. Her experiments were conducted on a solvent-free crystal form of a model dimeric tetranuclear complex containing silver(I) and copper(I) ($Ag_2Cu_2L_4$, L = $C_9H_7NPPh_2$, 2-diphenylphosphino-3-methylindole). This system exhibited red solid-state luminescence (650 nm at both room temperature and 90 K) with a lifetime of about 1 μs, one of the shortest-lived excited states that have ever been studied with the Laue technique. Katarzyna observed significant structural changes upon irradiation, such as Ag···Ag bond distance shortening of 0.38(3) Å for the excited state and even more pronounced change in one of the Cu···Ag distances, which suggests formation of new intermetallic bonds on excitation.

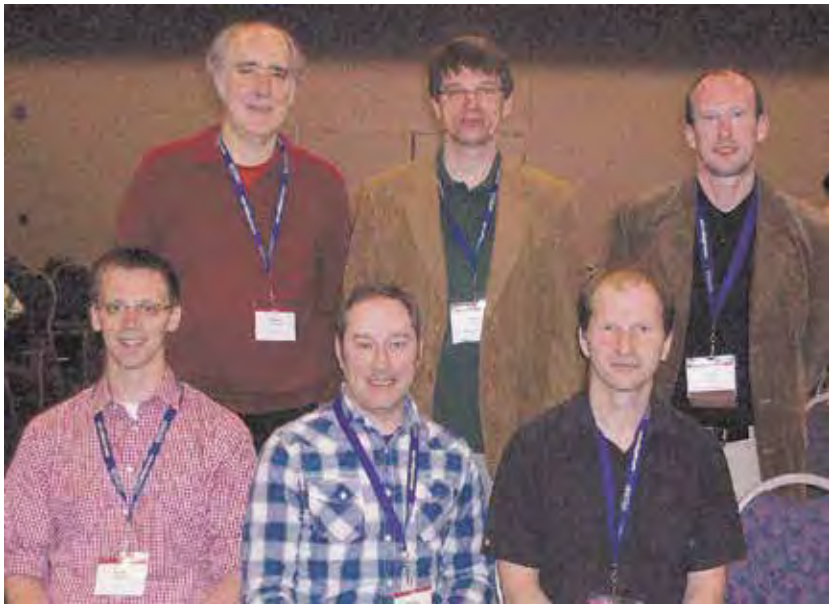
Yulia Sevryugina

Dan Anderson & David Sargent at the Opening Reception.

Note: The Etter Early Career Symposium received generous financial support from Bruker, Sigma-Aldrich, and the ACA.

Session 3.1.3: Solution Structure and Dynamics of Biomacromolecules (I)

Two sessions at the Albuquerque ACA focussed on **SS&DB**; the other session was **4.1.1** (see page 37). Both were co-sponsored by the small angle scattering SIG, the biological macromolecules SIG and the Canadian division.



Standing in the back, L to R: Tracy Nixon, Volker Urban, Frank Gabel. In front: Thomas Grant, Nicholas Clark, Thomas Weiss.

The opening talk by **Tracy Nixon**, Penn State U, described combining data from time-resolved small angle solution scattering, crystallography and electron microscopy in order to understand how typical homomeric ATPases associated with various cellular activities can perform mechanical work. Tracy explained how the closed hexameric ring of the bacterial enhancer binding protein NtrC1 transformed into a split ring in the presence of ATP and that this asymmetry imparts a unique identity and function to each subunit that is then harnessed to deliver mechanical work to asymmetric target molecules.

Nicholas Clark, National Institute of Standards and Technology (NIST), presented a study combining SAXS, (small angle x-ray scattering), and SANS, (small angle neutron scattering), data to investigate the intermolecular interaction of monoclonal antibodies (mAbs) in highly concentrated solutions. These highly concentrated solutions are typical for therapeutic formulations of mAbs and exhibit a range of problematic behaviors, *e.g.*, liquid-liquid phase separation, aggregation and time dependent precipitation. Nicholas discussed how solution scattering methods can be used to determine the intermolecular interactions of the mAbs molecules in these solutions, which should aid in understanding the effects of pH, salt and concentration on the behavior of these highly concentrated solutions.

Then **Thomas Grant**, Hauptman-Woodward Institute, discussed the structure and dynamics of the appended domain of the yeast glutaminyl-tRNA synthetase (Gln4). Although the 215-residue appended to the N-terminal domain of Gln4 was missing in the electron density of the full-length crystal structure, its presence could be confirmed using SAXS. Molecular dynamics simulations of the full-length bound enzyme coupled with SAXS analysis revealed a series of large conformational dynamics present in the Gln4 mechanism of aminoacylation.

Frank Gabel, Institut de Biologie Structurale, Grenoble, emphasized the power of combining SANS, SAXS and NMR data to study high molecular-weight biomacromolecular assemblies such as the Box C/D complex, which is responsible for the post-transcriptional methylation of ribosomal RNA. He also pointed out that SANS data, together with deuterium labeling and contrast variation, were crucial for determination of the respective positions of the protein and RNA subunits within the apo- and holo-complexes for the NMR-modeling process.

Finally, **Volker Urban**, Oak Ridge National Laboratory (ORNL), described the recent upgrade of the of the BioSANS instrument at ORNL and other developments including recently developed sample environments; a high pressure cell; a sample changer with 'tumbler' cells (continuously rotating the samples during the measurements), and a humidity controlled sample chamber for lipid studies. Volker also pointed out that the newly extended BioSANS instrument can perform experiments in grazing-incidence geometry on planar samples, such as substrate supported lipid bilayers.

Thomas Weiss

3.1.5: Earth and Environmental Sciences

Standing in back, L to R: Margit Fabian & Christine Beavers. In front, Hsiu-Wen Wang, Olaf Borkiewicz, Claudia Rawn.

This session was a joint collaboration between the Powder Diffraction SIG, the Materials SIG and the Neutron Scattering SIG. It provided a broad overview of neutron and x-ray scattering studies on materials that are of great significance to earth and environmental sciences.

Hsiu-Wen Wang, Los Alamos National Laboratory, began by describing her latest work on the local structure of opal. She pointed out that her findings have broad implications for diagenetic environments. Hsiu-Wen's multi-modal analytical approach, which involved x-ray diffraction combined with pair distribution function analysis and multi-level modeling, provided valuable new insights into the structure of opal.

Margit Fabian, Hungarian Academy of Sciences, discussed the applications of micro x-ray diffraction to phase determination in a special argillaceous rock formation located in south-eastern Hungary that is considered to be a potential host rock for a deep geological radioactive waste repository.

Christine Beavers, Lawrence Berkeley National Laboratory, presented and discussed in detail new developments, equipment upgrades and additions at the beamline 12.2.2 of the Advanced Light Source – a high-pressure diffraction beamline used frequently by the US geological community.

Claudia Rawn, U Tennessee-Knoxville, reported on the synthesis and crystal chemistry of mayenite doped with Fe. She described a new synthetic route that yields high-purity samples with high Fe concentration and presented x-ray and neturon scattering data elucidating the structure-property relationships of the new material.

Olaf Borkiewicz and Claudia Rawn

3.2.1 Flesh & Blood: Intact and *in situ* Connective Tissue Diffraction Studies of Animals, Plants and Insect Bodies, and 1.1.1: Pathological Fibers: Trions, Amyloids & Friends

Standing in back, L to R: Jiliang Liu, Paul Langan, Joseph Orgel, Rama Sashank Madhurapantula. In front: Brendan Sullivan, Olga Antipova, Robert Perc-Edwards, Tatiana Timofeeva.

Sessions 3.2.1 and 1.1.1, organized by the Fiber Diffraction SIG, were merged at the ACA meeting because they shared the theme of biological and biomedical research aided by diffraction methodology.

Several of the speakers in 3.2.1 discussed *in situ* tissue x-ray diffraction of brain, muscle and connective tissues as well as biomass conversion that complemented beautifully the discussions in 1.1.1 of anti-convulsant drug development and pathological brain disease. **Rama Sashank Madhurapantula,** Illinois Institute of Technology (IIT), was chosen by the Fiber SIG to receive the **Margaret C. Etter Student Lecturer Award**. Rama talked about glycation detection in collagen.

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Rama Sashank Madhurapantula (at left) being congratulated by Session Chair Joseph Orgel.

3.2.1 / 1.1.1 cont'd:

Joseph Orgel, IIT, gave an overview on the advances in prion structure and described their progress in amyloid and brain disease research.

Tatiana Timofeeva, New Mexico Highlands U, discussed their discovery that compounds that contain an (- substituted amide group as their main structural motif inhibit neuronal nicotinic acetylcholine receptors (nAChRs) and show promising anticonvulsant activity in several animal models of epilepsy.

Bendan Sullivan, Purdue University, characterized copper in neuronal stem cells.

Olga Antipova, IIT, and her colleagues used x-ray fiber diffraction techniques to study bovine cardiac collagenous tissues and observed different collagen types as well as different fibril distribution patterns in the leaflet and annulus of valves. Combined with Transmission Electron Microscopy, their data may reveal the correlation of collagen fibril structure with its macromolecular ligands and their effect on the mechanical properties of heart valves.

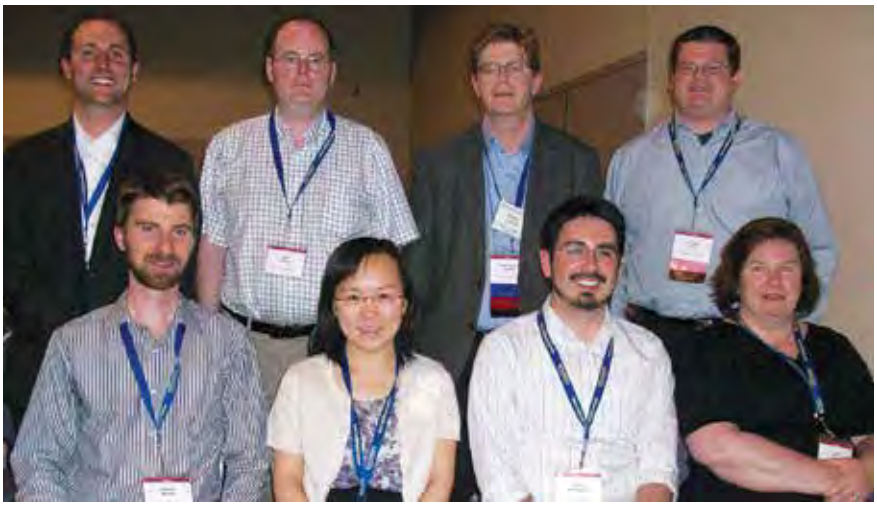
Paul Langan, ORNL, and coworkers combined x-ray and neutron fiber diffracion with molecular dynamics simulations, to reveal some of the processes responsible for the morphological changes in biomass during steam explosion pretreatment. Their results suggest some new pretreatments and plant modifications that will improve biomass conversion.

Joseph Orgel

3.2.2: Structural Studies of Radioelements

Christopher Cahill, George Washington U has focused on the hydrothermal synthesis of hybrid materials based on the uranyl cation for much of his career. As well as generating a large number of structures, their group has made real progress in relating reaction conditions to the structures they generated. Recently, the group has become interested in crystal engineering. Uranyl exhibits unique chemistry because it is capped by two nearly inert oxygen atoms, forcing all the coordination to happen in the plane around the ligand.

Because the team understood the unusual geometry around uranyl they were able to produce a rich vein of new compounds.



Standing in back, L to R: Paul Tobash, Paul Forster, Christopher Cahill, William Kerlin. In front: Helmut Matt Reiche, Jie Qiu, Efrain Rodriguez, Alice Smith.

Efrain Rodriguez, U Maryland, discussed several new ternary phases of technetium (Tc) oxides as well as basic new binary halides, and demonstrated the rich structural chemistry of Tc in the solid state. The development of Tc has lagged, primarily because the inherent radioactivity of all Tc isotopes has limited the number of laboratories that can safely study their chemistry.

Binary halides of transition metals are typically obtained by direct reaction of the metal and halogen at elevated temperature. Details of this reaction were provided, along with synthesis and structural characterization of $TcBr_3$ and $TcBr_4$, the first simple Tc halides to be reported in the past 40 years. The compound $TcBr_3$ is also the first trivalent technetium halide characterized to date.

William Kerlin, U Nevada Las Vegas, was chosen by the Materials Science SIG to receive the **Margaret C. Etter Student Lecturer Award**. William presented several crystal structures of new technetium compounds prepared hydrothermally. The reaction of potassium pertechnetate with glacial acetic acid plus either halo acids or halo salts under *in situ* hydrogen production by sodium borohydride yields multiple products. William described a new one-step solvothermal synthesis route for reduction of pertechnetate salts to low valent technetium metal-metal bonded dimers. Using this process, technetium readily formed metal-metal bonds with bond orders up to four. These one-step reductions provide high yield intermediates for potential waste forms, use in nuclear fuel cycle separations, and radiopharmaceuticals.

Paul Tobash, Los Alamos National Lab (LANL), reported on the physical properties of the three new In analog compounds in the $PuMGa_5$ (M=Co, Rh, Ir) family of superconductors. Since their discovery nearly a decade ago, plutonium-based superconductors have attracted considerable interest. The interest was heightened by the discovery of superconductivity in $PuCoIn_5$ (the Pu-intermetallic with the highest superconducting temperature). Some of the structural intricacies in the bonding environment around the Pu atom should provide insight into the structure and properties of superconductors and provide reasons why certain isostructural compounds exhibit superconducting behavior while others are just temperature independent paramagnets.

William Kerlin, at left, accepting the Margaret C. Etter Student Lecturer Award from Session Chair Paul Forster.

Jie Qiu, U Notre Dame, discussed work from their group on a series of uranium-based cluster compounds. In just a few years, their team has discovered more than 80 peroxide cage clusters and laid the groundwork for discovering a host of others.

Helmut Reiche, LANL, showed how time-of-flight neutron scattering was used to characterize the synthesis of uranium carbide at high temperatures.

Paul Forster and Alice Smith

It was on a short-cut through the hospital kitchens that Albert was first approached by a member of the Antibiotic Resistance.

Courtesy of Nick D. Kim, U Waikato, New Zealand.

Top of page, L to R: Patrice Kenfack Tsobnong; Andrew Torelli, Mariia Bauman, Yulia Sevryugina. Immediately above: George Phillips & Lu Han; James Neilson; and Claire White.

At left: Ram Seshadri.

Simon Billinge at left, and Nikita Ussin at right.

3.2.3: Computational, Chemical & Biological Crystallography: Complementary Methods Bridging the Divide

L to R: Jim Britten, Mark Presspich, Jason Mercer, Edward Snell, Louise Dawe, Victor Young, Gregory Warren, Herbert Bernstein, Gerald Audette.

This session brought together scientists who explored the application of techniques that encompass small molecule and macromolecular crystallography, and computational crystallography with emphasis on an interdisciplinary approach to resolving structural problems.

Gerald Audette, York U, provided a critical analysis of crystal structure prediction software for macromolecular systems.

Jim Britten, McMaster U, demonstrated a reciprocal space visualization package developed at McMaster (MAX3D), that enables better understanding of materials, with examples in diverse areas including aperiodic crystals, protein structures and engineered materials.

Other contributions evaluated new instrument hardware and software, the treatment of incommensurate structures, and the application of computational methods in structural refinement.

Louise Dawe and Jason Mercer

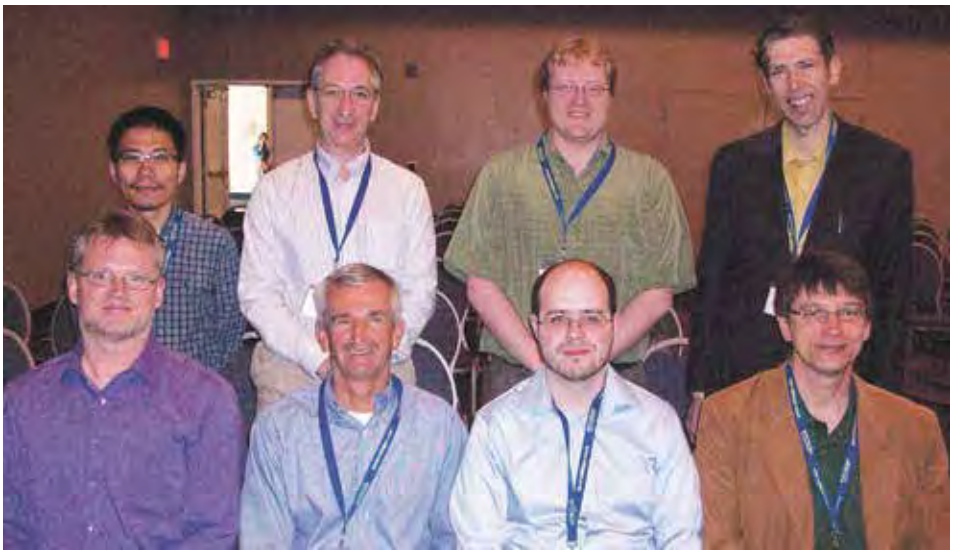
3.2.5: Chemistry and Biology with Novel Scattering Techniques

Axel Brunger, Stanford U, began by describing the LCLS x-ray free electron laser that produces 40 fs pulses with a 100 nm focus, which can be used to probe macromolecular crystal structure.

Michael Sawaya, UCLA, presented a new XFEL structure of a bacterial toxin crystallized in the living cell. The bacterial cells were flowed into the x-ray beam using a thin liquid stream, thus capturing the toxin structure in its native cellular environment.

Aaron Brewster, Lawrence Berkeley National Lab (LBNL), presented new software to analyze XFEL diffraction data. These compressed x-ray pulses also allow the study of free-floating molecules. The short duration of each pulse captures diffraction images from static molecules, rather than those tumbling in liquid.

Peter Zwart, LBNL, explained how this technique, called fluctuation scattering, will be useful in the study not only of biological samples, but chemical samples in material sciences.



Standing in the back, L to R: Chenhui Zhu, Nick Sauter, Aaron Brewster, Michael Sawaya. In front: Peter Zwart, Axel Brunger, Jesse Hopkins, Volker Urban

XFELs were not the only subject discussed. New work at other large facilities is also attempting to capture the overall shape of large molecules in solution using small angle x-ray scattering (SAXS). However, these samples are often sensitive to radiation damage from these powerful x-ray sources.

Chenhui Zhu, LBNL, presented work dealing with the chemistry of liquid-crystal display systems. X-rays enable the study of the molecules responsible for the change of polarization in response to applied electrical stimulus, *e.g.*, on a digital display. Hopefully these studies will lead to new ways of using these chiral molecules in display systems.

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Volker Urban, Oak Ridge National Laboratory (ORNL), presented new chemistries for preserving difficult to study membrane samples in a suspension suitable for x-ray diffraction studies.

Avoidance of damage through cryo-cooling was described by **Jesse Hopkins**, Cornell U, who was chosen by the Small Angle Scattering SIG to receive a **Margaret C. Etter Student Lecturer Award**. Jesse and his colleagues identifid SAXS-friendly cryoprotectant conditions that suppressed ice formation upon cooling, and compared cryoSAXS profiles obtained in window-free variable-path-length cells with room temperature measurements for a variety of standard molecules. They obtained data sufficient for envelope reconstructions using scattering volumes as small as 100 nL, with good agreement between cryoSAXS data and known atomic structures. They also worked on developing low-volume fixed path-length sample holders for cryoSAXS. While practical challenges remain, cryoSAXS is a step closer to studies that exploit high brightness x-ray sources and to mail-in high-throughput SAXS.

Jacob Urquidi

L to R: Seung Joong Kim, Farzaneh Todnevis, Mattia Rocco, Ximei Bu, Gerald Audette, Srinivas Charkravarthy, Tsutomu Matsui.

4.1.1: Solution Structure & Dynamics of Biomacromolecules II

Zimei Bu, City College of New York, spoke on the *Structure and dynamics of adapter proteins at the interface of cell membrane and actin cytoskeleton*.

Srinivas Chakravarthy, Illinois Institute of Technology, gave an overview of the advances in continuous flow SAXS at the BioCAT beamline of the APS. Following a discussion of the considerations of flow types and parameters for continuous flow SAXS, he presented some recent data on using this technique to study protein dynamics at the BioCAT beamline.

Seung Joong Kim, UCSF, described the use of the FOXS software (and web interface) as a suite of programs for the integrative modelling of multiple SAXS experiments. He detailed recent work using FOXS to examine the Nu192 protein of the yeast nuclear pore complex and the Nup84 complex.

Mattia Rocco, San Martino-IST, Genova, Italy, presented research into the coupling of multi-angle light scattering (MALS) and SAXS to elucidate protein oligomerization during fibrin assembly.

Tsutomu Matsui, Stanford U, presented advances at the SSRL in the development of SAXS methods with lower sample consumption, thereby enabling time resolved SAXS experiments.

Farzaneh Tondnevis, U Florida, described her work in characterizing the pH induced equilibrium shift mechanism of the *E. coli* β-clamp, which was also presented as a poster (and was awarded the Journal of Structural Dynamics Poster Prize, see the Poster Prize section preceding the start of the meeting reports). Farzaneh presented her characterization of the sliding β-clamp, which shifts between an open and closed conformation during DNA binding; the mechanism of this process was revealed through a series of SAXS studies of the protein under differing pH conditions showing a series of dynamic changes in the protein to facilitate DNA binding.

Gerald Audette

Colin Groom & Helen Berman deep in discussion in the Exhibit Area.

4.1.2: Innovative Ways of Finding Atoms from Powder Diffraction Data

Andrey Yakovenko, Argonne National Laboratory, showed how the diffraction signal from a specific phase generated during an *in situ* reaction can be isolated from that of any other phases present in the sample. This is done by periodically varying a parameter that drives the reaction forwards or backwards, such as flowing O_2 gas followed by CO gas, and then using Fourier analysis to isolate the diffraction pattern of the oxidation product that is only present during the flow of O_2.

Peter Stephens, SUNY Stony Brook, discussed some fundamental questions regarding the true uncertainties inherent in structures solved from powder diffraction data using several recent examples. His talk focused on errors other than counting statistics as well as assumptions made during refinements. This talk generated a useful dialog involving several others in the audience.

In back, L to R: Andrey Yakovenko, Graham King, Peter Stephens. In front: Branton Campbell, Olivier Gourdon, Allyson Fry.

Allyson Fry, Johns Hopkins U, showed how symmetry analysis, constraints, and many types of data were used to solve the remarkably complex structures of $K_3MoO_3F_3$ and $Rb_3MoO_3F_3$. These structures each have 104 symmetrically independent sites and unit cell volumes over 13,000 and 14,000 $Å^3$, respectively. This work demonstrates how the polar MoO_3F_3 units can stack to form a ferroelectric compound.

Branton Campbell, Brigham Young U, gave an overview of using the basis functions of irreducible representations to categorize and refine structures. This was applied to help solve several complicated multi-k magnetic structures.

Olivier Gourdon, Los Alamos National Laboratory, discussed the importance, in the refinement of powder data, of obtaining more structural details than normal. This includes the use of non-harmonic/anharmonic displacement parameters so that the distributions of atoms will be better understood, and the use of the superspace approach to describe modulated structures.

Graham King and Peter Stephens

4.1.3: Neutrons in Biology: New Instruments and New Structures

This was the second of two 'Neutrons in Biology' sessions (the first was 2.1.2, see page 26). With the recent world-wide renaissance of neutron crystallography of macromolecules, several new instruments have been commissioned and are now available to general users. BIODIFF at FRM-II is at Garching, Germany; in the United States there is IMAGINE at HFIR and MaNDi at SNS, Oak Ridge; and in Lund, Sweden at the European Spallation Source (ESS) there is a proposal for a new NMX instrument. **Flora Meilleur**, Oak Ridge National Laboratory (ORNL), described the recently commissioned IMAGINE quasi-Laue diffractometer installed at the High Flux Isotope Reactor at ORNL. Incoming neutrons are in the 2-10 Å range at the beam port and the flux is 3 x 10^7 neutrons/sec/cm^2 in the 2.8 - 4.0 Å wavelength range. The beam size appropriate for most data collections is a rectangular aperture measuring

Standing in back, L to R: Joseph Ng, Esko Oksanen, Leighton Coates, Flora Meilliur, Andrey Kovalevsky. In front: Katherine Sippel, Patricia Langan, Karen Allen, Zoë Fisher.

2 × 3.2 mm having the full beam divergence of 0.6 °. It is also possible to switch from quasi-Laue to full Laue mode for very rapid testing of crystal diffraction quality. The instrument was first used in June 2013 and the instrument team has since collected several high-impact data sets. IMAGINE is especially attractive to users who may be unable to grow large crystals: sample sizes for some of the data sets collected were in the 0.4 – 0.5 mm^3 range.

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Leighton Coates, ORNL, presented preliminary information on the new MaNDi macromolecular neutron diffractometer that is under commissioning at SNS (ORNL). This instrument has a 30m flight path and a variable wavelength bandwidth of 2.7 Å. The beam divergence ranges from 0.80 – 0.12° with incoming neutrons in the 1–10 Å range. MaNDi is optimized for samples in the 0.1 – 1.0 mm^3 range. Estimates for resolution are 1.5 Å for samples in this size range, and 2.0 – 2.5 Å for crystals with very large unit cells (up to 300 Å). Diagrams of the instrument cave and detector array were shown as well as information on the initial data collected at MaNDi. The instrument promises to dramatically increase the number of neutron projects and structures.

Zoë Fisher & Andrey Kovalevsky (at left) presenting the Margaret C. Etter Student Lecturer Award to Patricia Langan.

Esko Oksanen, ESS, presented the design of the instrument dedicated to the structure determination of macromolecules by neutron crystallography to be built in Lund. The aim is to locate the hydrogen atoms relevant to function. The instrument will be a time-of-flight (TOF) quasi-Laue diffractometer optimized for small samples and large unit cells. A long pulse structure well suited for quasi-Laue technique studies of smaller crystals or larger unit cell volumes will be used. As the background from incoherent scattering increases dramatically if all 1H cannot be replaced by 2H, ESS will have a significant advantage for those systems where perdeuteration cannot be achieved.

Karen Allen, Boston U, presented the first joint neutron and x-ray crystal structures of a haloalkanoate dehalogenase, KDN9PP, at pH 8.5 to 2.3 Å resolution, collected at BIODIFF (FRM-II, in Germany) and at pH 6.5 to 2.3 Å resolution, collected at IMAGINE at ORNL. Neutron diffraction was undertaken to determine the protonation states of residues that form the conserved catalytic motif of KDN9PP. The results clearly show that, in the unliganded enzyme, the Asp nucleophile is unprotonated and that the Asp general/acid base catalyst is in a salt bridge with a lysine residue. This supports a model for catalysis that can be extrapolated to the other phosphohydrolases in the superfamily and is consistent with ligand-induced conformational positioning of the catalytic residues. Knowing the protonation states of active-site residues in KDN9PP will facilitate the understanding of catalysis and further the development of superior docking protocols for structure-based substrate prediction in the enzyme family.

Katherine Sippel, Baylor College of Medicine, presented the first neutron structure of an *E. coli* periplasmic phosphate binding protein (PBP). PBP uses ion-dipole interactions to bind charged atoms exclusively through neutral protein dipoles. The study was done to answer questions about the mechanism by which PBP accommodates the second hydrogen of monobasic phosphate. A 2.5 Å resolution neutron data set was collected at the Protein Crystallography Station at the Los Alamos Neutron Science Center from a ~8 mm^3 H/D exchanged crystal of PBP. Results from the initial joint neutron/x-ray refinement show strong nuclear density for the phosphate D and excellent H/D exchange. Initial results indicate the need for lower pH studies and complementary NMR measurements.

Patricia Langan, U New Mexico, was chosen by the Neutron Scattering SIG to receive a **Margaret C. Etter Student Lecturer Award**. Patricia presented a 2.5 Å resolution neutron structure of engineered reversibly photo-switchable fluorescent protein, coded B-11. The data were collected from a large H/D exchanged crystal by a team as part of the MaNDi instrument commissioning at ORNL. B-11 chromoprotein is a variant of the thermostable green protein (TGP), with 4 amino acid residues mutated, that was evolved for improved solubility, thermostability, and enhanced crystallization properties. The neutron structure showed the location of important H atoms, including protonation of the chromophore, and revealed the position, orientation and protonation states of solvent molecules in the chromophore region as well as in surrounding amino acids, details that were not observed in x-ray crystal structures. The team also reported ground and light-induced state x-ray crystal structures of B11 to 1.65 Å resolution. B-11 differs from TGP by only 4 amino acids but has a weak fluorescence in its ground state. Upon irradiation with blue light, B-11 switches to a light-induced metastable state that has a distinct UV-Vis spectrum and is stable at room temperature, with $t_{½}$ of about 60 min. By analogy with other chromoproteins of the same family a cis-trans isomerization and deprotonation of the chromophore is expected to occur upon irradiation, and this did in fact occur. These structures will enhance future engineering of new and novel fluorescent proteins.

Joseph Ng, U Alabama-Huntsville, presented the 2.2 Å resolution neutron structure of inorganic pyrophosphatase (IPPase) from *Thermococcus thioreducens*. Analysis of this structure, along with a series of apo, holo and substrate-bound IPPase x-ray crystal structures, led to the proposal of a new structure-based catalytic mechanism associated with the hydrolysis of pyrophosphate. This team also has very ambitious plans for obtaining many more neutron structures of all the complexes obtained for x-ray diffraction studies. They would ultimately like to completely map, through neutrons, every possible intermediate in the reaction trajectory to gain a complete understanding of every player that controls catalysis in IPPase. This is feasible as IPPase crystals can be grown to large volumes; they are temperature and mechanically stable and diffract neutrons well. The presented neutron diffraction studies, along with molecular and biochemical studies, confirmed and clarified the involvement of the H atoms in the overall catalytic mechanism of IPPase. These are highly conserved enzymes suggesting that the proposed catalytic mechanism may represent the mechanism for all inorganic pyrophosphatases in this family.

Zoë Fisher and Andrey Kovalevsky

4.1.4: New Algorithms in SAXS/WAXS

Alex Hexemer, LBNL, opened with a presentation discussing results obtained with the high-performance GISAXS simulation code, HIPGIXAXS. Time resolved experiments generate data at very high rates, and GISAXS requires an added dimension. Combining GISAXS experiments with AFM greatly enhances the value of the GISAXS results and contributes to the generation of images from the scattering data.

Hailiang Zhang, NIST, discussed SASCALC, a fast calculator for use with both x-ray and neutron scattering experiments. SASCALC is a component of the widely used SASSIE software in which a very efficient algorithm is employed in order to carry out calculations that scale approximately linearly with the number of atoms.

Standing in back, L to R: Alexander Hexemer, Peter Zwart, Marc Allaire. In front: Emre Brookes, Cody Alsaker, Lee Makowski, Yuba Bhandari.

Lee Makowski, Northeastern U, described the sensitivity of WAXS data to structural fluctuations in proteins and introduced the concept of a sigma-r plot – a plot of the standard deviation of fluctuating interatomic distances as a function of interatomic distance. A major advantage of sigma-r plots is that they can be generated directly from both WAXS data and MD trajectories, making possible direct comparison of the results obtained by these two techniques.

Peter Zwart, Lawrence Berkeley National Laboratory, demonstrated their small angle scattering toolbox and discussed strategies for overcoming shortcomings of existing algorithms such as the problems in calculating the maximum interatomic vector length in a protein and removing fluctuations in p(r) through regularization. Peter also introduced software packages that carry out fast shape determination.

Emre Brookes, U Texas Health Science Center, talked about the use of *parsimonious spatial models* to fit SAXS data – a strategy to define the simplest model defined by the experimental parameters. This approach was demonstrated using examples comprised of multiple spheres and other well-defined geometric shapes.

Yuba Bhandari, NCI, presented his work on large RNAs using SAXS. Large RNAs are an important new application for SAXS, but there are significant technical challenges. Structural studies of RNA lag well behind those of proteins, just as their functional importance is being increasingly appreciated. Yuba's work demonstrates that SAXS can indeed have an important impact on understanding the structure and function of large RNA structures.

Cody Alsaker, Colorado State U, discussed the improvement and evaluation of uncertainty in estimates of the radius of gyration in SAXS data collections. In many cases, the Guinier plot is not sufficiently linear to allow for an accurate estimate of Rg. Cody introduced a new strategy for optimizing the accuracy and precision of radii of gyration estimates.

The development of software packages providing help in understanding the large scale structural changes that are so important in a broad range of biochemical processes will greatly increase the use of x-ray solution scattering techniques.

Lee Makowski

4.2.1 General Interest II

Zheng-Qing Fu, U Georgia, presented results from their tests on a new Rayonix MX300HS high-speed area detector that has been installed on beamline 22BM at SER-CAT. The new detector has a 4×4 taper/chip array and a 1-2 millisecond read-out time, which allows data collection in either the shuttered or the shutterless modes. Data collected at beamline 22BM should be significantly improved from now on!

Standing in back, L to R: Zheng-Qing Fu, John MacDonald, Mathias Meyer, Larry Falvello, Chunhua Hu. In front: A. David Rae, Charles Campana, Graciela Diaz de Delgado.

4.2.1 cont'd **Mathias Meyer,** Agilent Technologies, discussed the new S2 generation of area detectors as well as features of Agilent's CrysAlisPro software (version 37). The new data reduction software in version 37 has an approach for twinned samples that significantly improves the data quality for small molecules and proteins.

Larry Falvello, U Zaragoza, Spain, explored structures that presented variations on the water wire, *i.e.*, a continuous hydrogen-bonded chain of water molecules for which the potential for proton mobility has been attributed. By comparing the geometries of these with those found in a water-rich, channel-free structure, Larry was able to conclude that hydrogen-atom disorder at double-well H-bond sites may be a cause of the failure to detect H atoms in some water wires. He then went on to discuss the relationship between this disorder and proton mobility.

Charles Campana, Bruker AXS, described the new Bruker APEX3 Suite, an extensive update of the Bruker single crystal software. With this new release, Bruker will take advantage of new developments in computer hardware and operating systems, include new CIF requirements, upgrade the QT4 programming, support multi-CPU computers, and be compatible with SHELX-2013. SHELX-2013 has an improved graphical interface, an improved version of the intrinsic structure solution option, and a new and improved autostructure routine.

Alan David Rae, Australian National U, enlightened the audience with his discussion of data refinement considerations. Rae's ideas aim to avoid the 'maximum ignorance' concept that there is only a single global model for error distribution. For any least squares refinement cycle the direction in vector space of an observation is determined by an initial model that includes the background, and the least squares equations are evaluated using this direction. By evaluating the variance of the calculated model an observation can be partitioned into partial observations. The effective number of observations can be determined for any parameter after taking proper account of the duplication of partial observations. The estimated errors of parameters can then be individually adjusted.

Chunhua Hu, New York U, described his tunable, octahedral coordination molecular cages that have large permanent nanometer-size cavities. They are made using 6 units of thiocalix[4]arene or sulfonylcalix[4]arene that bears four-fold rotational symmetry, and eight tiles of tricarboxylate ligand that has a three-fold axis, glued together by six groups of $\{M_4Cl\}$ or $\{M_4O\}$ metal clusters. The size is tunable by changing the organic groups in the upper rim of calixarenes and using different sizes of tricarboxylates. These cage structures can be heated to ~400 °C before they decompose and can easily incorporate gases and small molecules such as I_2 and Ibuprofen. Chunhua presented the crystal structure of a large tripodal tricarboxylate ligand, BBB (4,4',4"-benzene-1,3,5-triyl-tris(benzene-4,1-diyl) tribenzoate), which was solved by structure modeling using isomorphous replacement. This approach would be particularly useful when the diffraction data resolution is greater than 1.3 Å.

Graciela Diaz de Delgado, Universidad de Los Andes-Venezuela, and coworkers studied thiocolchicoside (THC), a synthetic sulfur derivative of colchicoside, a muscle relaxant and analgesic that has anti-inflammatory effects. Graciela reported the structure as determined both from powder diffraction data using the program TALP, and from single crystal x-ray data. This work is part of the effort in her laboratory to characterize common active pharmaceutical ingredients and to document polymorphs under different crystallization conditions.

John MacDonald, Worcester Polytechnic Institute, and his colleagues investigated porous metal-organic frameworks (MOFs) that incorporate photosensitizers in their efforts to develop sorbent materials that generate singlet oxygen that will oxidatively decompose adsorbed organic guest molecules. They synthesized a small library of porous MOFs featuring porphyrins as the backbone, materials that should ultimately be useful for environmental remediation and treatment of contaminated water sources.

Graciela Diaz de Delgado

General Interest Posters

S-02: Bonding in group I citrate salts by James Kaduk and Alagappa Rammohan.

Citric acid, a naturally occurring acidity regulator, is of great importance to our metabolism, as well as to food and beverage manufacturers. On paper its structure has appealing simplicity: a central carbon atom bearing one OH, one COOH group, and two more CH_2COOH groups. Many questions come to mind such as: What are the conformational changes? How do hydrogen bonds balance against interactions with alkali metal (M) ions? This situation just cries out for crystallographic studies, yet there were only 10 studies of alkali metal (hydrogen) citrates in the literature.

Jim Kaduk and **Alagappa Rammohan** have determined an additional 15 crystal structures of alkali metal (hydrogen) citrates by single crystal or powder diffraction. They used B3LYP density functional theory to calculate total energies for a variety of citrates. This study provides solid backing for some of our suppositions and answers some questions. Very small M-O Mulliken overlap populations (MOP) demonstrate very small covalent character; thus M-O bonding is largely ionic. Coordination number increases with cation size, from 4-6 for Li to 7-10 for Cs. Ionized carboxylate groups are the most common ligands, but COOH groups sometimes participate and OH groups and water mainly bridge two M ions. The central COOH group generally is the first one to ionize, followed by one end and then the other. A preference for 'curled up' conformations shows the importance of intramolecular hydrogen bonding. A plot of MOP versus distance for all O–H and O…H bonds yields a single smooth curve; the hydrogen bond energy is proportional to the square root of the MOP. Finally, the mixed metal structures $NaK_2C_6H_5O_7$ and $NaKHC_6H_5O_7$ provided a challenge to powder diffraction techniques; the latter study was rewarded by finding two of the shortest ever O–H…O hydrogen bonds (2.414 and 2.400 Å).

Carl Schwalbe

4.2.2: Exciting Structures

Franziska Huschmann, U Otago, New Zealand, discussed Lanosterol 14α-demethylase (Erg11p), a membrane-anchored cytochrome P450 enzyme involved in ergosterol production and fungal cell membrane viability that is a common target of azole drugs. Franziska reported on the production of several Erg11p variants from *C. albicans, C. glabrata* and *S. cerevisiae*.

The crystal structure of full-length *S. cerevisiae* ERG11p was also presented and represents the first structure for a full-length cytochrome P450 enzyme showing resolution of the membrane spanning helix.

In back, L to R: Daouda Traore, Peter Randolph, John Rose, Stefan Gajewski, Nicholas Noinaj. In front: Franziska Huschmann, Lesa Offermann, Paulina Dziubanska, Tengchuan Jin, Amit Das.

Amit Das, Oak Ridge National Laboratory, gave an update on his work related to cation binding to the Protein Kinase A catalytic subunit (PKAc). He presented evidence that the enzyme was active in the absence of metals and, unlike the mechanism observed in metal-assisted catalysis, metal-free enzyme catalysis involves an ordered binding sequence of substrate followed by ATP. This work will aid in understanding the role that metals play in PKAc catalysis.

Paulina Dziubanska, U Virginia, reported her work on the C-terminal domain of the Ebola virus nucleoprotein (NP), which is thought to serve as a hub for protein-protein interactions important for NP incorporation into virus-like particles and for NP interaction with the matrix protein VP40. The crystal structure of the NP C-terminal domain revealed a novel fold, with topology distantly related to the β-grasp fold, which may provide a template for drug design.

Tengchuan Jin, NIAID/NIH, gave an informative talk on the structural basis of cytosolic DNA recognition by the PYHIN family innate immune receptors AIM2 and IFI16 including the first structure of an inflammasome in complex with its ligand. The work is important to understanding the molecular mechanism of DNA mediated inflammation under autoimmune conditions or during infection.

Peter Randolph, U Virginia, reported on the structural and biophysical studies of the Sm-like RNA binding protein SmAP2 from *P. aerophilum*. The crystal structures of SmAP2 have been determined in multiple space groups and revealed new and unexpected Sm assembly states. The SmAP2 is the last remaining Sm protein in *P. aerophilum* whose structure was unknown. Thus a complete picture of Sm structure and assembly in a single genome is now available, which will provide a basis for understanding structure/function relationships in the Sm superfamily.

Lesa Offermann, U South Carolina, presented her structural studies on the Ara h 8 allergen found in peanuts. Lesa presented a 1.60 Å structure of Ara h 8 that showed structural similarity to allergens from birch pollen, celery, strawberry, soy and cherry, supporting the idea that Ara h 8 could be contributing to the oral allergy syndrome between birch pollen and peanuts. Structures containing 2-(N-morpholino)ethanesulfonic acid, ANS, epicatechin and quercetin were also presented, suggesting that Ara h 8 could also be involved in the transport of signaling molecules important for plant development.

Stefan Gajewski, St. Jude Children's Hospital, gave an interesting talk on overcoming crystal twinning problems of the UvsY protein from bacteriophage T4. UvsY is involved in DNA synthesis and recombination and readily crystallizes in Laue class 4/mmm. However, only twinned crystals are obtained. Single crystals were produced by a combination of reductive alkylation and mutagenesis, which reduced the surface entropy. The structure was solved by Se-SAD at 5.4 Å resolution and, aided by ROSETTA and NCS averaging, an open lockwasher assembly of α-helical protomers was observed. The low-resolution structure was extended to 2.5 Å by molecular replacement against the data set collected from a P1 crystal form.

Nicholas Noinaj, NIDDK/NIH, presented a very interesting talk on the BAM complex, an outer membrane multi-component β-barrel protein involved in the assembly of β–membrane spanning pores. Using both the BamA crystal structure and molecular dynamics simulations, a mechanism for BamA folding and membrane insertion was proposed that included a lateral opening of the BamA β-barrel, and a substrate exit pore positioned above the lateral opening site.

John P. Rose and Daouda Traore

L to R: Nicolas Wolff, Sophie Zinn-Justin, Nigel Kirby, Alvin Acerbo, Srinivas Chakravarthy, Javier Pérez, Alexey Kikhney, Emre Brookes, Adam Round, David Lambright.

4.2.4: SAXS with Biomolecular Mixtures

This session discussed strategies designed to obtain reliable structural information from polydisperse mixtures using small angle x-ray scattering (SAXS). The talks elaborated on three separate beamline setups that allow online Size Exclusion Chromatography (SEC), two software developments that enable deconvolution of SAXS data from mixtures, and three examples of biological projects that unmistakably demonstrate the efficacy of SEC-SAXS. The consensus that emerged was that SEC-SAXS may become the standard data collection strategy for biological samples, as a large number of samples that were heretofore believed to be monodisperse have been shown to be polydisperse when analyzed with online SEC-SAXS setups.

Alexey Kikhney, European Molecular Biology Laboratory, Hamburg, pointed out that while monodispersity of the sample solution is a crucial prerequisite for reliable SAXS data analysis, some samples remain polydisperse despite cautious sample preparation. Recent additions to the ATSAS package (***http://www.embl-hamburg.de/biosaxs/software.html***) include tools for *ab initio* and rigid body modeling against data collected from polydisperse samples such as partially dissociating complexes, flexible systems, and dynamic equilibria between monomers and higher oligomers. Applicability of these tools and possible pitfalls were discussed.

Nigel Kirby, Australian Synchrotron SAXS-WAXS (wide angle x-ray scattering) beamline, gave an overview of the beamline's solution scattering capabilities including online SEC-SAXS/WAXS. He also described specific beamline features that allow low detection limits and automated data acquisition and processing, and its data analysis pipeline. A new method for performing sucrose gradient analysis using Analytical UltraCentrifugation (AUC), not online, in combination with SAXS is currently under development. Finally, Nigel gave an interesting example of SAXS analysis on tannins showing details about how accurate SAXS measurements of small molecules, well under 1 kDa, can be taken out to 2 $Å^{-1}$.

Adam Round, EMBL, Grenoble, and the ESRF Synchrotron, spoke about the online SEC-SAXS setups at those instruments. He emphasized the need for efficient data management strategies in light of the large volumes of data generated by SEC-SAXS experiments and elaborated on ISPyB, which is currently being implemented to improve all aspects of a SAXS experiment including sample preparation, experimental logging, data reduction, processing, analysis and interpretation.

Alvin Acerbo, MacCHESS, discussed recent upgrades of their bioSAXS beamline and the possibilities of coupling online SEC-SAXS and inline Multi Angle and Dynamic Light Scattering (MALS/DLS). In the current setup, now in use at CHESS beamline G1, a polydisperse sample is passed through an SEC column and the elution peaks are examined using both SAXS and MALS/DLS. In addition to offering an inherent concentration series as elution peaks pass by the x-ray and light scattering detectors, complementary structural information from these techniques can offer new insights for complex inhomogeneous samples.

Emre Brookes, U Texas Health Science Center, presented an overview of the US-SOMO HPLC SAXS (***http://somo.uthscsa.edu***) analysis tools. These tools utilize Gaussian decomposition techniques to separate overlapping species present in online SEC-SAXS data sets into single-species intensity curves suitable for further analysis and are invaluable for the difficult cases of overlapping species. A Single Value Decomposition (SVD) module assists the user in choosing the number of Gaussians. Recent additions to the toolkit include optional non-symmetric modified Gaussian functions to deal with skewed profiles and a novel integral baseline algorithm for removing the effects of capillary fouling.

David Lambright, U Mass Medical School, reported that SEC-SAXS is useful for investigating oligomeric mixtures and aggregation prone samples. His group has explored the potential of SEC-SAXS to characterize oligomeric and allosteric states of regulatory enzymes that control activation and deactivation of small GTPases. The data was collected on the online SEC-SAXS at BioCAT (sector 18ID, APS). They used SVD to determine two basis components and recombined them to optimize the linearity of the Guinier region, and subsequently processed the data with ATSAS tools.

Sophie Zinn, Laboratoire de Biologie Structurale et Radiobiologie, Gif-sur-Yvette, France, talked about her group's attempts to characterize the 3D structures of several nucleoplasmic regions of nuclear envelope proteins using NMR, AUC and SAXS. Their online SEC-SAXS data were collected at SWING/SOLEIL. The conformational space occupied by the protein globular domains and flexible linkers was thoroughly sampled by simulation to identify the conformations that best fit the scattering data.

Nicolas Wolff, Institute Pasteur, Paris, described their use of online SEC-SAXS at SWING/SOLEIL and AUC methods to study PTPN4, a human tyrosine phosphatase that protects cells against apoptosis. Their SAXS data was collected with the gel filtration column with PDZ ligand at high concentration, a very promising strategy to deal with low affinity complexes. Nicolas' group proposes that an allosteric effect leading to a more relaxed conformation of the PTPN4 bidomain restores the catalytic competence of the system.

Emre Brookes, Srinivas Chakravarthy, and Javier Pérez

4.2.5: Advances in X-ray and Neutron Scattering Techniques under Non-ambient Conditions

Antonio M. dos Santos, ORNL, gave an overview of the recent developments in high-pressure neutron science, both at the SNAP beamline and other instruments at the Spallation Neutron Source.

Cora Lind-Kovacs, U Toledo, presented structural studies on powder samples of some negative thermal expansion (NTE) materials, using both synchrotron and neutron scattering techniques, including high-pressure powder diffraction.

Angus Wilkinson, Georgia Tech, delved into an exploration of NTE materials, which are central to his group's quest to make ideal engineering materials with zero thermal expansion, and described how the thermal expansion properties of NTE materials can change under applied pressure. This work included the development of a new sample environment for simultaneous variable pressure (up to ~400 MPa) and temperature (~300-550 K) measurements using high-energy x-rays at the Advanced Photon Source.

In back, L to R: Antonio dos Santos, Tomislav Friscic, Christine Beavers, Karena Chapman. Sitting in front, L to R: Jordan Cox, Cora Lind-Kovacs, Angus Wilkinson, Saul Lapidus.

Tomislav Friscic, McGill U, presented his recent work at the European Synchrotron Radiation Facility on real-time, *in situ* methods for monitoring solid-state reactions. He also enlightened the audience about mechanochemistry, which employs grinding to induce substances to react and is much more environmentally friendly than solvent-fuelled wet chemistry.

Jordan Cox, U Buffalo, our student speaker for this session, presented a photocrystallographic exploration of dithienylethenes using synchrotron radiation to study microcrystal samples at the Advanced Photon Source. Photochromic diarylethene compounds can exhibit a UV-activated ring-closing phenomenon, which for the work Jordan presented showed a highly unusual temperature-dependent behavior. The U Buffalo group combined their *in situ* photocrystallography studies with spectroscopic analysis to elucidate the novel temperature dependence.

Saul Lapidus, ANL, described an unusual material, $Zn(CN)_2$, that expands instead of compressing when pressure is applied – increasing the material's volume by a factor of 2! On its own, such negative volume compressibility is impossible; however, in the case of $Zn(CN)_2$ the material transforms under pressure to a porous phase that contains molecules from the fluid surrounding the solid material. So, while the volume of the solid increases, the combined solid + fluid volume is reduced. The structure generated at high pressure depends on the shape of the fluid molecule, with the originally nonporous interpenetrated $Zn(CN)_2$ framework reconstructing to several different porous, non-interpenetrated frameworks in water or methanol.

Christine Beavers and Gregory Halder

Editor's note: The following session, 2.2.5, is out of order.

2.2.5: Automation: from Crystal to Solved Structure

Joseph Luft, HWMRI, described improvements in the visualization of crystals that identify crystallization hits that would otherwise be missed using only a standard microscope. Second Harmonic Generation (SHG) and Ultraviolet Two-Photon Excited Fluorescence (UV-TPEF) imaging were used to rapidly and very effectively detect sub-micron crystals produced from a 1536 cocktail assay.

David Sargent, ETH Zürich, presented a novel invention called 'RodBot'. A rod-shaped micro-robot driven by rotating magnetic fields, RodBod is steered through a remote control. When submerged in a low Reynolds number liquid, the rotating RodBod produces a gentle fluidic force above it that may be used to transport crystals for sample mounting.

Elizabeth Baxter, SSRL, described the use of high-density sample holders that contain 75 mounting ports for crystals and fit inside standard uni-pucks for efficient collection of diffraction datasets using multiple crystals at micro-focus synchrotron beamlines and x-ray free electron laser sources. Automated routines have been added to the Blu-Ice/DCSS experimental control software to support grids including the positioning of grid ports, rastering and data collection. Crystallization experiments have been set up on grids using commercial liquid handling robots including the **Art Robbins Gryphon LCP** and the **Labcyte Echo550**.

Jean-Luc Ferrer, IBS, presented an overview of the expanded functions of the G-Rob robot. In addition to sample exchange, G-Rob may also function as a goniometer for cryo-cooled samples, may position crystallization trays for *in situ* screening, and may even be used for remote controlled crystal harvesting.

Kay Perry, Cornell, described new software developed to address challenges of combining data from a large number of crystals. The Python-based program automates the analysis and merging of multiple datasets for both native and *de novo* structure solution and was developed for incorporation into the program RAPD at NE-CAT.

In back, L to R: Graeme Winter, Joe Luft, Jean-Luc Ferrer, David Sargent. Sitting in the front: Aina Cohen, Kay Perry, Elizabeth Baxter.

Graeme Winter, Diamond Light Source, described new algorithm developments within the xia2 and DIALS projects that tackle the challenges of data reduction using diffraction from multiple weakly diffracting crystals. Supporting structure determination efforts using sub-micron sized crystals at the Diamond micro-focus beamline I24, automated methods provide feedback during the experiment and help in selecting the optimum subset of diffraction for use in further analysis.

Aina Cohen

Editor's note: The following session, 3.1.2, is out of order.

3.1.2: Combined Techniques in One Beamline

Jan Kern, Lawrence Berkeley National Lab, summarized the use of synchrotron x-ray sources and cryogenic conditions to monitor photoreduction of the OEC poised in various S-states with x-ray absorption spectroscopy (XAS) and polarized single crystal XAS/XANES/EXAFS studies in his talk: *Combining x-ray spectroscopy and diffraction to study the catalytic cycle of photosystem II using synchrotron and XFEL sources*. Photosystem II (PS-II) is a multi-subunit membrane protein complex that couples one-electron photochemistry and charge separation at the reaction center with the four-electron water oxidation at the oxygen evolving complex (OEC). The OEC exploits a Mn_4O_5Ca cluster as a 'redox capacitor' wherein photons promote oxidation from S0–S1–S2–S3–S4 states, and from which the last transient intermediate, S4, catalyzes O–O bond formation and release of dioxygen. Jan also presented results from the Linac Coherent Light Source (LCLS). The team used pump-probe, serial femtosecond crystallographic methods at ambient temperature. They determined structures and obtained Mn(II, III, IV) valence-to-core x-ray emission spectroscopic results from slurries of PS-II microcrystals poised in various S-states by visible-light laser illumination(s) before the samples were probed by the LCLS x-ray pulse.

In back, L to R: Jan Kern, Allen Orville, Darren Sherrell, Pawel Growchulski. Sitting in front: Igor Petrik, Lu Huo, Erik Yukl.

Erik Yukl, New Mexico State U, presented crystallographic electronic absorption and resonance Raman results obtained under cryogenic conditions at NSLS beamline X26-C that are considered to be diagnostic of the Fe(IV) metal centers within the protein-protein complex. His talk, *Tracking reduction of the bis-Fe(IV) heme intermediate in MauG-MADH crystals using single crystal spectroscopy,* described crystallographic analysis and how the spectroscopic signatures changed as a function of absorbed x-ray dose. Indeed, the high valent iron centers appear to be reduced with a '$t_{½}$' of only about 50 KGy. This indicates that these metal centers are very sensitive to photoreduction by the x-ray beam.

Darren Sherrell, U Saskatchewan, showed how x-ray absorption is not only element specific, but also atom specific; for example, two atoms of the same element in different states or in different neighborhoods will have slightly different absorption characteristics. The impact of these energy dependent atomic form factors are manifest in x-ray diffraction intensities. His talk, *Active site redox assignments in metalloproteins using diffraction spectroscopy,* described diffraction spectroscopy as a means to site separate 2 atoms of iron from within a ferrodoxin protein crystal, building on prior small molecule diffraction anomalous fine structure experiments and utilizing the collection and processing software commonly used in large unit cell crystallography. Darren also talked about a technique (dev + PCA) that has been developed to retrieve the small signals from individual atoms out of the large and noisy background of real diffraction data collected at many synchrotron x-ray sources.

Igor Petrik, U Illinois, discussed the strategy of using myoglobin, a stable, easy-to-produce and well-characterized heme protein, as a scaffold for making structural and functional models of heme-copper oxidases such as cytochrome c oxidase (a large, membrane bound, multi-subunit, multi-heme containing enzyme). The results showed that several designed myoglobin-based reductases offer unique opportunities to probe structure and function for O_2 reduction chemistry. The single crystal electronic absorption and resonance Raman spectroscopic analysis as a function of x-ray dose provided by NSLS beamline X26-C enabled them to unambiguously assign iron redox state and ligand structures.

Lu Huo, Georgia State U, presented *Structural characterization of the Kynurenine enzyme trio and reaction cycle intermediates reveal novel metabolic connections*, describing tryptophan metabolism through the Kynerenine pathway. This pathway generates several neuroactive, toxic, and/or important metabolic intermediates that profoundly impact human health. She described the characterization of several enzymes in the pathway. In particular, α-amino-β-muconate-ε-semialdehyde dehydrogenase (AMSDH) poised at several stages around the reaction cycle was studied by several complementary methods at the APS and the NSLS. Single crystal electronic absorption spectroscopy and mass spectrometry were used to verify the otherwise somewhat ambiguous electron density maps calculated for five cryo-trapped steps along the enzyme reaction cycle. These snapshots enabled Lu and her colleagues to propose a novel isomerase activity for the enzyme family that had not been characterized previously.

Allen Orville and Pawel Growchulski

Clockwise from top right corner:

Listeners, with Vivian Stroganoff, W. Robert Scheidt & Larry Falvello, prominent; and Frances & Herbert Bernstein.
Can anyone name this 'mystery man'?
Richard Bromund taking pictures;
Katherine Sippel;
Martha Teeter at the podium;
?? and,
just to the right of her, Alisa Glukhova receiving her poster prize from Ilia Guzei;
and Jessica Addiss & Marcia Colquhoun accepting their presents from Martha Teeter.

Structural Basis of Pharmacology: Deeper Understanding of Drug Discovery through Crystallography

Amid the hilltop castles and monasteries of Erice, more than 150 students and 25 lecturers from around the world gathered in attendance at the Ettore Majorana Foundation and Centre for Scientific Culture. The course organized by **Eddy Arnold**, Rutgers, **Richard Pauptit**, AstraZeneca, **Giovanna Scapin**, Merck, and **Robert Stroud**, UCSF, focused on the development of new treatments and methodologies to target the challenges associated with drug discovery and design. Generous support was provided by **NATO, ECA, IUCr, OPWC, CCDC, Art Robbins Instruments, Beryllium, Emerald Bio, Rigaku**, and **PANalytical**. IT support was provided by **Erin Bolstad**, **Fred Boyle**, and **Gianni Grassi**, in addition to the Centre Majorana staff.

The local team of 'orange scarves' led by **Paola Spadon**, U Padua, and **Annalisa Guerri**, U Florence, were essential in ensuring that the week long course ran smoothly and created a warm, welcoming environment in which students were free to engage in scientific discussion with their peers and scientific experts attending the course. Thought provoking and at times spirited conversations often extended into the informal meals at local restaurants. In the evenings, many participants convened at the 'Marsala Room' at the San Rocco Center, where music and conversation, as well as Sicilian marsala wine and pastries, would often flow late into the night.

Professor Tom Blundell, Director of the Erice International School of Crystallography, describing advances in his laboratory's program in drug discovery. Photo courtesy of Jeff Blaney.

The organizers and 'orange scarves' planned a series of events to celebrate both the **International Year of Crystallography** and the **40th anniversary of the Erice International School of Crystallography**. Personal accounts, reflections, and history eloquently delivered by **Tom Blundell**, U Cambridge, **Helen Berman**, Protein Data Bank, Rutgers U, **Judith Howard**, Durham U, and **Martin Schmidt**, Johann Wolfgang Goethe-Universität, highlighted some of the scientific and technical contributions of notable crystallographers and allowed students to appreciate how crystallography has evolved. The 'Game of the Goose' challenged students about their knowledge of local culture and crystallography as well as their singing skills! At the dance party following the game, attendees were able to show off their creative side with their red hats, which were designed to reference some crystallographic concept. Planned excursions to the nearby archeological sites in Mozia, Segesta and Selinunte provided the attendees an opportunity to appreciate some of the local culture and deep history of beautiful Sicily.

Erice course participants learning history on one of the outings to the ancient archaeological site in Selinunte. Photo courtesy of Disha Patel.

Through a combination of lectures and hands-on workshops, students were able to engage in an active exploration of current challenges in drug discovery and the new methodologies or experimental approaches for overcoming these obstacles. Lectures covered a wide range of topics including targeting protein-protein interactions (**Tom Blundell**), G-protein coupled receptors (GPCRs, **Miles Congreve**, Heptares, and **Andrew Kruse**, Stanford U), and other membrane protein structures (**Robert Stroud**), biopharmaceuticals (**Richard Pauptit**), epigenetic processes (**Chun-wa Chung**, Glaxo-SmithKline), kinases (**Dirk Bussiere**, Novartis) and ribosomes (**Raz Zarivach**, Ben-Gurion U).

Students learned about protein-ligand interactions through multiple perspectives. **Alberto Podjarny**, IGBMC, CNRS, used high-resolution protein structures from x-ray and neutron crystallography to demonstrate the importance of water molecules and protons in protein-ligand interactions. **Gerhard Klebe**, U Marburg, and **Helena Danielson**, Uppsala U, described protein-ligand interactions from thermodynamic and kinetic perspectives, respectively.

Different approaches for drug discovery and development were highlighted by several talks. **Giovanna Scapin** described drug discovery and design in pharmaceuticals using real-life examples while **James Wells**, UCSF, and **Joseph Bauman**, Rutgers U, described alternative approaches to drug discovery through protein engineering and crystallographic fragment screening, respectively. In talks that also addressed the problem of drug resistance, **Stephen Cusack**, EMBL, Grenoble, spoke about drug design targeting influenza virus and bacteria, and **Eddy Arnold**, Rutgers U, described the discovery of two drugs targeting HIV-1 reverse transcriptase.

Discussion was not solely limited to experimental approaches. **Anna Tramantano**, Sapienza U of Rome, described computational approaches for structural bioinformatics and **Salvador Ventura**, Autonomous U of Barcelona, discussed how one can predict protein aggregation using a combination of protein sequence and structure. **Jeff Blaney**, Genentech, demonstrated how molecular modeling and data mining could facilitate lead optimization. **Mike Hann**, GlaxoSmith-Kline, provided food for thought while describing favorable properties of drugs and drug-like molecules. New advances in software and concepts for computational lead generation (**John Irwin**, UCSF) and crystallographic phasing and refinement (**Oliver Smart**, Global Phasing Ltd.) were also discussed. **Helen Berman**, PDB, and **Colin Groom**, Cambridge Crystallographic Data Centre, spoke about the evolving roles of structural databases to ensure all data are

Erice School, Cont'd:

properly archived and optimally accessible to the public. Afternoon sessions consisted of workshops aimed to provide hands-on experience in using new bio-informatics tools to probe the databases of CCDC and PDB as well as computational approaches using DOCK and Buster.

'Orange scarves' and teams of students in 'The Game of the Goose,' part of the International Year of Crystallography Celebration.

Photo courtesy of Disha Patel.

Students were given an opportunity to share their own research experiences through poster sessions. In addition, based on the abstracts submitted for the poster presentations, eight students were invited to present their work as part of the lecture sessions. The week-long course included a session in which students had the opportunity to engage in a discussion with a panel of the lecturers consisting of **Eddy Arnold**, **Helen Berman**, **Jeff Blaney**, **Tom Blundell**, **Chun-wa Chung**, **Colin Groom**, **Richard Pauptit**, **Giovanna Scapin**, and **Robert Stroud**. The topic of the panel discussion was: **Career and Intellectual Development.**

The course concluded with recognition of some of the exceptional work done by students with awards for Best Poster to **Taiana Oliveira**, EMBL, Grenoble, and **Mirella Vivoli**, U Exeter. The Lodovico Prize for the most active student both inside and outside the lecture hall was awarded to **Anthony Bradley**, Oxford U.

Disha Patel and Eddy Arnold

Validation Reports Available for All X-ray Structures in the PDB

The Worldwide Protein Data Bank (wwPDB) partners are pleased to announce that validation reports for all x-ray crystal structures in the PDB archive are now publicly available.

"*The new validation reports are sure to become an indispensable resource for all x-ray crystallographers. Most importantly, we hope they will be really useful for all the end users of structural models, who increasingly need to critically assess and compare PDB entries*," said Anastassis Perrakis, Netherlands Cancer Institute, whose research focuses both on analyzing macromolecular structures relevant for cancer, and also on developing the tools needed to decipher these structures.

The reports implement the recommendations of a large group of community experts on validation and include the results of geometric checks, structure-factor assessment and ligand validation. The reports include results from tried and tested software including MolProbity, Xtriage, Mogul, EDS and various CCP4 programs. They summarize the quality of the structure and highlight specific concerns by considering the coordinates of the model, the diffraction data and the fit between the two. Easily interpretable summary information that compares the quality of a structure with that of other structures in the archive is also provided. The figures on the facing page show an example of the type of at-a-glance summary that is provided, along with a sample residue-property plot.

Validating structures prior to deposition and publication

The new x-ray structure-validation reports have been provided to depositors as part of the structure-annotation process since August 2013. More recently, a stand-alone wwPDB x-ray structure validation server was launched (***http://wwpdb-validation.wwpdb.org/***). The server allows crystallographers to check early, intermediate and near-final models on demand and helps identify any potential problems that need addressing prior to structure analysis, deposition and publication.

"*The stand-alone validation server will run exactly the same validation tests that have recently been introduced for the annotation of new depositions*," says Randy Read of Cambridge University. Read chairs the wwPDB X-ray Validation Task Force (VTF) that has produced detailed recommendations to the wwPDB about how macromolecular crystal structures should be validated [1]. "*With the stand-alone server, crystallographers won't have any last-minute surprises when they deposit their structures just before submitting the paper*," Read adds.

Accessing validation reports for archived structures

Validation reports for x-ray structures archived in the PDB are accessible from the following FTP sites:

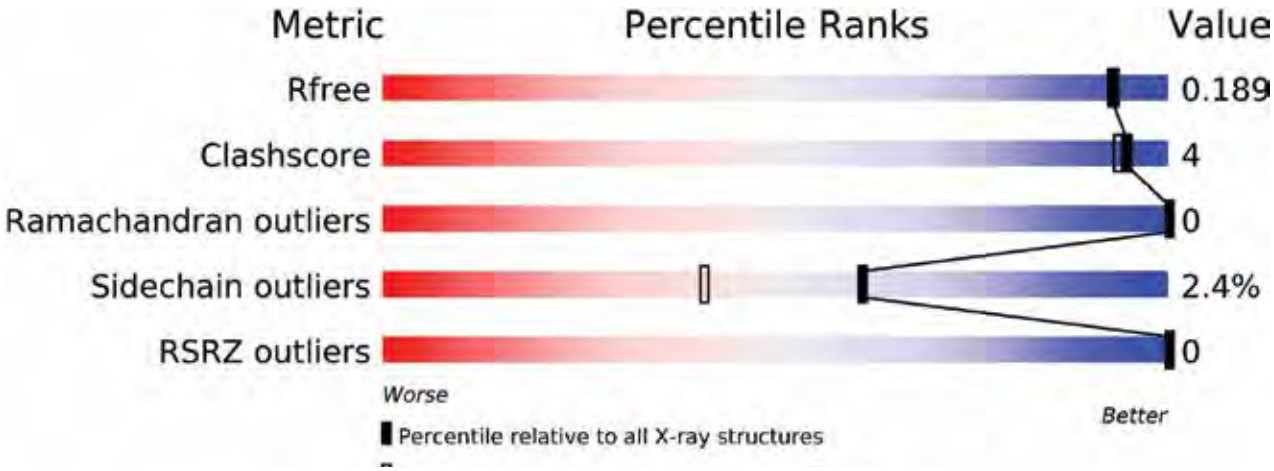
- *ftp://ftp.wwpdb.org/pub/pdb/validation_reports/* (wwPDB/RCSB PDB)
- *ftp://ftp.ebi.ac.uk/pub/databases/pdb/validation_reports/* (PDBe)
- *ftp://ftp.pdbj.org/pub/pdb/validation_reports/* (PDBj)

The reports have been developed in the context of a larger initiative, the new wwPDB Deposition and Annotation system (*http://wwpdb.org/system_info.html*), which was created to unify the annotation tools and practices used across all wwPDB deposition centers and for all common structure-determination methods.

About wwPDB

The wwPDB (*http://wwpdb.org*) is the international partnership that manages the PDB archive. It consists of: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; *http://rcsb.org*) and BioMagResBank (BMRB; *http://bmrb.wisc.edu*) in the USA, the Protein Data Bank in Europe (PDBe; *http://pdbe.org*) and the Protein Data Bank Japan (PDBj; *http://pdbj.org*). Together, the wwPDB partners are committed to ensuring high standards of quality, integrity and consistency of this uniquely important archive and to make it freely available for the benefit of scientists worldwide.

[**1**] Read R. J., Adams P. D., Arendall III W. D., Brünger A. T., Emsley P., Joosten R. P., Kleywegt G. J., Krissinel E. B., Lütteke T., Otwinowski Z., Perrakis A., Richardson J. S., Sheffler W. H., Smith J. L., Tickle I. J., Vriend G., and Zwart P. H. A new generation of crystallographic validation tools for the Protein Data Bank. *Structure*, **19**, 1395-1412, 2011. DOI: 10.1016/j.str.2011.08.006



The validation reports provide at-a-glance summary information that compares the quality of a model with that of other models in the archive.

The reports contain residue-property plots. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ>2).

YSSIG Activities

With Albuquerque in the rearview mirror, we have begun to plan numerous events for next year's meeting in Philadelphia. We have already secured chairs for YSSIG staples, like the *Etter Early Career Symposium* and the *Career Odysseys Panel*. We will also chair/co-chair sessions on SAXS/SANS methods, molecular machines, practical crystallization, structural enzymology, hot structures, small molecules, membrane systems, publication practices, cool structures, structured nucleic acids, diversity in science, and ambient and cryogenic approaches. Crystal McLaughlin will once again host an undergraduate symposium (a follow-up to last year's inaugural success), and Jarrod French and Andrew Torelli are in the early stages of planning a new career development workshop (with a tentative program focus on 'communicating science').

So many sessions… made possible by so many active YSSIG members!

Be sure to vote in this fall's election of new YSSIG officers. The offices of Chair-elect and Secretary will be up for grabs in the election. We thank outgoing chair Yulia Servrygina and secretary Jarrod French for their years of service. We are pleased to report that Yulia will join the ACA Council as the YSSIG Representative when Eric Montemayor's term concludes at the end of 2014.

As always, we look forward to next year's YSSIG mixer. We are still scouting venues; so, if there are any members in Philadelphia that know of a great place, please let us know!

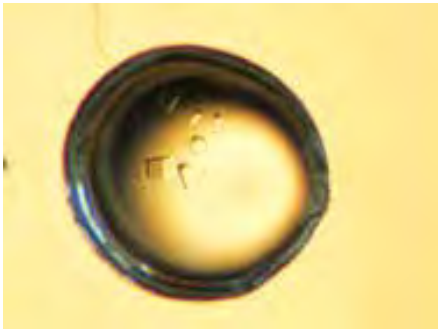
The ACA recently approved a change to the Etter Student Lecturer Award, which is given by each SIG in the ACA to an exceptional young scientist yet to complete a PhD. This award involves a scheduled talk at the ACA meeting and a monetary prize. Next year, the award will additionally provide waived registration at the following year's ACA meeting, and all recipients will be invited to serve on a panel that selects the YSSIG's awardee in the following year.

The high-school outreach continues to thrive, and many previous events have become self-sustaining programs that do not require an annual ACA meeting to be held in that location. For example, the Hawaii outreach that kicked off with the 2013 ACA meeting repeated again in 2014 (see photos below from a field trip hosted by Ho Lueng Ng).

McKinley High School students visit Ho Leung Ng's lab on a field trip to UH-Manoa.

McKinley students growing lysozyme crystals using materials generously donated by Hampton Research.

This spring, YSSIG also teamed up with Kyle Rizzo's AP Biology class at Lansing High School in Lansing, NY, to oversee a three-day project on crystallization. On the first day students learned the basics of crystallization and the impact of structural biology on understanding protein function. The final two days involved leading students through a rigorous study of variables that affect crystallization and x-ray diffraction.



Kyle Rizzo's AP Biology class from Lansing High School, Lansing, NY (top) and the beautiful lysozyme crystals (bottom) they generated during a three-day crystallography workshop.

The students' crystals were then sent to Cornell's High Energy Synchrotron Source (CHESS), and with invaluable help from the MacCHESS group, crystals were used to determine complete three-dimensional structures of lysozyme. We plan to expand this project next year to a high school in the Philadelphia area, and we hope that participating teachers and students can join us at the ACA meeting to present a poster. The outreach would not be possible without generous support from Hampton Research!

Amadeo Biter and Kimberly Stanek

HAMPTON RESEARCH

Many thanks to Hampton Research for their continued support of our high-school outreach. It would not be possible without them!

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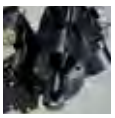

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Edward Snell

Senior scientist, Hauptman-Woodward Medical Research Institute, Buffalo, NY.

Education: PhD, The University of Manchester, England (1996), BSc (Hons 1st), Applied Physics, John Moore University, Liverpool (1992). Postdoc, NRC Resident Research Associate at the NASA Laboratory for Structural Biology, Marshall Space Flight Center, Huntsville, AL.

Professional activities: Council member, International Organization for Biological Crystallization; Member of the American Institute of Physics News and Media Services Advisory Committee, SSRL Users Executive Committee, Referee for numerous international journals and both national and international funding agencies.

Research interests: Macromolecular crystallization, metalloproteins and complexes, radiation damage, technique development and complementary structural methods, *e.g.*, small angle solution scattering.

Statement: Wandering around a meeting can be dangerous especially when nominating committee members are on the prowl. So it happened that I received a polite request to stand for election as ACA Secretary. The secretary keeps minutes of all the ACA council meetings, keeps an eye on the membership files, deals with correspondence related to the ACA, and keeps track of precedents and procedures for council members, committee chairs and program chairs. One of my weaknesses is not to say "no" enough and I agreed on the condition that other people would also be standing. I've been involved with the ACA since 1996 and have attended every meeting if you can count spending only one day in Chicago when my sister had the temerity to schedule a wedding to overlap with important talks! I have told her not to do it again. More recently I've become interested in seeing what goes on in the ACA, how meetings are put together, and what happens after the talks have finished. I've been attending Special Interest Group (SIG) meetings, the business meetings, and ended up chairing a SIG last year and serving on the Communications Committee. It's been fun and I've meet great people, maybe had a little influence in shaping future meetings, and more importantly seen a little on how the organization functions. I've also been a big proponent of encouraging new members to get involved at an early stage from just attending the SIG meetings and voicing an opinion on future topics to attending the general business meeting. The ACA is its members – to maintain a thriving organization everyone should be prepared to give something back so it can continue into the future, and members should be aware that the ACA is more than organizing an annual meeting: it serves to promote crystallography (and increasingly complementary structural techniques) within North America. The ACA has been around since 1945, 70 years old in 2015. I'm happy to stand as the potential secretary for a society that has such a long history; I've seen others doing the job, and I promise I'll do my best!

Diana Tomchick

Professor, Departments of Biophysics & Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX.

Education: BS, Chemistry, Washington State University (1983); PhD, Chemistry, University of Wisconsin-Madison (1990); American Heart Association Postdoctoral Fellow, Department of Biochemistry, University of Wisconsin-Madison (1990-1993); postdoc, Department of Biology, Purdue University with Janet Smith (1993-1997).

Professional activities: Director of The Structural Biology Laboratory at the University of Texas Southwestern Medical Center; member of the ACA since 1986; synchrotron beamtime proposal reviewer for the Advanced Photon Source (2011-present).

Research interests: The use of structural biology and x-ray crystallography in the study of molecular mechanisms of neurotransmitter release, bacterial pathogenicity, cell signaling and division, and enzymology; improved methods of protein crystallization, data collection and phasing of data from poorly diffracting crystals.

Statement: I would be delighted to serve the ACA as Secretary! This is an organization I have belonged to for almost 30 years, and I gladly support its activities and am proud of its role in the crystallographic community. I would welcome the opportunity to actively assist the ACA as Secretary, and as a member of the ACA Council. My crystallographic experience began with small molecules as an inorganic chemist, and I was a recipient of a student travel award to the 14th IUCr Congress in 1987 in Australia, as well as a recipient of a Pauling Prize in 1990. My training eventually led me to my current position as the Director of a campus-wide core facility that provides expertise in macromolecular structure. This position requires significant organizational skills as well as scientific expertise, and for many campus research groups I am the professional 'face' of crystallography. Perhaps my most important role is as an educator, as I provide expertise in current crystallographic methods to members of the campus community through the classroom and individual consultation on structural projects. The ACA provides a critical resource for crystallographers to network and keep abreast of scientific and technical advancements, and to educate the next generation of scientists as well as the general public. As Secretary I would work diligently to support the efforts of the organization as well as the other officers and various committee chairs in furthering these goals.

2015 ASBMB Medals Awarded to ACA Members Ian Wilson and David Eisenberg

The ASBMB has announced the winners of the 2015 ASBMB medals, which will be bestowed at the society's annual meeting in Boston in April. Two eminent ACA members, Ian Wilson, from The Scripps Research Institute in La Jolla, and David Eisenberg, from the University of California, Los Angeles, are among the winners of the prestigious awards.

Ian Wilson is the Hansen Professor of Structural Biology in the Department of Molecular Biology and at The Skaggs Institute for Chemical Biology at The Scripps Research Institute. His research focuses on viruses and on the mechanisms that human cells have developed to deal with viral attack. He has determined the high-resolution x-ray structures of several key molecules involved in the cellular immune response; in particular, one of his major achievements is the determination of the 3D structure of the T cell receptor (TCR), the 'Holy Grail for cellular immunologists'. T cell receptors reside on the surface of T lymphocytes, a particular type of immune cell, and recognize foreign bodies (antigens) previously tagged by the immune system. Once bound to the antigen, TCRs trigger a chain of signals within the cell that activate the cellular defense response. In particular, Ian has conducted important research on HIV and influenza viruses. His work has provided invaluable insights into antibody-antigen recognition and into virus neutralization, paving the way for the design and the development of new vaccines.

David Eisenberg is the recipient of the ASBMB Bert and Natalie Vallee Award in Biomedical Sciences. He is Professor of Chemistry and Biochemistry in the Department of Molecular Biology at the University of California, Los Angeles, and the director of the UCLA-DOE Institute for Genomics and Proteomics. He is a member of the National Academy of Sciences and has been a Howard Hughes Medical Institute investigator since 2001. His breakthrough research on amyloidogenic proteins has been recognized by an impressive number of medals and awards. He uses a structural, biochemical and bioinformatics multidisciplinary approach to understand the determinants of protein aggregation and the basis of amyloid toxicity. His goal is to identify the key molecular features that characterize each amyloidogenic disease and to develop possible curative agents. In 2005 David's group determined the first x-ray structure of an amyloid fiber, which allowed them to gain insights into the aggregation process and to understand why only certain proteins form amyloids. Since then his group has produced more than 90 structures of amyloid fibers from proteins involved in different diseases, contributing enormously to the progress of the field.

Fields Medal: A Woman, at Last

Photo courtesy of Maryam Mirzakhani

This year, for the first time in history, a woman has won the Fields Medal – the highest honor for a mathematician. **Maryam Mirzakhani**, a young Iranian professor at Stanford University, has earned this prestigious recognition for her "outstanding contributions to the dynamics and geometry of Riemann surfaces and their moduli spaces". The prize recognizes her efforts to understand the symmetry of curved surfaces, in particular of complicated non-Euclidean hyperbolic objects. Examples of real objects displaying non-Euclidean hyperbolic geometries are doughnuts, amoebae, the tip of the kale leaf, and the intricate arrangements of corals in coral reefs. (For an artistic rendering of the math of coral reefs, check the hyperbolic crochet coral reef project at The Institute for Figuring.)

Initially drawn to literature, Maryam started appreciating the elegance and beauty of mathematics when she was in high school. She won two consecutive Math Olympiads, in 1994 and 1995, and she earned her bachelor's degree in mathematics at the Sharif University of Technology in Tehran in 1999. She pursued her graduate studies at Harvard University, under the mentorship of Fields Medal winner Curtis McMullen. From 2004 to 2008 she was a Clay Mathematics Institute Research Fellow and an assistant professor at Princeton University. In 2008, she became Professor of Mathematics at Stanford.

Great Barrier Reef coral displaying hyperbolic geometry. Image taken from Wikipedia, shot by photographer Toby Hudson.

Although her research might have applications in several fields of science, such as cryptography, physics, and material science, she is mostly driven by the sheer curiosity of answering challenging questions regarding basic mathematical structures. In the news page from Stanford University, she is reported saying, "...doing research is challenging as well as attractive. It is like being lost in a jungle and trying to use all the knowledge that you can gather to come up with some new tricks, and with some luck you might find a way out."

The Fields Medal was established in 1936 and was initially a rather obscure recognition. Only

at the end of the 1960s, for reasons not related to science but rather to cold war politics, it started being associated with the Nobel Prize and became the most coveted award in mathematics. On August 8, 2014, The New York Times published an entertaining and illuminating account of how the Fields Medal reached its fame: ***http://www.nytimes.com/2014/08/10/opinion/sunday/how-math-got-its-nobel-.html***. The award is given every four years to two to four outstanding mathematicians younger than 40 years of age.

Sexual bias in mathematics is perhaps even more blatant than in other realms of research, and female mathematicians who have greatly contributed to the development of the field have often so far failed to receive public recognition for their merits. The Fields Medal prize to Maryam is a sign that, hopefully, the situation is changing: "I will be happy if it encourages young female scientists and mathematicians," she said. "I am sure there will be many more women winning this kind of award in coming years."

Geologist Frank Hawthorne Wins Roebling Medal

Frank C. Hawthorne, of the University of Manitoba, is the recipient of the 2013 Roebling Medal of the Mineralogical Society of America. He is one of the most brilliant Earth scientists of our times: he has published over 600 scientific papers and 30 book chapters; he was ranked as the world's most cited geoscientist of the decade 1996-2007. He contributed to the discovery of 48 new minerals and has a leafy-green copper tellurate named after him – the frankhawthorneite. His research and keen interest in the architecture of crystal-structure arrangements at the atomic level greatly expanded our current knowledge on mineral chemistry and on the factors that affect the structure and chemical composition of minerals and rocks.

Frank undertook his undergraduate degree in geology at the Royal School of Mines, Imperial College London, and earned a PhD in the same subject at McMaster University. In 1973 he moved to the University of Manitoba for a post-doctoral fellowship; there, he became an Assistant Researcher in 1975, University Research Fellow in 1980, Associate Professor in 1984, Full Professor in 1985 and Distinguished Professor in 1997. In 2001 he was appointed Canada Research Chair in Crystallography and Mineralogy. He is a Fellow of the Royal Society of Canada and has received all the principal medals awarded by the Society; he has also received the highest recognitions from the Mineralogical Association of Canada, from the Mineralogical Society of Great Britain, and from the Geological Association of Canada. In 2009 he won the IMA medal from the International Mineralogical Association, and the Carnegie Medal from the Carnegie Museum of Natural History.

His first and long-lasting love was with amphiboles, a large group of rock-forming silicate minerals characterized by complex chemical compositions and atomic structures, but he has also researched a wide variety of other complex minerals, such as tourmaline, vesuvianite, staurolite, pyroxenes and beryllate minerals. He uses microbeam analytical techniques to characterize the chemical compositions of mineralogical samples, and different structural approaches (such as single-crystal structure solution, Mössbauer, Raman, infrared and NMR spectroscopies) to determine their atomic arrangements. The goal of his research is to relate the specific bond topology of each specimen (*i.e.*, the spatial organization of their atomic bonds) to the physical processes that led to their formation.

Using bond topology and chemical composition, he has developed an improved theoretical treatment for the interpretation of new data. Through his meticulous work, he has opened a new door for geological research and has shifted the perspective towards the core problems in mineralogy. His theoretical approach, in fact, allows researchers to make predictions on many aspects of the structure and of the chemical formulae of complex minerals. Furthermore his work enables mineralogists to ask important questions that are deeply rooted in the essence of the Earth's processes, such as why minerals have their specific chemical composition and structural arrangement or why they are stable over a certain range of pH, temperature and pressure values.

Marilyn Olmstead Named ACS Fellow

Marilyn Olmstead, Professor of Chemistry at the University of California, Davis, has been named a 2014 Fellow of the American Chemical Society. A long-time member of ACA , and a constant presence over the years at our annual meetings, Marilyn was recognized by ACS for her contributions to the structural chemistry of inorganic, bioinorganic, and especially fullerene molecules through application of small molecule x-ray crystallography. In talks at ACA meetings, Marilyn has presented to crystallographers the fascinating intracacies and wide variety of her beautiful fullerene structures.

The ACS Fellows Program was created by the ACS Board of Directors to recognize members of ACS for outstanding achievements in and contributions to science, the profession, and the Society. Marilyn was cited for her contributions to the ACS community as an advisor to the UC, Davis Chemistry Club, where she has influenced the promotion of chemical science to local schools, clubs, science museums and alumni.

Stories, Videos and More: What's New on the ACA History Portal

In the 2014 *ACA RefleXions* spring issue, the *Editor's Desk* column hosted the very first testimonial to the ***ACA History Portal***. In his letter to *RefleXions*, Don Caspar related his serendipitous encounter with the website. While browsing for photographs of Dorothy Hodgkin, he found an unlabelled picture of Penelope Codding and Jenny Glusker that was linked to Jenny's memoir published in the History Portal. After reading it, he moved on to read Marjorie Senechal's and Jack Dunitz's memoirs, and finally he stumbled across the video of his very own *Origins of structural biology* presentation from the 2012 ACA meeting. Don described his surprise and delight in seeing the slides from his presentation "wonderfully displayed" on the website, and wrote that he would do his best to treat us with a text that could complement and explain the images.

This testimonial perfectly captures the spirit of the History Portal, created to collect precious historical material and to make it readily available to the public *via* simple Internet searches. Since the last issue of *RefleXions*, the History Portal team has prepared and uploaded new items.

Two new award videos, recorded at the 2014 ACA meeting in Albuquerque and at the 2013 ACA meeting in Honolulu, are now available on the ACA YouTube channel: John Helliwell's 2014 Patterson Award talk, *Synchrotron radiation macromolecular crystallography: instrumentation, methods and applications* – which is also linked in the History Portal website – and Tom Koetzle's 2013 Bau Award seminar, *From the amino acid structures to metal hydrides: four decades of single-crystal neutron diffraction*. Besides the videos, readers can also enjoy two new memoirs: Abraham Clearfield's *A life in crystallography* and Richard Marsh's *My crystallographic history*.

A new page called 'Nobel Prizes in the News' has been introduced under the main 'Nobel Prizes' tab. At the moment, the page contains the link to the 2009 *RefleXions* article on the Nobel Prize to Ada Yonath, Thomas Steitz and Venkatraman Ramakrishnan, but many more will soon be added. As the beautiful poster, *Highlights on the many Nobel Prizes awarded to crystallographers*, reminds us, the 2009 Prize is only one of the many Nobels that dot the incredible 100-year journey of crystallography. The poster is now accessible from the main Nobel Prizes tab and can be downloaded as a pdf file. It was designed by Vanessa Reitz (***vjreitz.prosite.com***) and prepared by S. Narasinga Rao.

Editor's note: If you've enjoyed the 'Living History' articles in *RefleXions* and online at the ACA History Portal, or if you've watched a video on the ACA YouTube Channel, perhaps you'd like to volunteer for the newly established *Ad Hoc* History Committee (Chair, Virginia Pett; Members, Ilia Guzei, Judith Flippen-Anderson and Patti Potter). There are opportunities for varied talents: identifying authors, editing memoirs for the newsletter, recording videos at ACA meetings, making movies that combine speaker and slides. If you are interested in joining this committee, please contact Virginia Pett, ***pett@wooster.edu***.

Stephen Burley Succeeds Helen Berman as RCSB Protein Data Bank Director

In July 2014 **Stephen K. Burley** succeeded Helen M. Berman as the director of the RCSB Protein Data Bank organization. Burley is a well-known physician-chemist, expert in structural biology and proteomics, structure/fragment drug discovery, and clinical medicine/oncology. In January 2013 he joined Rutgers University, The State University of New Jersey, to direct the Center for Integrative Proteomic Research and the BioMaPS Institute for Quantitative Biology. At Rutgers he is also Distinguished Professor in the Department of Chemistry and Chemical Biology, and he is a member of the Cancer Institute of New Jersey.

Burley has wide experience in both academia and industry. He received an MD degree from Harvard University and a DPhil in molecular biophysics from the University of Oxford. In Boston he interned at the Brigham and Women's Hospital and did research as a post-doctoral fellow in the laboratories of Gregory Petsko at MIT and William Lipscomb at Harvard University. In 1990 he became the Richard M. and Isabel P. Furlaud Professor at The Rockefeller University, and an investigator at the Howard Hughes Medical Institute. From 2002 to 2013 he took a hiatus from academia to venture into the biotech sector; he was chief scientific officer at Structural GenomiX Pharmaceuticals, Inc., and subsequently served as Distinguished Lilly Research Scholar in Lilly Research Laboratories.

Helen M. Berman, who stepped down from her role as director of the PDB after 16 years of leadership, will still be involved as associate director. She will continue to lead the Nucleic Acid Database, the Structural Biology Knowledgebase and the EMDataBank, and she will be in charge of coordinating external partnerships and activities related to hybrid or integrative structure determination methods.

Back to the Future: Beware the Giant Virus

Among its peers, *Pithovirus sibericum* is a sleeping giant. It has been dormant for 30,000 years, well preserved by the favorable environment of the arctic permafrost: no oxygen, neutral pH, and an optimal temperature of around -10 °C. It belongs to a newly discovered species of ancestral giant DNA viruses that a team of Russian and French scientists revived from an ancient Siberian soil sample and that they describe in a paper published in March in *Proceedings of the National Academy of Sciences* **2014**, *111*, 4274-4279.

The researchers isolated the viral DNA from the sample and inoculated it into a particular type of amoeba that is susceptible to infection. Despite its age, the virus revived inside its host cells, replicating and propagating in 10-20 h cycles. The name *Pithovirus* comes from the word *pithos*, the large pottery jar used by ancient Greeks to store oil, grains or wine, and refers to the shape adopted by the virus. Incidentally, it is also a pun built on the myth of Pandora: when Zeus used Pandora to punish Prometheus for stealing the fire from the gods, he gave her a pithos full of evils. Similar to another family of giant viruses named pandoraviruses, pithoviruses form amphora-shaped particles so big that they can be observed under a light microscope. Their genome contains 500 genes – not the record breaking 2500 of the pandoravirus genome, but a respectable number, considering that the HIV's genome consists of only 12 genes.

Image © Julia Bartoli and Chantal Abergel, IGS/CNRS/AMU. Transmission electron microscopy of a Pithovirus sibericum cross-section. The specimen is 1.5 µm long and 0.5 µm wide.

Pithovirus is not harmful to humans or animals, but the research proved that DNA viruses can be infectious over a very long time-scale. About 28,000 years ago Neanderthals inhabited the Arctic and presumably suffered from illnesses caused by different microbes, pretty much the way we do. The question now arises of what will happen if those same pathogens are freed from their icy cages: will they represent a danger for human health? As science fiction as it might sound, this is a real possibility, since global warming and human exploitation of the arctic regions are leading to the melting of increasingly thicker layers of permafrost, with the consequent release of microorganisms into the environment. The parallelism with the myth of Pandora appears even more pertinent here.

The authors of the *PNAS* study are monitoring the permafrost to identify other possible dormant pathogens, sampling even older layers. Their aim is to isolate and to revive amoeba-infecting viruses, to analyze their genetic content and to study their life cycle; this will help in assessing the threat posed by ancient pathogens that may eventually find their way out into the modern world, for which humans and animals have no immune defenses.

Chiara Pastore

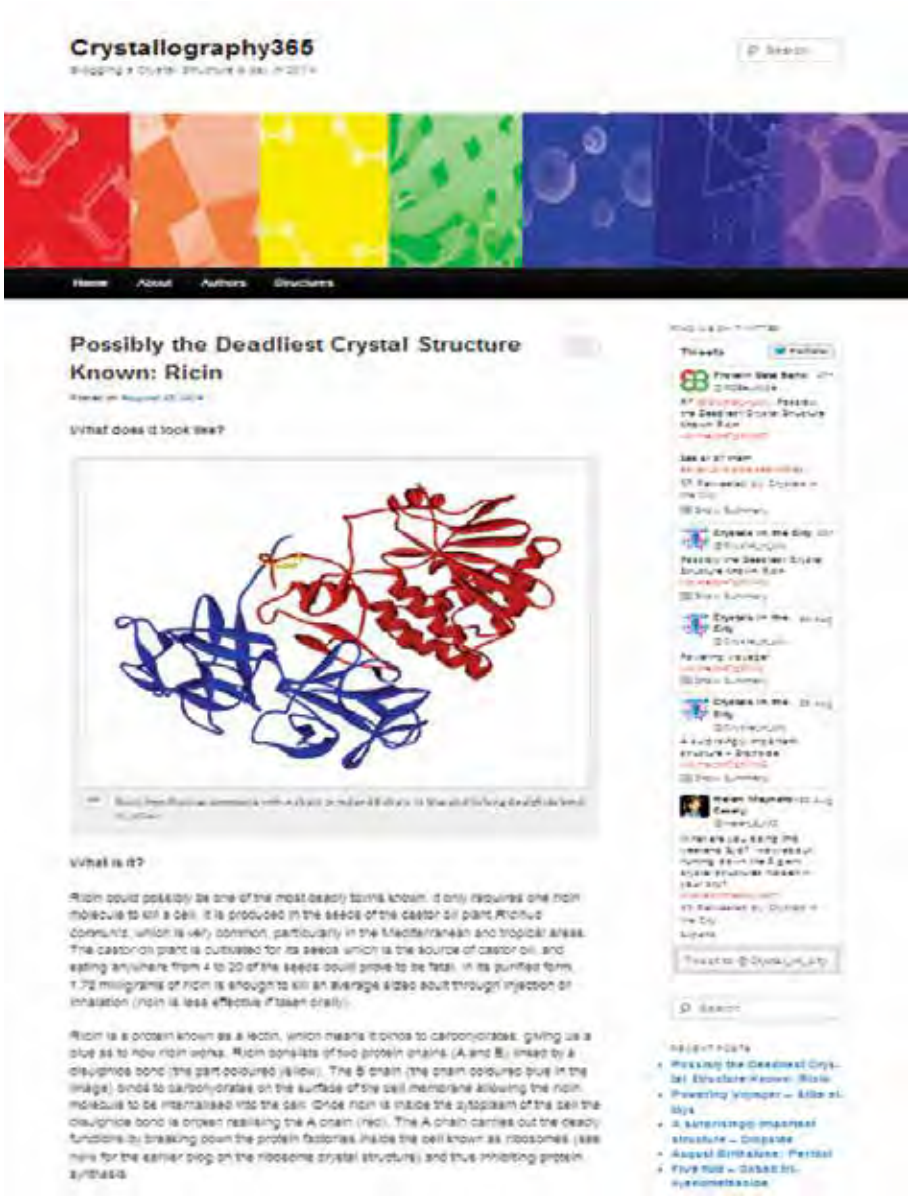
Net RefleXions

Net Reflexions author Amy Sarjeant and coordinator of Crystallography365 Helen Maynard-Casely catching up at the IUCr Congress in Montreal.

As crystallographers around the world find new ways to celebrate this International Year, many excellent sites dedicated to bringing crystallography to the masses are popping up around the web. Crystallography365 (***http://crystallography365.wordpress.com/***) – a blog featuring one new crystal structure for every day of the IYCr2014 – is one such site. Helen Maynard-Casely, the coordinator of Crystallography365, took some time out of her busy schedule to answer a few questions for *Net RefleXions*:

Net RefleXions: This is an excellent way to celebrate the IYCr2014 and a fun way to bring crystallography to the general public. Have you seen much interest from non-research scientists at your website?

Helen Maynard-Caseley: Thanks very much. I was inspired by another Australian-based blog [***http://philosophicallydisturbed.wordpress.com/chemistry365/***] that did something similar during the International Year of Chemistry in 2011. It occurred to me that, given the common factor of the CIF format for crystal structures across crystallography and the number of databases housing them, it would be a little more straightforward for us crystallographers to do something similar. Judging from our Twitter followers (tweeting from @Crystal_in_City) most of our visitors are scientists themselves. That said, we often get promoted on ANSTO's (my employers, the Australian Nuclear Science and Technology Organisation) Facebook page, which brings in a mainly non-research scientist audience. Over the year there's a competition as to which author can bring in the most (normalized) readers to their posts – there's some inventive promotion going on!



NR: How did your team of crystallographic bloggers assemble?

HMC: Kind of organically, really, and we're still growing as the project finds the ears of others around the world. Also, I'm always happy to get new authors on board! One of the aims of the blog was to be a place for early career crystallographic researchers – ECR's – [to have] a 'playground' to try out writing for a different audience. Though the blog isn't just ECR's, and I've been grateful to all my colleagues who've contributed. I figured if we had about 30 authors, then if everyone wrote about a post a month then that would see us through. We're a relatively small community here in Australia, and my positions (I've worked both at Australian Synchrotron and now at the Bragg Institute, ANSTO) meant that I'd come into contact with many of the groups. So, I emailed out to a few people in November to test the water and see who might be interested in contributing, with a basic structure (the What does it look like? What is it? and Where did the structure come from?) that worked for all themes. I've less contact with the biological community in Australia, so I was really grateful to a few of the principal investigators in the field here who distributed the idea to their group.

NR: Crystallography365 includes a wide variety of structures. Are there any particular motivations for choosing the structures included in the blog such as following current events or is it just personal preference?

HMC: Not really. I've definitely encouraged people to write about their own structures – and ones that they are working on. The thought was that this would be the best way to get a unique spin on things. Generally though, they are just the structures the authors are interested in. I update all the authors monthly on how things are going, and now set a bit of a theme for each month that people can work to. August's is 'Crystal growing', but we've not had any inspired by that yet! Personally I like to write about structures with a bit of a story behind them, whether it be how they were solved or how they are used in everyday life.

NR: Are you involved in any other public-facing events for IYCr2014?

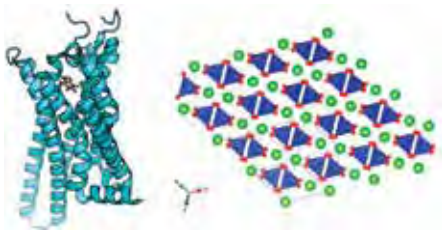
HMC: Yes! The sister project to Crystallography365 is 'Crystals in the City' [***www.crystalsinthecity.com***] which is a travelling exhibition of giant crystal structure sculptures that will be moving around Australia. We're launching it in National Science Week (which starts August 16th in Australia), and will continue into 2015.

NR: Crystallography365 is a wonderful resource for all sorts of researchers and teachers. Do you have plans to continue the blog after the IYCr2014 has ended?

HMC: I think the plan would be, rather than continuing to blog, to tidy up and package what has been done to be more of a useful resource for lecturers and teachers. What we'll end up with will be a great database of stories of cutting edge and historic crystal structures featured. It would be nice to put it all in a book – that would be my dream!

Check out the wonderful crystal structures featured daily at Crystallography365, for even more crystallographic inspiration!

Amy Sarjeant



Structures from Crystallography365, from 'A' to 'Z'.

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The Cambridge Crystallographic Data Centre - Making it Easier to Deposit Data into the CSD

The Cambridge Crystallographic Data Centre (CCDC; ***www.ccdc.cam.ac.uk***) launched a new improved service in June 2014 to make it easy and fast for researchers to deposit their structural data into the CSD.

The CCDC creates and distributes the Cambridge Structural Database[1] (CSD), the world's repository of small molecule crystal structures, so that the crystallographic community can store and share their structures with scientists across the globe. Since its inception nearly 50 years ago, the CSD has grown considerably and now contains over 730,000 entries; the complexity of these entries is also on the increase. As the size of the CSD has grown, so too has the number of depositions, revisions and publications that go alongside the entries in the CSD. Today nearly 10,000 different individuals deposit data at the CCDC every year – a record 9,622 structures were processed into the CSD during the month of May 2014 alone. This figure demonstrates how much the crystallographic community has advanced since 1990 when less than 9,000 small molecule crystal structures were published in the entire year. With all these structures and so many depositors storing data at the CCDC, it is essential there is a quick, easy process to deposit data and ensure that high quality, comprehensive structural data are made more readily available to the scientific community.

The new deposition process

The CCDC launched its new CSD web-based data deposition facility (***www.ccdc.cam.ac.uk/deposit***) on June 23, 2014, to address these challenges, making the whole process of depositing small molecule data faster, easier and more intuitive[2]. The service incorporates the CCDC's enCIFer syntax checking and editing functionality to enable straightforward review and correction of deposited CIFs. This makes the process more efficient for depositors, and also ensures the integrity of the data stored at the CCDC for the world's community of structural chemists. To further ensure the quality of the crystallographic data and to help with the peer review process, the inclusion of structure factors is now a prominent part of the deposition. In addition to this, users are able to review, edit and add to the metadata during the process. This ensures the quality of the metadata received and provides the community with a more enriched CSD entry. The CCDC has plans to build on this new deposition process in the coming months; one of the many enhancements on the horizon is to incorporate sophisticated CCDC diagram generation code.

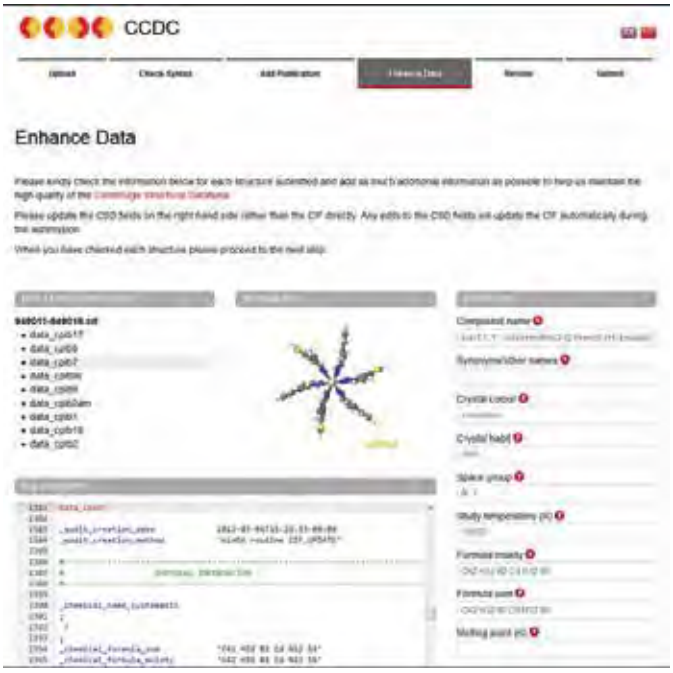


Figure 1: The new deposition process allows users to easily check and update the metadata during the process.

"*Depositors will be delighted to discover how quick and easy it is to deposit their data with the CCDC now that the new, interactive, web-based data deposition facility has been launched. The IUCr is particularly pleased that the new process highlights the importance of including structure factors in the deposition process, which should help to ensure the quality of the reported science*," said **Peter Strickland**, Managing Editor at the IUCr.

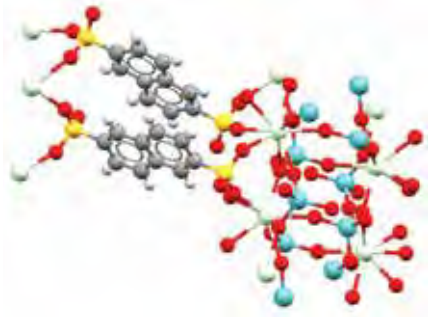


Figure 2: A molybdenum neodymium naphthalene polymer, CSD refcode XAFLEX01, which has the 500,000th CCDC DOI (http://dx.doi.org/10.5517/CC12X6BJ)

Maximizing accessibility of crystallographic data

The new deposition form is just one of the latest developments of an ongoing process to maximize accessibility of crystallographic data in the CSD. We have been working with DataCite (***http://www.datacite.org/***), and in March 2014 the CCDC started assigning Digital Object Identifiers (DOIs) to datasets of crystal structures deposited with the CCDC[3]. Now over half a million CCDC data DOIs have been assigned. Not only do DOIs provide a stable linking mechanism that helps ensure the preservation of data, they also provide a way to increase the discoverability of data. For example, the CCDC will be utilizing the workflow that was developed between DataCite and Thomson Reuters to populate the Data Citation Index (***http://wokinfo.com/products_tools/multidisciplinary/dci/***).

The metadata available through DataCite will also allow authors in the CSD to add data to their researcher or institutional IDs to make sure the appropriate credit is received for data as well as publications.

The CCDC is committed to adding to the array of free services that are available to the scientific community, to aid the discoverability of research data. With the April 2013 launch of CSD-Xpedite[4], the new infrastructure used to manage depositions and process entries into the CSD, the CCDC is now prepared for the rapid growth of the CSD into the next decade.

The crystallographic community is now able to experience some of the benefits of this new architecture with the release of CCDC DOIs and the new deposition process. Furthermore the CCDC is looking forward to expanding the opportunities for crystallographers worldwide to gain high value insights from their experimental data.

Suzanna Ward

[1] F. H. Allen, *Acta Cryst*., **B58**, 380-388, 2002 "The Cambridge Structural Database: a quarter of a million crystal structures and rising" DOI: ***10.1107/S0108768102003890***

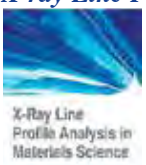
[2] ***http://www.ccdc.cam.ac.uk/NewsandEvents/News/Pages/NewsItem.aspx?newsid=29***

[3] ***http://www.ccdc.cam.ac.uk/NewsandEvents/News/Pages/NewsItem.aspx?newsid=28***

[4] ***http://www.ccdc.cam.ac.uk/NewsandEvents/News/pages/NewsItem.aspx?newsid=23***

Book Reviews

X-ray Line Profile Analysis in Material Science: Jenö Gubicza, Engineering Science Reference, Hershey, 2014, 343 pp., ISBN 978-1-466-65852-3.



The author set out to provide a survey of the field of x-ray line profile analysis (XLPA) for the materials sciences. The book covers the basics and advanced XLPA and attempts to fill in the gaps in the current literature. From my perspective the author has done a reasonably good job. The book is divided into nine chapters. Each chapter provides an introduction and a conclusion, which nicely complement the meat of the chapter. Each chapter has its own list of references, and a compilation of references is provided at the end of the book.

Chapter 1 discusses the fundamentals of kinematical x-ray scattering including derivation of scattering intensity, the reciprocal lattice, the Ewald construction and Bragg's law. Chapter 2 covers broadening of diffraction profiles as result of crystallite size, ending with analyses of spherical and anisotropic crystallites. Chapter 3 looks at the effects of strain on broadening of peaks, discusses the results for dislocations for cubic, hexagonal and orthorhombic systems, and gives three practical examples. Chapter 4 covers broadening from planar faults, while chapter 5 looks at the effects of chemical inhomogeneities.

Chapter 6 reviews the methods for the evaluation of profiles including the classical and modified Warren-Averbach method, multiple whole profile fitting, classical and modified Williamson-Hall method, variance methods, whole powder pattern fitting and modeling, and finally convolutional multiple whole profile fitting.

Chapter 7 discusses profile evaluation for thin films, and chapter 8 does the same for single crystals. Chapter 9 reviews the importance of the instrument function and its impact on the line shape, and then surveys a number of practical examples.

The editors should have taken a little more time to ensure the English is correctly written. There are a few places where a reader might break stride to go back and double check what they have just read. I did not find any errors in the equations, but there are a few places where the font becomes so small it is barely legible.

Joseph Ferrara

Celestial Sleuth: Using Astronomy to Solve Mysteries in Art, History and Literature: Donald W. Olson, Springer Praxis Books, New York, 2014, 355 pp., ISBN 978-1-4614-8403-5.

It may not seem as if the unsolved mysteries of art, history, and literature could have anything to do with astronomy, but physicist Donald W. Olson seeks to prove otherwise in his new book, *Celestial Sleuth*. As the title suggests, Olson implements the tools of astronomy to solve a select number of mysteries in art, history, and literature. The book should be just as enjoyable for a lover of art as a fan of physics. Despite the somewhat complicated astronomical theories applied to solve these 'mysteries,' Olson does a decent job of explaining these concepts so that the average layman can understand how exactly he solves each one.

I found it particularly helpful that the book has a wide variety of illustrations, including reproductions of the paintings Olson discusses, and relevant photographs of the night sky and landscape, as well as a few documentary photographs of Olson and his team from Texas State University.

First, Olson seeks to answer a number of questions about the time and location, as well as the celestial accuracy of a number of famous paintings, including masterpieces by Monet, van Gogh and Munch. Olson and his team have used celestial markers in the paintings to determine the exact time and location of the scenes that are depicted.

Then, Olson approaches a series of historical questions. I found his interest in debunking the urban legend that the Boston Tea Party occurred under a full moon quite intriguing. As Olson and his team eventually proved, the Boston Tea Party really occurred under the cover of almost total darkness, as the moon would have been a thin waxing crescent on the night of the Tea Party.

Finally, Olson wraps up the book with an astronomically driven approach to literature, which he breaks into two categories, pre-1800 and post-1800. Of these discussions, I was especially fascinated by Olson's interest in Shakespeare's *Hamlet* and its description of a 'bright star' burning in the first act. He ultimately reaches the conclusion that Shakespeare was actually describing a famous supernova that occurred in 1572. As a budding Shakespearean scholar, I found it particularly interesting that such a brief yet iconic moment in one of his works could in fact be rooted in a real-life astronomical event.

I certainly wasn't sure what to expect when I began reading this book, and although at times it seemed to me like Olson used astronomy as an umbrella concept under which to draw conclusions about art, history, and literature, it was a good and relatively quick read.

Jeanette Ferrara

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In conjunction with the International Year of Crystallography, Rigaku is proud to announce the new

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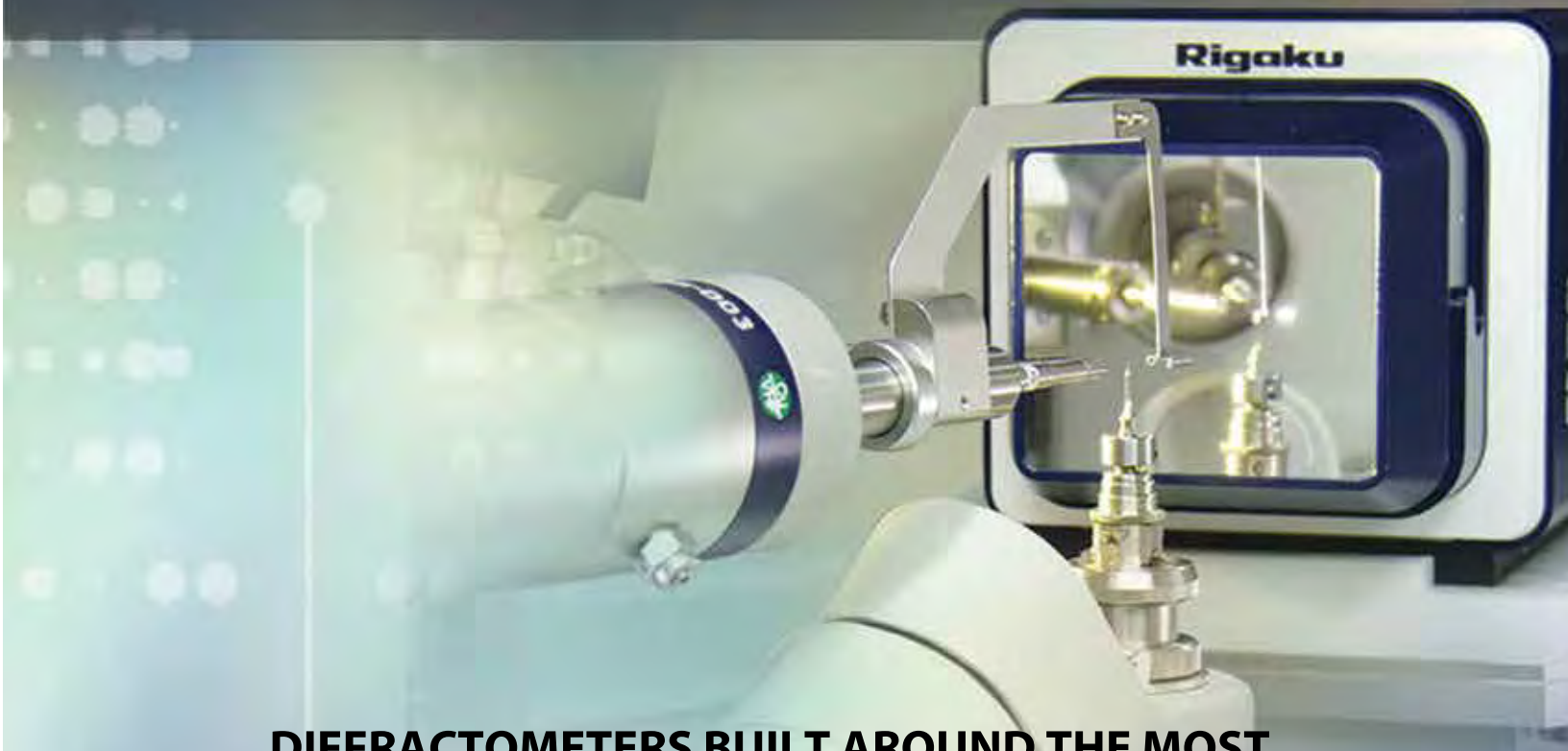

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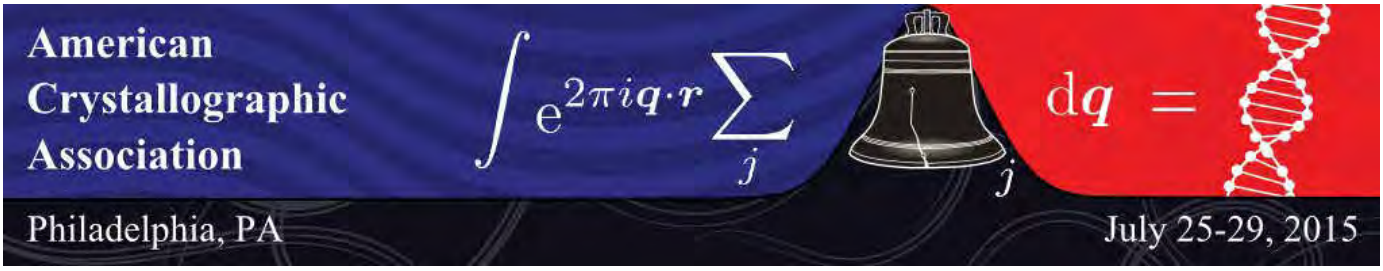

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Advances in Serial Crystallography
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Ambient and Cryogenic Approaches
Porous and Meso-Scale structures

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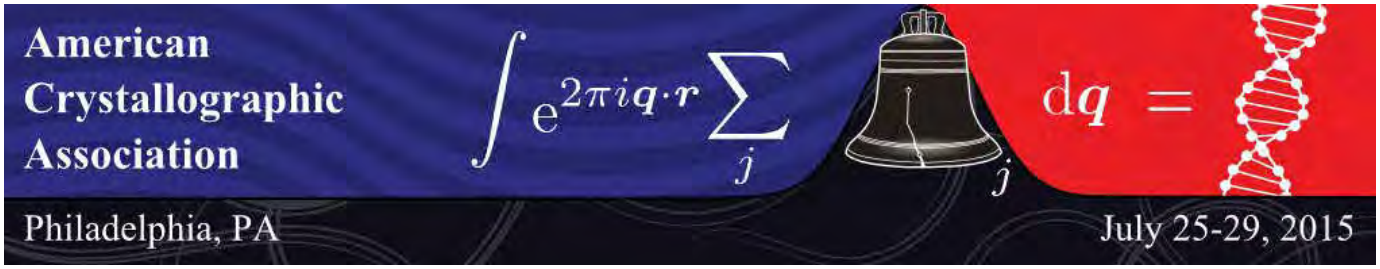
Jason Mercer (Memorial University of Newfoundland)



Transactions Symposium
Crystallography for Sustainability

Organizers: Cora Lind-Kovacs (University of Toledo; ***cora.lind@utoledo.edu***); Robin D. Rogers (University of Alabama; ***rdrogers@ua.edu***)

This multidisciplinary symposium will be focused on the cutting edge impact of crystallography-based research on global aspects of the sustainability of world resources, including green chemistry, the globalization of chemistry, and responsibilities and opportunities to serve the broader public. In particular, the symposium will cover such aspects as the lead role of crystallography in the design of materials and in the design of processes that reduce energy consumption, protect clean water supplies, provide unique environmental benefits, enable new medicines, or provide new greener routes to chemicals and materials. The *Transactions Symposium* will highlight the unique roles of crystallography in achieving major societal goals. Special attention will be given to providing international perspectives related to both areas of critical need, such as the supply of medicines and clean water and energy to all citizens of the world, and to overcoming the limitations or restrictions of raw materials for products that lead to improved quality of life. Possible topics are:

Crystallography in the design of sustainable materials

In situ characterization of materials and analysis to reduce waste

Crystal engineering

Energy-related materials (batteries, fuel cells, solar cells)

Crystallography in the design of sustainable processes

Design of catalysts for reduced chemical consumption

Photosynthesis as alternative production methods

Water purification

Catalysis

CO_2 capture

Crystallography used for a sustainable society

Food

Energy

Medicines

Drinking water

Learning lessons from nature about sustainability

Photosynthesis / the artificial leaf

General Meeting Information

The US Declaration of Independence was signed in Philadelphia in July 1776, and Pennsylvania was the second state to join the Union in 1787. It is a very walkable city. You will not need a car to visit the Liberty Bell (Independence Hall), the Franklin Institute, the Philadelphia Museum of Art and many other local attractions. Philadelphia is also a 'foodie' town, and you will find palate pleasing repasts in all price ranges. The lower end need not be fast food, not with the myraid of eclectic food trucks that you will find all over the city. Sadly, the legendary Le Bec Fin is no more but upper end appetites will find restaurants like Alma de Cuba and a variety of tastes and prices featured in restaurants by Jose Garces and other celebrity chefs.

Obtaining a VISA: Advanced planning by foreign travelers is critical. For those travelers who will requre a VISA: ***applications should be made at least 90 days in advance of the travel date. For further information contact: the US Department of State (travel.state.gov/visa/visa_1750.html).***

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

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

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

Financial Support: Travel support will be available for young scientists. Applications should be made by the abstract deadline on the meeting web site.

The meeing 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.

Puzzle Corner

In this issue, we have the solution to the last DISORDERED puzzle, a new DISORDERED puzzle, comments on the poetry puzzle from the summer issue, and a new *Crystal Connections* puzzle.

Poetry Puzzle Comments

We gave a few lines from a poem and asked what is the title and who is the author. There were no responses with the correct answer. The lines were:

A crystal assembles itself out of its own constituent
disarray: the puzzle puts itself together, each piece
falling as though by chance into its correct location.

A crystal is nothing more
than a breeze blowing sand
into the form of a castle
or a film played backwards
of a window being smashed.

The poem is entitled *Crystals* and is one of several with that title contained in the poetry book, *Crystallography* by Christian Bök, originally published in 1994. The full poem can be found online, and the book (not to be mistaken for a textbook) is available, reprinted in 2003 by Coach House Books. The author explains that, from its etymology, the title 'crystallography' can be taken to mean 'lucid writing'. The book contains poetic tributes to René Just-Haüy, W. H. Miller, A. Bravais, M. von Laue, W. L. Bragg and others, and is an interesting read.

Crystal Connections Puzzle

The six answers have something in common, meaningful to crystallographers. What is it?

(1) Number of U.S. constitutional amendment ratified in 1868

(2) "____ can be as bad as one," according to Three Dog Night

(3) Most stable F isotope

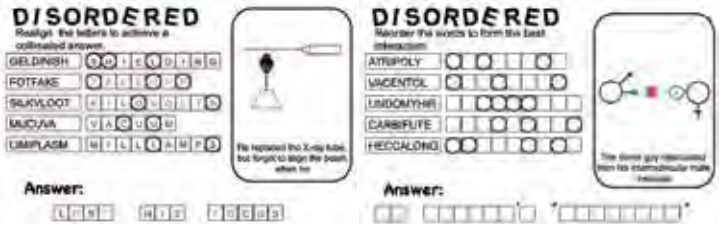
(4) The Ides of March

(5) 53Mod7

(6) 2001 Roger Maris movie

The solution will be given in the winter *ACA RefleXions*, but send the answer to me by email (***ffronc@lsu.edu***) when you figure it out. You will be mentioned in the Puzzle Corner if you are the first to respond with the correct answer.

Frank Fronczek



OCTOBER 2014

26-28 **72nd Annual Pittsburgh Diffraction Conference**. University of Georgia, Athens, GA. ***pdc14.bmb.uga.edu/Home.html***

26-31 **12th International Conference on X-Ray Microscopy**. Melbourne, Australia. ***www.xrm2014.com***

NOVEMBER 2014

30-5 Dec **MRS Fall Meeting & Exhibit.** Boston, MA. ***www.mrs.org/fall2014***

JANUARY 2015

14-16 **BioXFEL STC Annual Conference.** Ponce, Puerto Rico. ***www.bioxfel.org/events/details/6***

MARCH 2015

8-12 **Ultrafast Dynamic Imaging of Matter.** Grindelwald, Switzerland. ***www.udim2015.ethz.ch***

30-2 Apr **BCA Spring Meeting.** University of York, UK. ***www.crystallography.org.uk***

JUNE 2015

7-11 **International Conference on Structural Genomics 2015: Deep Sequencing Meets Structural Biology**. Rehovot, Israel. ***www.weizmann.ac.il/conferences/ICSG2015***

JULY 2015

25-29 **ACA 2015 Annual Meeting**. Philadelphia, PA, Sheraton Philadelphia Downtown. Program Chairs: Kraig Wheeler & Louise Dawe. ***www.AmerCrystalAssn.org***

AUGUST 2015

23-28 **19th European Crystallographic Meeting, ECM29**. Rovinj, Croatia. ***ecm29.ecanews.org***

DECEMBER 2015

5-8 **AsCA2015 Science City.** Kolkata, India. ***asca.iucr.org***

JULY 2016

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

The AIP State Department Science Fellowship

Most of the foreign policy issues faced by the US Department of State have a scientific or technical component. This fellowship is intended to enhance the S&T capacity of the Department by enabling at least one scientist annually to work at the Department's Washington, DC headquarters for a one-year term.

This is a unique opportunity for a scientist to contribute scientific and technical expertise to the Department and raise awareness of the value of scientific input. In turn, scientists broaden their experience by interacting with policymakers in the federal government and learning about the foreign policy process.

Application deadline: November 1 of the year prior to the fellowship term of the year applied for.

The AIP Congressional Science Fellowship Program

The American Institute of Physics, in partnership with the Acoustical Society of America (ASA), annually sponsors one scientist to spend a year providing analytical expertise and scientific advice to Congress. A second fellowship is sponsored by the American Physical Society. The program enables scientists to broaden their experience through direct involvement with the legislative and policy processes.

Fellows gain a perspective which, ideally, will enhance not only their own careers but also the physics community's ability to more effectively communicate with its representatives in Congress.

Benefits: Stipend of $70,000 - $72,000 per year. Relocation allowance. Allowance for in-service travel for professional development. Reimbursement for health insurance premiums up to specified maximum.

Application deadline: January 15 of the year of the fellowship term. Fellowships are for one year, usually running September through August.

Scientists at all career stages, including mid- and late-career professionals, are encouraged to apply. Although the fellowship is a full-time position, arrangements to supplement the stipend by continuing to receive a salary from a current employer while taking a sabbatical or leave of absence during the fellowship term may be worked out on a case-by-case basis.

www.aip.org/gov/fellowships/both_apply.html

2016 ACA Meeting Is Set for Denver

The 2016 ACA Annual Meeting will be held July 22-26, 2016, in Denver, CO, as is noted in the calendar of future meetings (see above). ACA has just signed on with the Sheraton Downtown Denver, which will be the 2016 meeting site. The meeting will begin on ***Friday, July 22***. The workshops will be scheduled for all-day on Friday with the opening reception on Friday evening. Sessions will end on Tuesday with the banquet scheduled for Tuesday evening. ***Please note that this is a new meeting schedule for 2016!***

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